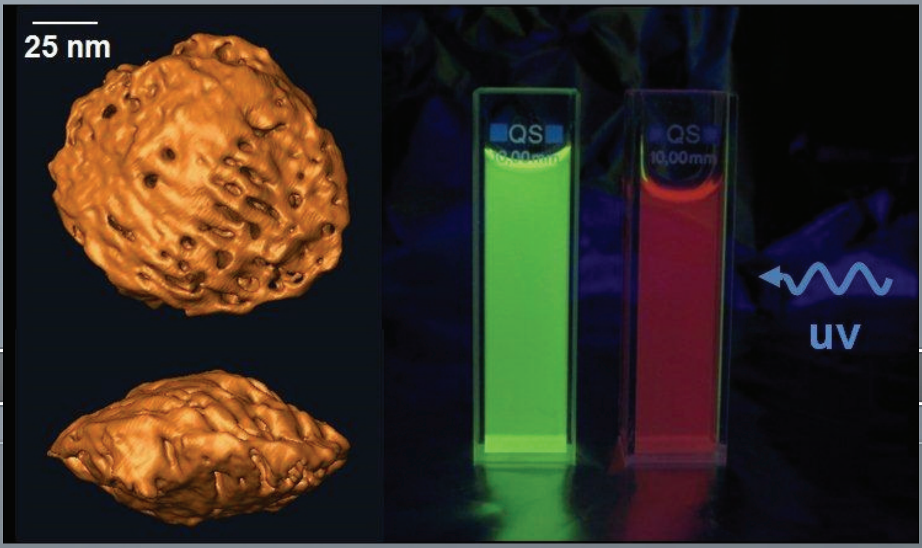
Instituto de Ciencia de Materiales de Sevilla



Consejo
Superior de
Investigaciones
Científicas

Universidad
de Sevilla

Junta de
Andalucía

Memoria de Actividades

Annual Report

2011

Consejo Superior de Investigaciones Científicas
Universidad de Sevilla
Junta de Andalucía

INSTITUTO DE CIENCIA DE MATERIALES DE SEVILLA

Memoria de Actividades
Annual Report
2011

Centro de Investigaciones Científicas "Isla de la Cartuja"
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EDITA
Instituto de Ciencia de Materiales de Sevilla (ICMS)
Centro Mixto entre el Consejo Superior de Investigaciones
Científicas y la Universidad de Sevilla
Centro de Investigaciones Científicas Isla de la Cartuja
c/ Americo Vespucio, 49
41092 Isla de la Cartuja, Sevilla
http://www.icmse.csic.es

COMISIÓN MEMORIA-ICMS
Hernán R. Míguez García – Manuel Ocaña Jurado – Pedro José Sánchez Soto

INDICE

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El ICMS en 2011

ICMS in 2011

Presentación Presentation

A través de esta Memoria 2011, el Instituto de Ciencia de Materiales de Sevilla pretende comunicar lo mejor de las actividades científicas realizadas a lo largo del periodo.

Nuestro Instituto, un Centro Mixto del Consejo Superior de Investigaciones Científicas (CSIC) y la Universidad de Sevilla (US), y cofinanciado por la Junta de Andalucía, está incluido en el Área de Ciencia y Tecnología de Materiales, una de las 8 en las que el CSIC estructura sus actividades científicas. Integrado por tanto por personal científico del CSIC y la Universidad de Sevilla, cuenta en la actualidad con 135 personas, 49 de las cuales son científicos permanentes.

El Plan Estratégico 2010-2013, actualmente vigente, organiza nuestro centro en 5 líneas de investigación, las que enraizando en disciplinas de la Química y Física del Estado Sólido, así como de la Ingeniería de Materiales, pretenden abarcar los aspectos más modernos y novedosos de la Ciencia de Materiales actual. Nuestro empeño fundamental para los años venideros es el apoyo en la medida de lo posible al desarrollo de un nuevo sistema económico en el que la base científica y tecnológica pase a ser un pilar fundamental de la misma. Por tanto, el desarrollo de una actividad de I+D acorde con el estado del arte, es la prioridad más importante, si no la única, de nuestro centro de investigación.

A pesar de las limitaciones de espacio que venimos padeciendo, tanto para la ubicación de personal científico y técnico como para la instalación de equipamiento científico, la promoción de la actividad científica, la instalación del equipamiento científico más innovador y la incorporación de jóvenes científicos seguirá siendo nuestro gran objetivo diario.

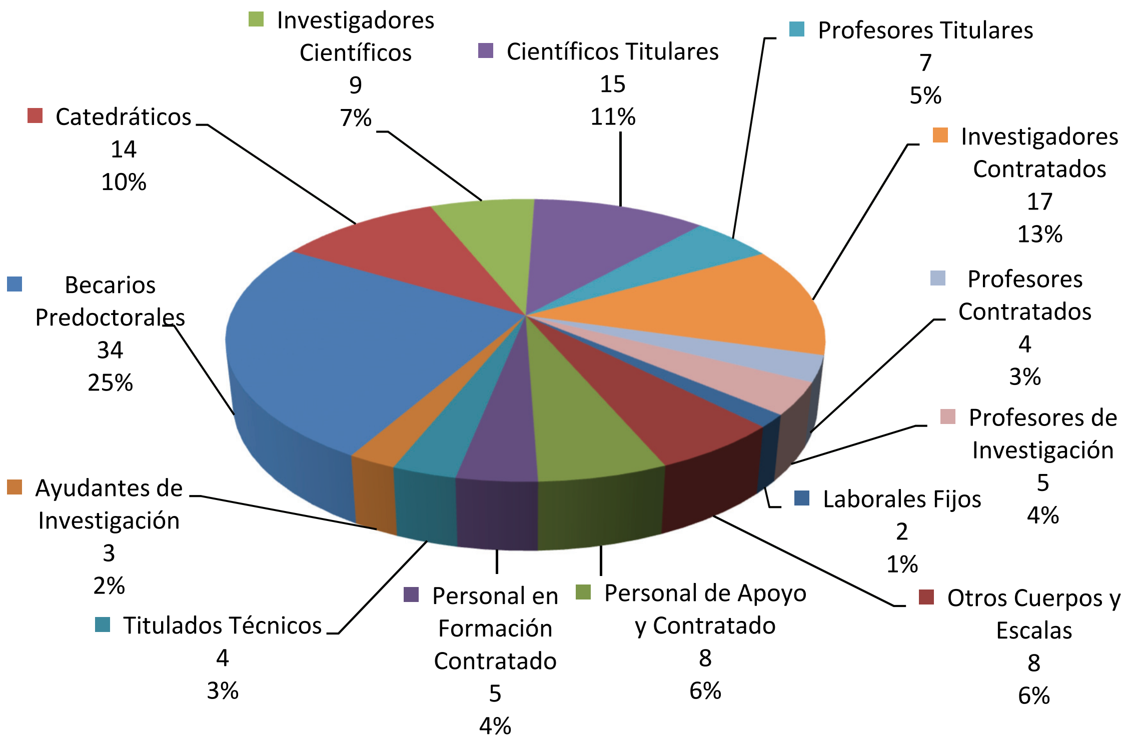
Through this Activity Report 2011, the Institute of Materials Science of Seville is trying to communicate the best of its scientific activities for the period. Our Institute, a joint Center of the Spanish Research Council (CSIC) and the University of Seville (US), also funded by the Junta de Andalucia, is included in the “Field of Science and Technology of Materials”, one of the eight within the scientific framework of the CSIC. Integrated therefore by scientific staff of the CSIC and the University of Seville, includes today more than 135 people, 49 of which are permanent scientific staff. The current Strategic Plan 2010-2013 organizes our Center in 5 lines of research, which related with disciplines of solid state chemistry and physic, as well as materials engineering subjects, are intended to cover the most modern and innovative aspects of the current material science. Our basic commitment for years to come is to support, as far as possible, the development of a new economic system, in which the scientific and technological basis should become a fundamental pillar of the same. Therefore, development of a R+D activity according to the State of the Art, is the top priority, if not the only, of our research centre. In spite of the limitations of space we are suffering today, both for the location of scientific and technical staff and for the installation of scientific equipment, the promotion of the scientific activity, the installation of the most innovative scientific equipment and the incorporation of young scientist staff will remain our great daily goal.

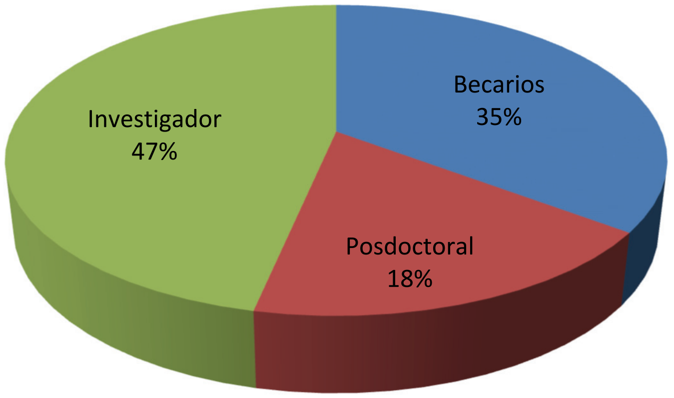
Dr. **Alfonso Caballero Martínez**
Director del Instituto de Ciencia de Materiales de Sevilla

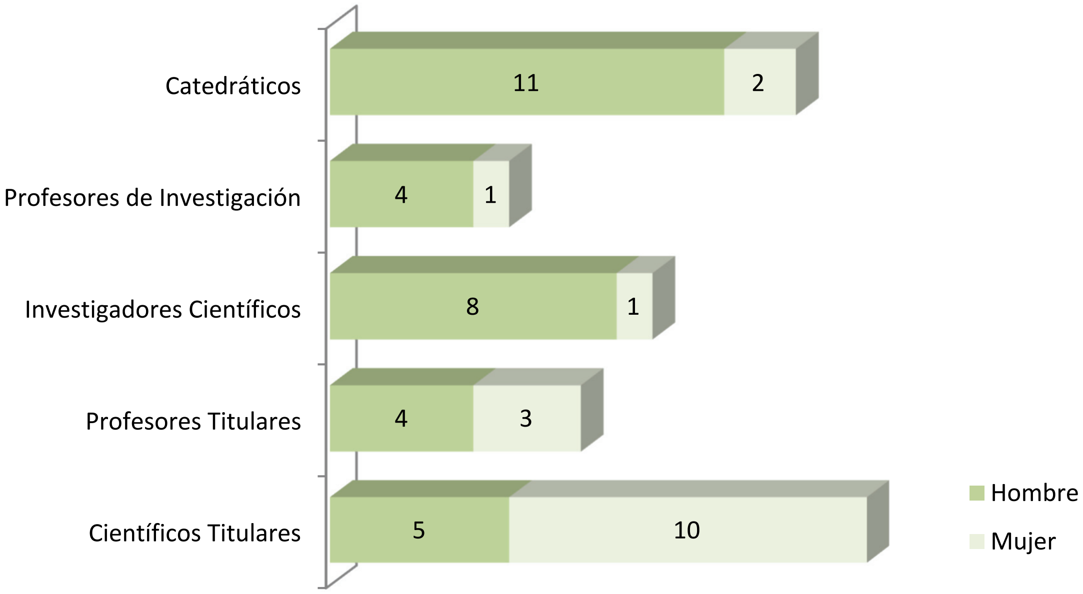
Datos Estadísticos del ICMS
Statistical Data of ICMS

RECURSOS HUMANOS / HUMAN RESOURCES

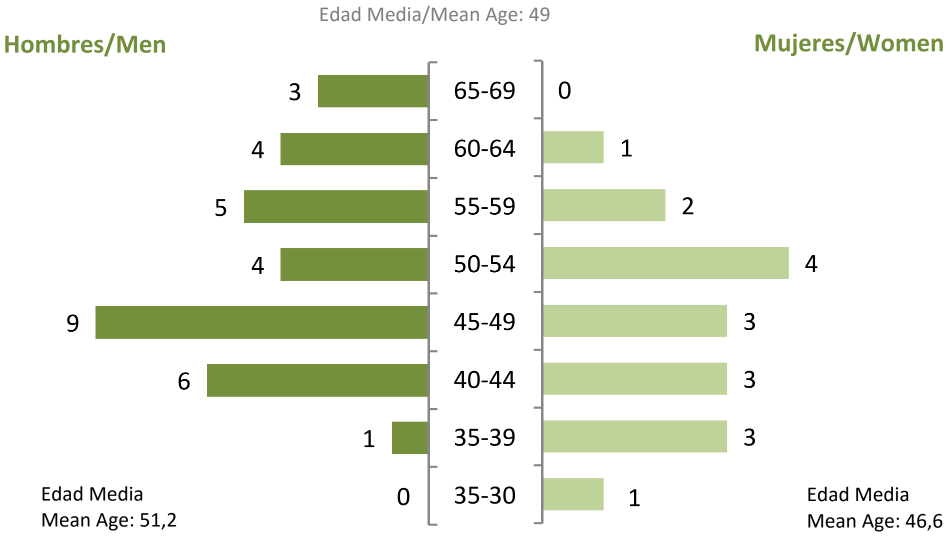
Distribución del personal por categorías
Distribution of by cathegories





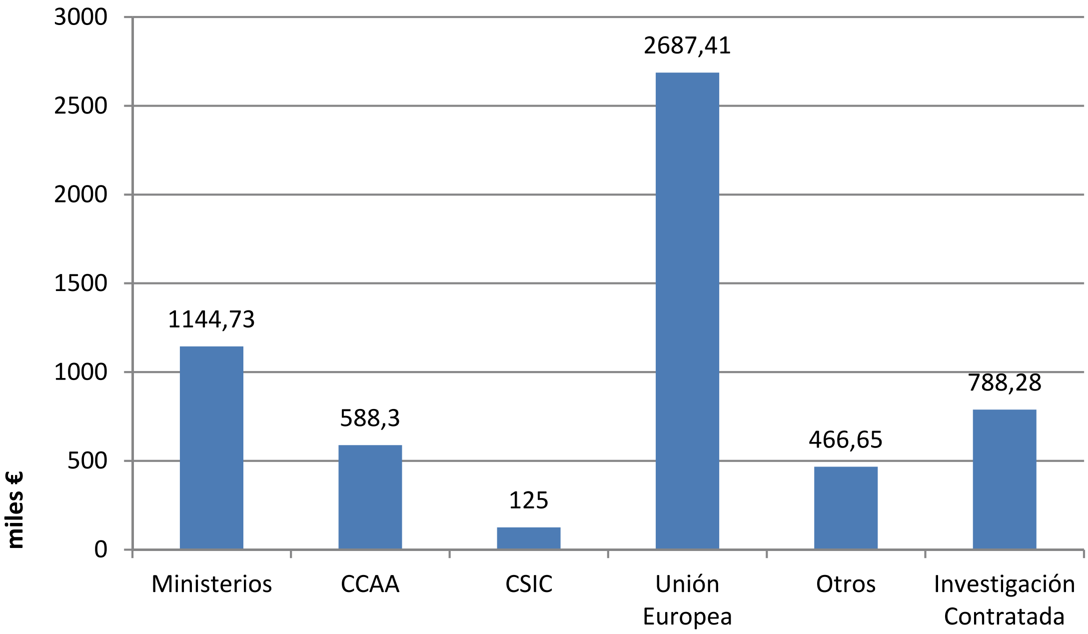


Distribución del personal investigador por edad
Scientific staff by age

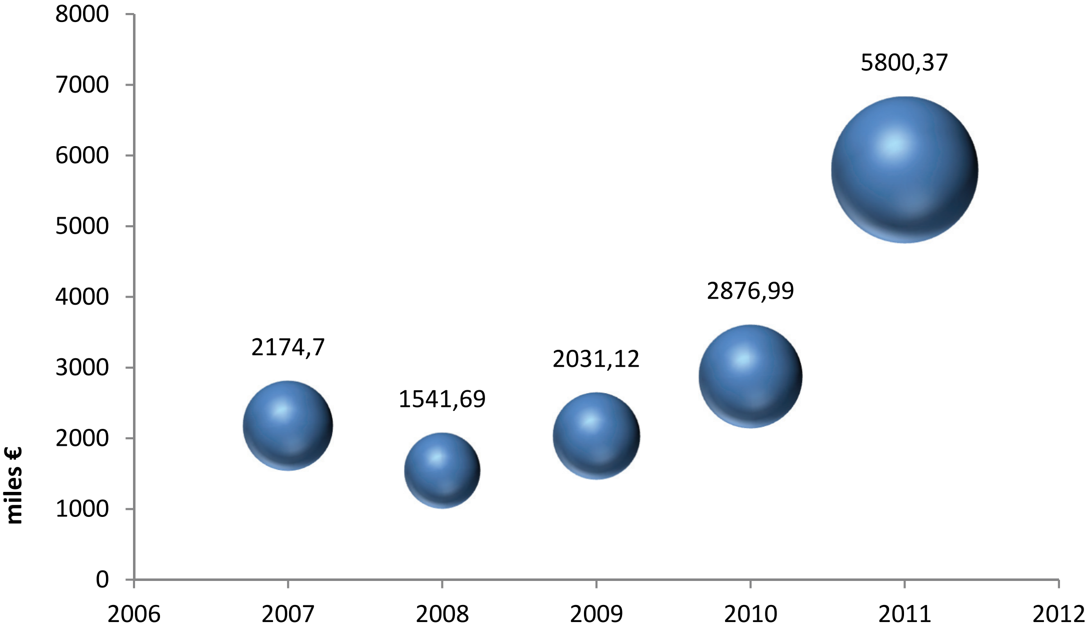


FINANCIACIÓN / FUNDING

Financiación del ICMS por Organismo Financiador 2011 (Sede-CicCartuja)
Funding of ICMS classified by source 2011 (Sede-CicCartuja)



Evolución 2007-2011 de la Financiación del ICMS (PCO)
Evolution of the funding of the ICMS in the period 2007-2011



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Revistas SCI en las que se ha publicado algún artículo, por orden de Factor de Impacto
Number of Scientific Papers published in a Specific Journal Arranged by Their Impact Factor (SCI)

REVISTA JOURNAL	ARTÍCULOS PAPERS	FACTOR DE IMPACTO IMPACT FACTOR (*)
ADVANCED MATERIALS	3	13,877
ADVANCED FUNCTIONAL MATERIALS	1	10,179
ENERGY ENVIRONMENTAL SCIENCE	2	9,61
NEW PHYTOLOGIST	1	6,645
PLANT PHYSIOLOGY	1	6,535
CHEMICAL COMMUNICATIONS	1	6,169
JOURNAL OF MATERIALS CHEMISTRY	1	5,968
APPLIED CATALYSIS B ENVIRONMENTAL	3	5,968
NANOSCALE	2	5,914
ANALYTICAL CHEMISTRY	1	5,856
CHEMCATCHEM	1	5,207
JOURNAL OF APPLIED CRYSTALLOGRAPHY	1	5,152
JOURNAL OF POWER SOURCES	2	4,951
JOURNAL OF PHYSICAL CHEMISTRY C	4	4,805
ANALYTICA CHIMICA ACTA	1	4,555
SOFT MATTER	1	4,39
LANGMUIR	4	4,186
JOURNAL OF HAZARDOUS MATERIALS	3	4,173
INTERNATIONAL JOURNAL OF HYDROGEN ENERGY	1	4,054
NANOTECHNOLOGY	1	3,979
APPLIED CATALYSIS A GENERAL	3	3,903
APPLIED PHYSICS LETTERS	1	3,844
ACTA MATERIALIA	1	3,755
JOURNAL OF PHYSICAL CHEMISTRY B	1	3,696
CELLULOSE	1	3,6
PHYSICAL CHEMISTRY CHEMICAL PHYSICS	1	3,573
CHEMICAL ENGINEERING JOURNAL	4	3,461
CHEMPHYSCHEM	1	3,412
CATALYSIS TODAY	2	3,407
CHEMOSPHERE	1	3,206
DYES AND PIGMENTS	1	3,126
JOURNAL OF RAMAN SPECTROSCOPY	1	3,087

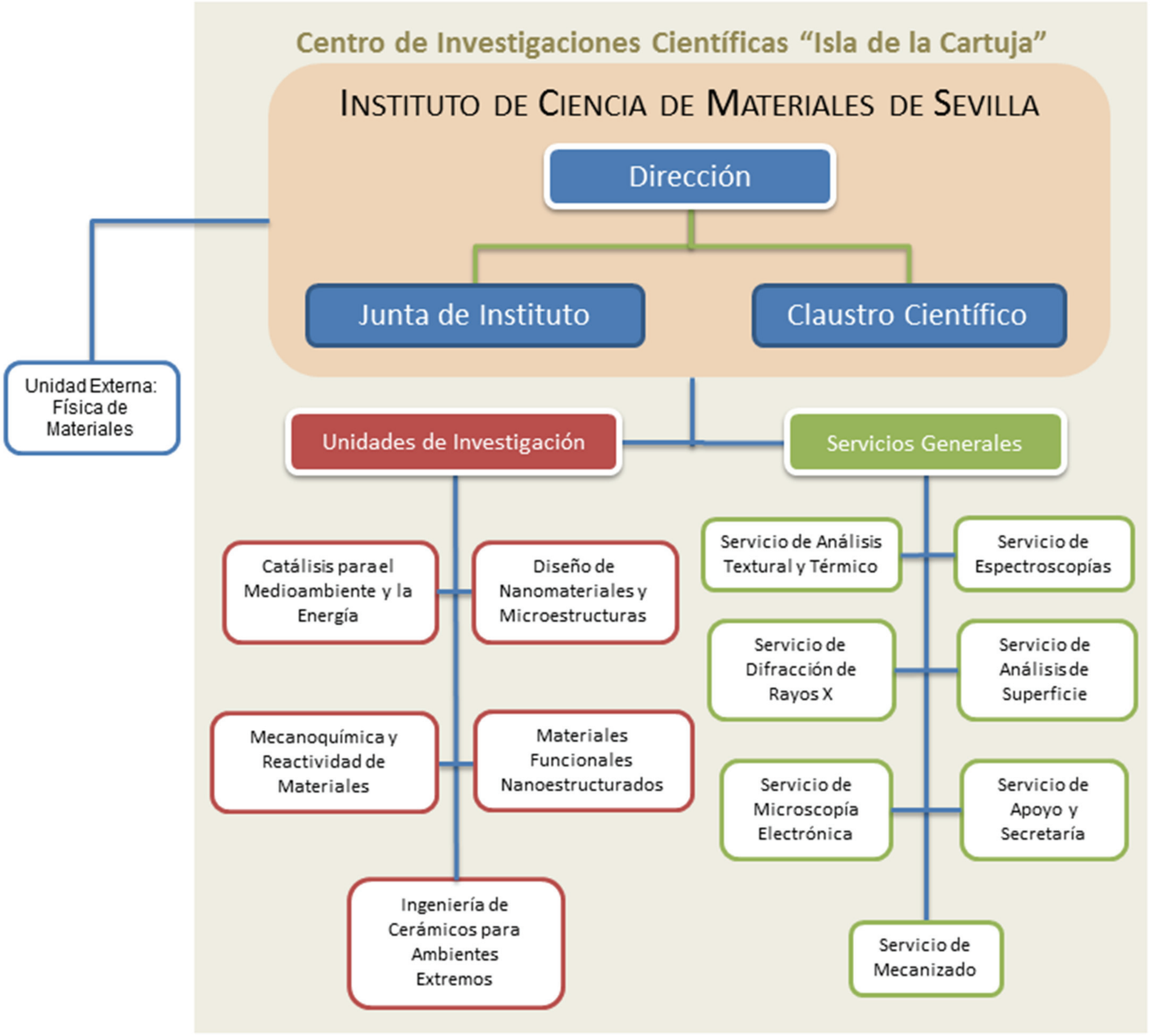
REVISTA **JOURNAL**	ARTÍCULOS PAPERS	FACTOR DE IMPACTO IMPACT FACTOR (*)
CATALYSIS COMMUNICATIONS	1	2,986
POLYMER DEGRADATION AND STABILITY	1	2,769
SCRIPTA MATERIALIA	1	2,699
SOLID STATE IONICS	1	2,646
TOPICS IN CATALYSIS	1	2,624
JOURNAL OF PHYSICS D APPLIED PHYSICS	2	2,544
APPLIED CLAY SCIENCE	3	2,474
PLASMA PROCESSES AND POLYMERS	2	2,468
JOURNAL OF PHOTOCHEMISTRY AND PHOTOBIOLOGY A CHEMISTRY	2	2,421
JOURNAL OF THE EUROPEAN CERAMIC SOCIETY	7	2,353
JOURNAL OF MATERIALS SCIENCE MATERIALS IN MEDICINE	1	2,316
JOURNAL OF THE AMERICAN CERAMIC SOCIETY	1	2,272
CATALYSIS LETTERS	1	2,242
INDUSTRIAL ENGINEERING CHEMISTRY RESEARCH	1	2,237
MATERIALS CHEMISTRY AND PHYSICS	2	2,234
AMERICAN MINERALOGIST	1	2,169
JOURNAL OF APPLIED PHYSICS	2	2,168
JOURNAL OF SOLID STATE CHEMISTRY	2	2,159
JOURNAL OF SOLID STATE ELECTROCHEMISTRY	1	2,131
JOURNAL OF ARCHAEOLOGICAL SCIENCE	1	1,914
DIAMOND AND RELATED MATERIALS	1	1,913
THIN SOLID FILMS	3	1,89
WEAR	1	1,872
SURFACE COATINGS TECHNOLOGY	5	1,867
THERMOCHIMICA ACTA	3	1,805
INTERNATIONAL JOURNAL OF PHOTOENERGY	1	1,769
CERAMICS INTERNATIONAL	1	1,751
INTERMETALLICS	1	1,649
JOURNAL OF SOL GEL SCIENCE AND TECHNOLOGY	1	1,632
JOURNAL OF THERMAL ANALYSIS AND CALORIMETRY	1	1,604
TRIBOLOGY INTERNATIONAL	1	1,553
SOLID STATE NUCLEAR MAGNETIC RESONANCE	1	1,172
SPECTROSCOPY LETTERS	2	0,719
PHYSICS OF THE SOLID STATE	1	0,711
BOLETIN DE LA SOCIEDAD ESPAÑOLA DE CERAMICA Y VIDRIO	1	0,432

REVISTA JOURNAL	ARTÍCULOS PAPERS	FACTOR DE IMPACTO IMPACT FACTOR (*)
ACTA MICROSCOPICA	1	0,202
ACS CATALYSIS	1	---
JOURNAL OF NANOBIOTECHNOLOGY	1	---
OPTICAL MATERIALS EXPRESS	1	---

(*) Factor de Impacto correspondiente al año 2011
Journal Citation Reports of 2011

COMPOSICIÓN Y ESTRUCTURA
STRUCTURE AND ORGANISATION

ORGANIGRAMA / ORGANIZATION CHART



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PROYECTOS DE INVESTIGACIÓN / RESEARCH PROJECTS

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Fondo Europeo de Desarrollo Regional
"Una manera de hacer Europa"
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Desarrollo de estrategias para la preparación y optimización de materiales altamente fotoactivos Development of photocatalytic-materials highly activ in the visible for environmental applications

Código/Code: CTQ2008-05961-C02-01
Periodo/Period: 01-01-2009 / 31-12-2011
Organismo Financiador/Financial source: Ministerio de Ciencia e Innovación
Importe total/Total amount: 102.850 €
Investigador responsable/Research head: José Antonio Navío Santos
Componentes/Research group: Gerardo Colón Ibáñez, M. Carmen Hidalgo López, Manuel Macías Azaña, Marina Maicu

RESUMEN / ABSTRACT

El objetivo general de este proyecto coordinado es "diseñar una nueva generación de materiales en forma de polvo con tamaño nanométrico basados en TiO_2, SnO_2 y ZnO simples, mixtos y/o dopados con otros iones, con alta actividad fotocatalítica en el visible y su fijación en otros materiales (membranas, vidrios, arcillas y láminas metálicas) que permitan emplearlos, de manera eficiente y competitiva en procesos de descontaminación fotocatalítica de efluentes líquidos y gases contaminados". La hipótesis fundamental de la que se parte es que existen pigmentos inorgánicos (tales como el TiO_2, SnO_2, ZnO, etc.) con actividad fotocatalítica en UV capaces de degradar de forma no selectiva a especies tóxicas presentes en nuestro medio ambiente. El reto es superar los problemas derivados de la utilización sólo de la parte UV del espectro solar y extender la respuesta hacia el visible, implementando al mismo tiempo, las propiedades fisicoquímicas de los fotocatalizadores.

Para realizar este estudio se proponen dos bloques principales de actividad que serán el diseño y desarrollo de catalizadores heterogéneos de tamaño nanométricos altamente fotoactivos, basados en TiO_2, SnO_2 y ZnO que puedan hacer las transformaciones de degradación de contaminantes mediante el concurso de luz solar visible (Química Solar Medioambiental) y la inmovilización de nanopartículas de estos semiconductores, simples, mixtos y/o dopados, en soportes adecuados (membranas, vidrios, láminas metálicas, fibras, placas cerámicas, etc,) con el fin de desarrollar dispositivos fotocatalíticos con alta actividad para el tratamiento de contaminantes en gases y aguas, para la generación de superficies autolimpiables.

The main goal of this coordinated project is "the tailoring of a new generation of powdered materials having nanometer size based on TiO_2, SnO_2 and ZnO single, mixed an/or doped showing high photoactivity in the visible region (nanophotocatalysts), eventually immobilized on other selected materials (membranes, glass, ceramic tiles, clays and metal films) in order to be used in a competitive and efficiently way to the treatment of pollutants in water and air by using the solar energy". The principal hypothesis is the existence of inorganic pigments such as TiO_2, SnO_2 ZnO having high oxidizing power in the UV region that are capable of degrading toxic species present in our environment. The project intends to develop new heterogeneous

TiO_2, SnO_2 and ZnO nanocatalysts exhibiting good optoelectronic properties in the visible region at the same time that the physicochemical properties are being implemented.

Two main research activities will be proposed to cover the development of heterogeneous nanosized TiO_2, SnO_2 and ZnO powders (nanocatalysts) capable to design and develop the photodegradation of pollutants in water and air, by the use of Solar Light (Environmental Solar Chemistry). The project also will address the immobilization of different semiconductor nanoparticles (single, mixed and/or doped) on selected supports (membranes, glass and metal films) with the intention of developing heterogeneous systems exhibiting high photocatalytic activity for their applicability to the treatment of pollutants that would represent an improvement in the catalyst filtration and at the same time, with the generation of self-cleaning surfaces.

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Catalizadores nanoestructurados basados en Au para reacciones de oxidación selectiva

Gold based nanostructured catalysts for selective oxidation reactions

Código/Code:	CTQ2010-21348-C02-01
Periodo/Period:	1-01-2011 / 31-12-2011
Organismo Financiador/Financial source:	Otros Programas del Plan Nacional I+D. Ministerio de Ciencia y Tecnología
Importe total/Total amount:	10.890 €
Investigador responsable/Research head:	Juan Pedro Holgado Vázquez
Componentes/Research group:	Alfonso Caballero Martínez, Víctor Manuel González de la Cruz, Fátima Ternero Fernández, Richard M. Lambert

RESUMEN / ABSTRACT

El objetivo del proyecto es el desarrollo de catalizadores con base oro, con alta reactividad en los procesos de oxidación selectiva. En este contexto, se abordan reacciones tales como la oxidación selectiva del alcohol bencílico (y derivados) o la oxidación selectiva de CO. esta última conectada con su aplicación en Catálisis Ambiental como es el control de la calidad del aire y en aplicaciones energéticas como la purificación de corriente de H2 procedente de procesos de reformado (PROX).

Las propiedades del oro, metal biocompatible y no tóxico, puede ser explotadas en catálisis cuando se usa en forma soportada y muy dispersa. Se pretende optimizar el rendimiento de los catalizadores mediante el control del tamaño, forma de las nanopartículas y su interacción con el soporte, en base a la “dependencia de la estructura” de estas reacciones. Así, se preparan catalizadores basados en Au, doblemente nanoestructurados (tanto a nivel de la fase activa como del soporte) soportados sobre CeO2 y TiO2 (Al2O3 y SiO2 como referencia) mediante distintas estrategias de síntesis; evaluando sus propiedades mediante técnicas de caracterización avanzadas y evaluando su comportamiento en reactividad (en régimen estacionario y transitorio) en procesos de oxidación. En el mismo contexto, y considerando la reciente apa-

rición de catalizadores bimetálicos (AuCu, AuPd) para estas reacciones con elevados rendimientos, se prepararan sistemas AuPt, AuCu y Au Ni con control del tamaño y la composición de la fase activa.

The aim of the proposed project is the development of highly active gold-based catalysts for selective oxidation processes. In these context, benzyl alcohol oxidation (and derivatives) under mild conditions and low temperature CO oxidation in connection with applications in Environment Catalysis as the air control (CO-removal from air) and applications in Catalysis for Energy as the purification of H_2 produced by reforming (CO removal from H_2) will be considered.

The outstanding properties of gold, a biocompatible non-toxic metal, can be exploited in catalysis when used in highly dispersed form. In order to get elevated yields and selectivities, doubly nanostructured (considering both the active phase and support) gold-based catalysts deposited onto CeO_2 and TiO_2 (Al_2O_3 and SiO_2 as references) will be prepared. Monometallic gold catalysts will be prepared with control of size and shape of the Au particles, taking advantage of the observed “structure sensitivity” of the proposed reactions. In the same context, it has been recently reported that bimetallic composition based on Gold (AuPd, AuCu, etc) may enhance the performance of these catalysts. Therefore bimetallic catalysts such as AuPt, AuCu and AuNi, will be explored and tested.

Producción de gas de síntesis e hidrógeno mediante reformado de hidrocarburo con catalizadores nanoestructurados de niquel

Syngas and Hydrogen Production by Hydrocarbon Reforming on Nickel Nanostructured Catalysts (SYNANOCAT)

Código/Code:	ENE2007-67926-C02-01
Periodo/Period:	1-12-2007/30-11-2011
Organismo Financiador/Financial source:	Ministerio de Educación y Ciencia
Importe total/Total amount:	119.790 €
Investigador responsable/Research head:	Alfonso Caballero Martínez
Componentes/Research group:	Juan Pedro Holgado Vázquez, Agustín R. González-Elipe, Victor Manuel González de la Cruz, Rosa Pereñiguez Rodríguez

RESUMEN / ABSTRACT

Este proyecto coordinado de investigación, que puede considerarse como extensión de los anteriores ENE2004-01660 y ENE2004-06176, pretende la preparación de nuevos sistemas catalíticos,con tamaños de partícula discretos y con alta resistencia a la desactivación. El objetivo ultimo es la mejora de la reacción de reformado de hidrocarburos para producción de H_2(+CO), principalmente metano y propano, al ser esta una reacción dependiente de la estructura, y por tanto sensible al tamaño de partícula.

Para ello, se prepararán diferentes series de nanopartículas de níquel de tamaño y morfología bien definidos, utilizando métodos ex-situ como la irradiación mediante plasma de microondas, líquidos iónicos, microemulsión inversa o la impregnación con modificación externa del soporte por sililación.

Estos métodos nos permitirán obtener partículas con un rango de tamaños muy amplio, desde menos de 10nm hasta valores entorno a los 100nm y con una estrecha distribución de tamaños de partícula.

La actividad catalítica de estas nanopartículas, una vez depositadas en soportes como ZrO_2 or Al_2O_3, será evaluada en las reacciones de reformado de metano y propano; estableciendo una correlación estructura-reactividad. Se estudiarán con una especial atención los procesos de deposición de carbón sobre los catalizadores en condiciones de reacción, ya que son los principales responsables de la disminución en la eficiencia de estos sistemas catalíticos. El control estricto de la morfología de las nanopartículas metálicas nos permitirá, por tanto, correlacionar la cinética de estos procesos de desactivación con sus características estructurales. Por otro lado, estudiaremos el efecto en la mejora de las prestaciones catalíticas globales de la adición de promotores como Pt, Au, Sr, K, etc.

Alternativamente, se realizará un estudio de la reacción de reformado inducida por un plasma de microondas, con el fin último de desarrollar un sistema integrado térmico-plasma, que esperamos mejore las condiciones de reacción, reduciendo la temperatura necesaria y/o disminuyendo los procesos de deposición de coque sobre los catalizadores.

The coordinated proposed research project, that seek to be an extension of the references ENE2004- 01660 and ENE2004-06176,pretends to prepare new catalytic systems, with a discrete crystallite size and a higher resistance to deactivation. The aim is to obtain catalysts for an optimum performance in the reforming reaction of hydrocarbons to yield H2(+CO), principally from methane and propane. These reactions being structure-sensitive, are affected by the size of metallic particles.

Nanoparticles of nickel with well controlled size and morphology will be prepared by ex-situ methods as microwave plasma irradiation, ionic liquid, reverse microemulsion or impregnation with external surface modification by silylation. These methods will allow us to obtain metal particles of a very different range of size: from less than 10nm to sizes about 100nm and a narrow particle size distribution. The catalytic activity of these nanoparticles, supported on different oxides as ZrO_2 or Al_2O_3, will be evaluated in the reforming reactions of methane and propane to establish a structure-reactivity relationship. Special attention will be devoted to the carbon deposition over the catalyst in reaction conditions, the more important process hindering the performances of these kind of catalysts. The strict control of the morphology of the particles must allow us to correlate the kinetic of the deactivation process to the different type of nanoparticles. Also, we will evaluate the effect of different kind of additives, as Pt, Au, Sr, K, etc., reported in the literature as beneficial for the overall activity of these materials.

The reforming reactions of hydrocarbon will be alternatively studied in the presence of a microwave generated plasma. We expect finally to develop an integrated thermal-plasma reactor that could permit the reaction at a lower temperature and/or with less deposition of coke over the catalyst.

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Integración de reactores catalíticos de microcanales para la producción de hidrógeno a partir de alcoholes
Integration of microchannel catalytic reactors for hydrogen production from alcohols

Código/Code:	ENE2009-14522-C05-01 (subprograma CON)
Periodo/Period:	1-08-2009 / 31-07-2012
Organismo Financiador/Financial source:	Programa Nacional de Proyectos de Investigación Fundamental, Subprograma de Proyectos de Investigación Fundamental no Orientada (Ministerio de Ciencia e Innovación)
Importe total/Total amount:	314.600 €
Investigador responsable/Research head:	José Antonio Odriozola Gordón
Componentes/Research group:	M.A. Centeno, S. Ivanova, F. Romero Sarria, M.I. Domínguez, Sandra Palma, Oscar Laguna, Ana Penkova, Sylvia Cruz, W.Yesid Hernández, Luis Bobadilla

RESUMEN / ABSTRACT

El uso masivo y generalizado de dispositivos eléctricos y electrónicos portátiles aumenta la necesidad de fuentes de potencia autónomas y eficientes, de hasta unos 50 We, capaces de reemplazar la tecnología actual basada en el uso de baterías. El uso de combustibles o productos químicos convencionales, hidrocarburos o alcoholes por ejemplo, es una alternativa prometedora cuando se combina con los recientes desarrollos en intensificación de procesos basados en la tecnología de reactores de microcanales.

El desarrollo de la tecnología de microcanales para la producción de hidrógeno, in situ y a demanda, a partir de alcoholes, se comenzó a estudiar en el proyecto anterior (MAT2006-12386-C05). Este estudio permitió la construcción de reactores de microcanales para las reacciones de reformado catalítico de metanol y oxidación preferente de CO (PROX).

En el presente proyecto se pretenden aplicar los conocimientos adquiridos para acoplar los microrreactores entre sí integrando flujos térmicos y materiales, escalarlos, y unirlos a una celda de combustible comercial de 50 We (PEMFC). En paralelo, se desarrollarán reactores de microcanales para el reformado catalítico de etanol y la reacción de desplazamiento del gas de agua (WGS) lo que permite aumentar la versatilidad el dispositivo diseñado.

La viabilidad de estas fuentes de potencia autónomas requiere el estudio no sólo de la fabricación, escalado de los microreactores e integración de los flujos térmicos y materiales sino también explorar el uso de materiales de mayor disponibilidad (aceros ferríticos adaptados al uso), su durabilidad (aceros, catalizadores, soldaduras, juntas, …) y el desarrollo de un algoritmo de control para el conjunto formado por el procesador de combustible (reformado + eliminación de CO) y la pila de combustible.

The widespread use of portable electric and electronic devices increases the need for efficient autonomous power supplies (up to 50 We) that replace the currently predominant battery technology. The use of common fuels/chemicals, such as hydrocarbons or alcohols, as an energy source is a promising alternative when combined with the recent developments in microchannel reactor technology.

In the previous project (MAT2006-12386-C05) we began to explore the use of microchannel reactor technology to generate hydrogen on site and on demand by processing alcohols which has allowed the manufacturing of microreactors for the catalytic steam reforming of methanol and CO preferential oxidation (PROX) reactions.

In the present project, the main focus is set on the scaling up of the already designed microreactors which will allow the fueling of a 50 We commercial fuel cell (PEMFC) and the integration of both, the material and thermal flows generated in the fuel processor and the fuel cell, including the production and cleaning steps required by the PEMFC. In addition to this, the development of microreactors for the catalytic steam reforming of ethanol and the water-gas-shift (WGS) reactions is considered in this project for increasing the versatility of the designed device.

The feasibility of this kind of autonomous power supplies would require the study of the manufacturing, scaling up of the microreactors and material and thermal flows integration, but also to explore the use of easily available materials (new steels adapted to use), the ageing behaviour of devices (steel, catalysts, sealings, …) and the development of a control algorithm of the fuel processor/fuel cell system

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Desarrollo de nuevos procesos industriales basados en sistemas catalíticos para la obtención sostenible de ingredientes base en fragancias y aromas

Development of new industrial processes based on catalytic systems for Sustainable production of base compounds of fragrances and aromas

Código/Code:	IPT-2011-1553-420000
Periodo/Period:	04-05-2011 / 31-12-2014
Organismo Financiador/Financial source:	Programa INNPACTO. Ministerio de Economía y Competitividad
Importe total/Total amount:	183.423 €
Investigador responsable/Research head:	Juan Pedro Holgado Vázquez
Componentes/Research group:	Alfonso Caballero Martínez, Víctor Manuel González de la Cruz, Rosa Pereñíguez Rodríguez, Gerardo Colón Ibáñez

RESUMEN / ABSTRACT

En la actualidad, los procesos industriales utilizados para la transformación de muchos compuestos utilizados en el campo de las fragancias y los aromas ofrecen bajos rendimientos y

generan una enorme cantidad de residuos peligrosos, que requieren varias etapas de segregación y tratamiento de los mismos durante el proceso. La mayor parte de estos procesos se basan en reacciones de oxidación/reducción de compuestos estequiometricos, o están basados en sistemas de catálisis homogénea, los cuales presentan inconvenientes asociados con la corrosión, la recuperación del catalizador de la mezcla de reacción y su regeneración para su posible reutilización. En este contexto "eco-amigable", existe un interés creciente para el uso de oxidantes menos contaminantes, tales como el peróxido de hidrógeno o el oxígeno molecular, y la integración de dichos oxidantes en sistemas de catálisis heterogénea. Obviamente uno de los mayores retos que presentan las reacciones basadas en sistemas catalíticos es lograr el máximo rendimiento (producto de conversión por selectividad) con objeto de reducir el consumo de reactivos (materias primas), y minimizar los procesos de separación y eliminación de subproductos no deseados fruto de la ineficacia del proceso. En este tipo de reacciones (con compuestos principalmente orgánicos, muchos de origen natural), no es, en general, difícil obtener una alta conversión, pero dado que estos compuestos presentan multiples funcionalidades y/o puntos susceptibles de ser oxidados, el reto se centra en la obtención de una alta selectividad, generalmente incluso a nivel enantiomérico.

En el marco del proyecto, se han seleccionado procesos de interés en la industria cosmética y alimentaria, con objeto de conseguir el desarrollo a escala industrial de procesos basados en sistemas de catálisis heterogénea para la obtención de compuestos intermedios de gran valor añadido en el mercado de los perfumes y aromas, como son, entre otros, el proceso de obtención de la l-carvona a partir de la oxidación catalítica del d-limoneno.

Nowadays, most of the industrial processes used for transformations of many compounds used in the field of fragrances and aromas have low yields, and generate a lot of environmentally noxious products, being necessary to accomplish several stages of segregation and treatment during the process of production of these chemicals. Most of these processes are done by reduction or oxidation reactions using stoichiometric compounds, or are based in homogeneous catalysis, that present associated hitches associated with corrosion, recovery of the catalysts from reaction media and its regeneration for its possible recycle. In this "environmentally friendly" context, there is a growing interest in the use of oxidants less contaminants, such as molecular oxygen or hydrogen peroxide, and the integration of these oxidants into heterogeneous catalysis processes. Obviously, one of the big challenges for catalytic systems is to maximize the yield (conversion times selectivity), in order to reduce the consumption of reactants (raw material), and minimize the separation and elimination of undesired sub-products obtained as consequence of process inefficacy. In these type of reactions (with mainly organic products, many from natural sources), it is not, as a general rule, difficult to obtain a high conversion, but as the starting materials present many functionalities and/or points susceptible to be oxidized, the main challenge is to obtain a (very) high selectivity, in many cases even at enantiomer level.

In this project, we have selected processes and reactions with a direct interest in the food and cosmetic industry, with the scope to develop processes, at industrial scale, based on heterogeneous catalysts to obtain compounds with high added value in the aromas and fragrances fields, such as the production of l-carvone from catalytic oxidation of d-limonene.

Reformado Catalítico de Glicerina
Catalytic reforming of glycerol

Código/Code:	P09-TEP-5454 (Proyecto de Excelencia)
Periodo/Period:	01-01-2010 / 31-12-2012
Organismo Financiador/Financial source:	Junta de Andalucía
Importe total/Total amount:	284.545,68 €
Investigador responsable/Research head:	José Antonio Odriozola Gordón
Componentes/Research group:	Luis F. Bobadilla Baladrón, Sylvia A. Cruz Torres, M. Isabel Domínguez Leal, Anna D. Penkova, Francisca Romero Sarria, Andrea Alvarez Moreno

RESUMEN / ABSTRACT

Este proyecto pretende la producción de hidrógeno a partir del reformado de glicerina. La glicerina es el producto secundario principal en la producción de bio-diesel a través de la transesterificatión de ácidos grasos. Si tenemos en cuenta el desarrollo actual, la producción de bio-combustibles se estima en 9.9 Mtoe para 2010, lo que representa el 50% de los objetivos de la Unión Europea.

Los sistemas de energía actuales necesita el desarrollo de modelos energéticos alternativos. El empleo de hidrógeno como vector energético representa una de esas alternativas, aunque para asegurar la sostenibilidad se requiere que el hidrógeno se produzca a partir de fuentes renovables. La principal ventaja del planteamiento que proponemos, aprovechamiento de la glicerina, reside en que además de sostenible el balance de carbono es prácticamente neutro. Además, su valorización debe conducir a aumentar la rentabilidad de las bio-refinerías que de otro modo se verían afectadas por el incremento de costes asociados a la eliminación de este producto

The main objective of this Project is the production of Hydrogen from glicerol steam reforming. Glycerol is the most important by-product of the biodiesel production from the transterification of fatty acids. In the year 2010, the estimated production of biofuels was about 9.9 millions of tonnes, which represents 50% of the aims of the European Union objectives. The current energy system needs the development of alternative energetic models. The use of hydrogen as energetic vector is one of these alternatives, but, to assure the sustainability, its production must be from renewable sources. Among the possible renewable sources of hydrogen, the main advantage of the use of glycerol is the almost neutral carbon balance. In addition, the glycerol valorisation must lead to increase the profitability of the bio-refineries that, differently, would meet affected by the increase of costs associated with the elimination of this product.

Nuevos fotocatalizadores basados en compuestos de Bi^{3+} altamente fotoactivos en el visible

New Bi^{3+} based photocatalysts highly active in the visible

Código/Code:	P09-FQM-4570 (Proyecto de Excelencia)
Periodo/Period:	11-03-2011 / 31-03- 2015
Organismo Financiador/Financial source:	Junta de Andalucía
Importe total/Total amount:	82.000 €
Investigador responsable/Research head:	Gerardo Colón Ibáñez
Componentes/Research group:	M. Carmen Hidalgo López, J. Antonio Navío Santos, Manuel Macías Azaña, Sebastián Murcia

RESUMEN / ABSTRACT

El objetivo principal de este proyecto es el desarrollo de una nueva generación de materiales nanoestructurados alternativos al TiO_2 que presenten una alta fotoactividad en la región del visible y que puedan ser utilizados de forma competitiva y eficiente en procesos de tratamiento de efluentes líquidos y gaseosos mediante el aprovechamiento de la luz solar. El presente proyecto pretende desarrollar nuevos sistemas de nanocatalizadores heterogéneos basados en Bi^{3+} (Bi_2WO_4, Bi_2MoO_6, $BiVO_4$, Bi_3O_4Cl, $CaBi_2O_4$, $PbBi_2Nb_2O_9$,…) que presenten unas propiedades optoelectrónicas adecuadas para el aprovechamiento de la energía solar en el rango del visible (Fotocatálisis Solar) y que al mismo tiempo exhiban unas propiedades fisicoquímicas mejoradas que optimicen el proceso fotocatalítico desde el punto de vista de difusión y transferencia de portadores de carga fotogenerados.

The main objective of this project is the development of a new generation of nanostructured materials alternative to TiO_2 with high photoactivity in the visible region that could be efficiently used in liquid or gaseous effluent treatment. The present project intent to develop new heterogeneous nanocatalytic systems based on Bi^{3+} (Bi_2WO_4, Bi_2MoO_6, $BiVO_4$, Bi_3O_4Cl, $CaBi_2O_4$, $PbBi_2Nb_2O_9$,…) exhibiting appropriated optoelectronic properties for the solar light use in the visible range (Solar Photocatalysis). Moreover, from the point of view of the photoinduced charge carriers diffusion and transfer, the improved physicochemical properties would optimize the photocatalytic process.

Otros Proyectos / Other Projects

Desarrollo de nuevos catalizadores a partir de fosfatos naturales marroquíes para las reacciones de oxidación de alcoholes y producción de hidrógeno

Código/Code:	C/030491/10
Periodo/Period:	27-01-2011 / 27-01-2012
Organismo Financiador/Financial source:	Otros programas de la Agencia Española de Cooperación Internacional (AECI), Ministerio de Asuntos Exteriores y Cooperación
Importe total/Total amount:	11.000 €
Investigador responsable/Research head:	Alfonso Caballero Martínez

Valorización de fosfatos naturales marroquíes en aplicaciones catalíticas energéticas y medioambientales

Código/Code: A1/035614/11
Periodo/Period: 13-12-2011 / 12-12-2012
Organismo Financiador/Financial source: Otros programas de la Agencia Española de Cooperación Internacional (AECI), Ministerio de Asuntos Exteriores y Cooperación
Importe total/Total amount: 55.650 €
Investigador responsable/Research head: Alfonso Caballero Martínez

COOPERACIÓN INTERNACIONAL Y OTROS

INTERNATIONAL COOPERATION AND OTHERS

Reformado catalítico de glicerol: Estudio IR de la influencia de las propiedades de los sólidos sobre el mecanismo de reacción

Código/Code: FR2009-0105
Periodo/Period: 1-01-2010 / 31-12-2011
Entidad Financiadora/Financial source: ACCIONES INTEGRADAS (Ministerio de Ciencia e Innovación) con Francia
Importe total/Total amount: 12.000 €
Investigador responsable/Research head: Francisca Romero Sarria

Design and characterization of gold catalysts for pure hydrogen production for fuel cell application

Código/Code: 2009BG0024
Periodo/Period: 01-01-2011 / 31-12-2012
Organismo Financiador/Financial source: Proyecto conjunto con instituciones extranjeras CSIC-Academia de Ciencias Búlgara
Importe total/Total amount: 3.300 €
Investigador responsable/Research head: José Antonio Odriozola Gordón
Componentes/Research group: Svetlana Ivanova, Francisca Romero Sarria, Miguel Angel Centeno Gallego, Anna Penkova

Transferencia / Technological Transfer

Convenios y Contratos / Contracts and Agreements

Estudio de los parámetros críticos para soldadura de materiales metálicos y verificación de la soldadura obtenida y apoyo en las labores de especificación de producto y definición de sistema

Código/Code: 1185/0017
Periodo/Period: 01-03-2011 / 31-12-2011
Organismo Financiador/Financial source: IMPROEQUIPO INGENIERIA, SL
Importe total/Total amount: 35.400 €
Investigador responsable/Research head: José Antonio Odriozola Gordón
Componentes/Research group: Alicia Corrales Miralles, M. Isabel Domínguez Leal

Estudio en ambientes agresivos de aceros inoxidables ferríticos con adiciones especiales de determinados elementos de aleación

Código/Code: 0802/0017
Periodo/Period: 15-04-2010 / 30-06-2011
Organismo Financiador/Financial source: ACERINOX, S.A.
Importe total/Total amount: 66.481,20 €
Investigador responsable/Research head: José Antonio Odriozola Gordón
Componentes/Research group: Alicia Corrales Miralles

Desarrollo de sistemas catalíticos compactos para aplicaciones energéticas

Código/Code: 1211/0017
Periodo/Period: 25-04-2011 / 10-12-2013
Organismo Financiador/Financial source: Técnicas Reunidas, SA
Importe total/Total amount: 415.041,40 €
Investigador responsable/Research head: José Antonio Odriozola Gordón

Oxidación selectiva de diferentes terpenos de interés en química de fragancias

Código/Code: 020165110009
Periodo/Period: 09-05-2011 / 09-05-2012
Organismo Financiador/Financial source: Destilaciones Bordas Chinchurreta, SA
Importe total/Total amount: 38.940 €
Investigador responsable/Research head: Juan Pedro Holgado Vázquez

Evaluación del riesgo de incendio por autocombustión de neumáticos usados almacenados al aire libre

Periodo/Period:	15-06-2011 / 30-06-2011
Organismo Financiador/Financial source:	Neumáticos Antonio, SLU
Importe total/Total amount:	4.000 €
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PUBLICACIONES / PUBLICATIONS

ARTÍCULOS PUBLICADOS EN REVISTAS SCI / PAPERS IN SCI JOURNALS

Effect of thermal treatments on the catalytic behaviour in the CO preferential oxidation of a CuO-CeO2-ZrO2 catalyst with a flower-like morphology

Moretti, E; Storaro, L; Talon, A; Lenarda, M; Riello, P; Frattini, R; de Yuso, MDM; Jimenez-Lopez, A; Rodriguez-Castellon, E; Ternero, F; Caballero, A; Holgado, JP

Applied Catalysis B-Environmental, **102** (2011) 627-637

DOI: 10.1016/j.apcatb.2011.01.004

A Ce-Zr-Cu oxide system with a flower-like morphology was prepared by a slow co-precipitation method in the absence of any structure directing agent. Four portions of the oxide were thermally treated at four different temperatures (350 degrees C, 450 degrees C, 550 degrees C, 650 degrees C). The resulting materials samples were characterized by quantitative XRD, adsorption-desorption of N-2 at-196 degrees C, SEM and TEM microscopy, -H-2-TPR, XPS and Operando-XANES. All samples were tested in the preferential CO oxidation (CO-PROX) in the 40-190 degrees C temperature range. Thermal treatments were found to induce slight structural changes without altering the starting morphology of the samples. The samples treated at higher temperature 550-650 degrees C showed a quite interesting CO-PROX activity and selectivity in a temperature range suitable for a practical use within the FEMFC technology.

CO oxidation at low temperature on Au/CePO(4): Mechanistic aspects

Romero-Sarria, F; Dominguez, MI; Centeno, MA; Odriozola, JA

Applied Catalysis B-Environmental, **107** (2011) 268-273

DOI: 10.1016/j.apcatb.2011.07.022

This work reports the synthesis and characterization of a cerium phosphate supported gold catalyst as well as its catalytic activity for the oxidation of CO. A precipitation method in the presence of an organic modifier followed by a hydrothermal treatment was used for the support synthesis, resulting in high surface area nanometric particles. Gold/cerium phosphate catalyst with a 1% (w/w) nominal gold content was characterized using XRF, XRD, N(2) adsorption-desorption measurements, TEM and DRIFTS-MS. The catalyst shows good catalytic activity at low temperature. The activity is related to the generation of oxygen vacancies in the support caused by the elimination of structural oxygen. In situ studies revealed that the reaction of the oxygen vacancies with gaseous oxygen resulted in the formation of peroxo species. These species are responsible for the activity detected at room temperature in both the catalyst and the support. Moreover, the presence of carbonate and hydrogen carbonate acting as reaction intermediates have been observed.

Fe-doped ceria solids synthesized by the microemulsion method for CO oxidation reactions
Laguna, OH; Centeno, MA; Boutonnet, M; Odriozola, JA
Applied Catalysis B-Environmental, **106** (2011) 621-629
DOI: 10.1016/j.apcatb.2011.06.025

A series of Ce-Fe mixed oxides as well as the pure oxides were synthesized by the microemulsions method. The solid solution formation was established for all the Fe-doped systems and only a hardly noticeable segregation of alpha-Fe(2)O(3) was appreciated for the solid with the maximum iron content (50 at.% Fe). The oxygen exchange is improved for all the Fe-doped systems; however the 10 at.% Fe appears as the optimal iron content for achieving the maximum oxygen vacancies concentration and the higher reducibility efficiency. The CO oxidation (TOX. PROX) is especially achieved for the solids with the lower iron contents but with a superior oxygen vacancies proportion. These Ce-Fe systems prepared from microemulsions are very attractive to be considered as supports for depositing active phases capable of enhancing oxygen exchange ability of the whole system, allowing higher CO oxidation abilities.

Well-Defined Negatively Charged Gold Carbonyls on Au/SiO(2)
Chakarova, K; Mihaylov, M; Ivanova, S; Centeno, MA; Hadjiivanov, K
Journal Of Physical Chemistry C, **115** (2011) 21273-21282
DOI: 10.1021/jp2070562

A Au/SiO(2) sample was prepared by ammonia-assisted grafting using HAuCl(4) as a gold precursor. Gold on the sample evacuated at 673 K is essentially in metallic form: adsorption of CO at 100 K results in formation of Au(0)-CO species (IR band at 2122 cm(-1) shifting to 2103 cm(-1) at high coverage). Coadsorption of CO and O(2) even at ambient temperature leads to creation of Au(delta+) sites and oxidation of CO. On the contrary, increase of the contact time between CO and the sample leads to a gradual reduction of Au(0) to Au(delta-) species. The process is slightly favored by the presence of water and strongly enhanced in the presence of hydrogen. Back oxidation of Au(delta-) to Au(0) and to Au(delta+) occurs in the presence of oxygen. The Au(delta-) sites strongly adsorb CO and form different interconverting carbonyls observed in the 2080-2050 cm(-1) region. On the basis of adsorption of CO-(13)CO and CO-(13)C(18)O isotopic mixtures, it is concluded that all Au(delta-)-CO species are linear, and probably ordered structures are formed. Intensity transfer phenomena are nicely monitored during adsorption of CO isotopic mixtures. The eventual role of negatively charged gold in catalysis is discussed.

Structural, catalytic/redox and electrical characterization of systems combining Cu-Fe with CeO2 or Ce1-xMxO2-delta (M = Gd or Tb) for direct methane oxidation

Hornes, A.; Munuera, G.; Fuerte, A.; Escudero, M. J.; Daza, L.; Martinez-Arias, A.
Journal Of Power Sources, **196** (2011) 4218-4225
DOI: 10.1016/j.jpowsour.2010.10.042

The present work analyses bimetallic Cu-Fe formulations combined with CeO2 or other structurally related mixed oxides resulting from doping of the former with Gd or Tb, focusing to its possible use as anodes of solid oxide fuel cells (SOFC) for direct oxidation of methane. The main objective is the characterization of the various formulations at structural level as well as with regard to redox changes taking place in the systems upon interaction with methane, in order to evaluate the effects induced by the presence of the mentioned dopants. In the same sense, an analysis of thermal expansion and electrical properties of the systems as well as their chemical compatibilities with several electrolytic materials is performed, considering its possible implantation in SOFC single cells. For the mentioned purposes, the systems have been analysed by means of CH4-TPR tests subsequently followed by TPO tests, as well as by XRD, Raman and XPS, with the aim of exploring structural and redox changes produced in the systems and the formation of carbon deposits during interaction with methane. The results reveal significant modifications in the structural, catalytic/redox and electrical properties of the systems as a function of the presence of Fe and/or Gd and Tb dopants in the formulation.

Novel Bi2WO6-TiO2 heterostructures for Rhodamine B degradation under sunlike irradiation

Lopez, SM; Hidalgo, MC; Navio, JA; Colon, G
Journal Of Hazardous Materials, **185** (2011) 1425-1434
DOI: 10.1016/j.jhazmat.2010.10.065

Highly efficient Bi2WO6-TiO2 heterostructure is synthesized by means of a hydrothermal method having highly photoactivity for the degradation of Rhodamine B under sunlike irradiation. From the structural characterization it has been demonstrated that TiO2 is incorporated on the Aurivillius structure. Interesting synergetic effect between TiO2 and Bi2WO6 leads to an improved charge carrier separation mechanism, causing the excellent photocatalytic performance under sunlike irradiation. The photocatalytic performance of Bi2WO6 and Bi2WO6-TiO2 was compared under different irradiation conditions and using increasing Rhodamine B concentration up to 25 ppm. After the photocatalytic analysis of both systems, the mineralization efficiency of the heterostructure appears significantly higher with respect to Bi2WO6.

Hydrogen production by methanol steam reforming on NiSn/MgO-Al2O3 catalysts: The role of MgO addition

Penkova, A; Bobadilla, L; Ivanova, S; Dominguez, MI; Romero-Sarria, F; Roger, AC; Centeno, MA; Odriozola, JA
Applied Catalysis A-General, **392** (2011) 184-191
DOI: 10.1016/j.apcata.2010.11.016

The effect of the magnesia loading on the surface structure and catalytic properties of NiSn/MgO-Al2O3 catalysts for hydrogen production by methanol steam reforming has been investigated. The catalysts have been obtained by impregnation of gamma-Al2O3 by the incipient wetness method, with variation of the MgO content. X-ray diffraction (XRD), BET surface area and H-2-temperature programmed reduction (TPR) have been used to characterise the prepared catalysts. From this, it has been concluded that the incorporation of MgO results in the formation of MgAl2O4 spinet, which modifies the acid-base properties of the catalysts. The formation of Ni-Sn alloys after the reductive pre-treatment has also been evidenced. The influence of the temperature of reaction and of the MgO loading on the hydrogen production by reforming of methanol has been established. Moreover, tests of catalytic stability have been carried out for more than 20 h. The carbonaceous deposits have been examined by temperature-programmed oxidation (TPO). The analysis of the catalysts after reaction has confirmed the low level of carbon formation on these catalysts. In no case, carbon nanotubes have been detected on the solids.

Photodeposition of gold on titanium dioxide for photocatalytic phenol oxidation
Hidalgo, MC; Murcia, JJ; Navio, JA; Colon, G
Applied Catalysis A-General, **397** (2011) 112-120
DOI: 10.1016/j.apcata.2011.02.030

The influence of experimental conditions during the photodeposition in the preparation of supported Au on TiO2 has been studied. Besides preparation pH, light intensity and deposition time showed to have a high influence on the final properties of gold deposits. Photodeposition using illumination with a high light intensity UV-vis lamp (140 W/m(2) UVA range) resulted to be an ineffective method for obtaining nanoparticles of gold on the titania, producing very large and poorly distributed gold deposits. Thus obtained materials did not show any important improvement of their photocatalytic activity tested for phenol oxidation. By contrast, photodeposition using a low light intensity of illumination (0.15 W/m(2) UVA range), produced materials with notably improved photocatalytic activity. The illumination with such a low light intensity allowed the control of the amount, aggregation and oxidation state of gold by changing deposition time, enabling a feasible method of tailoring Au-TiO2 with the appropriate properties for a high photocatalytic activity. Best photocatalytic behaviour for phenol photodegradation was obtained for Au-TiO2 samples prepared by photodeposition at low light intensity with 120 min photodeposition time for catalysts with a 0.5% and 1% nominal content of gold and with 60 min photodeposition time for catalyst with a 2% nominal content of gold.

Synthesis, characterization and photocatalytic activity of Bi-doped TiO(2) photocatalysts under simulated solar irradiation
Murcia-Lopez, S; Hidalgo, MC; Navio, JA
Applied Catalysis A-General, **404** (2011) 59-67
DOI: 10.1016/j.apcata.2011.07.008

A series of Bi(3+)-doped TiO(2) catalysts with a doping concentration up to 2 wt% were prepared by a sol-gel hydrothermal method. The prepared photocatalysts were characterized by different techniques to determine their structure, morphology and light absorption properties. The activities were evaluated in the photocatalytic oxidation of phenol in aqueous solution under UV-vis illumination. The experimental results indicate that the presence of Bi(3+) in TiO(2) catalysts enhances the photocatalytic reaction of phenol degradation, although the efficiency of the process markedly depends on the nominal content of the Bi(3+) and on the calcination temperature. It was found that the optimal dosage of 0.5 wt% Bi(3+) in TiO(2) and calcinations at 600 degrees C 4h achieved the fastest reaction of phenol degradation under the experimental conditions. From the comparison of the initial rates of the photocatalytic degradation of phenol between home prepared undoped and Bi(3+)-doped TiO(2) with commercial TiO(2) Degussa P25, it can be inferred that home prepared TiO(2) calcined at temperatures above 500 degrees C clearly exceed the photocatalytic performance of P25. When bismuth is incorporated, the reaction rate values are even higher, especially at 600 degrees C. Even when Bi(3+)-doped TiO(2) (0.5 wt% Bi(3+)) calcined at 600 degrees C has almost the same BET surface than P25, its activity is better. In particular, the reaction rate for the sample with a 0.5% mass content of Bi(3+) calcined at 600 degrees C not only present higher value with respect to the other series but also a degree of mineralization close to 100%.

Selective CO removal over Au/CeFe and CeCu catalysts in microreactors studied through kinetic analysis and CFD simulations

Arzamendi, G; Uriz, I; Dieguez, PM; Laguna, OH; Hernandez, WV; Alvarez, A; Centeno, MA; Odriozola, JA; Montes, M; Gandia, LM

Chemical Engineering Journal, **167** (2011) 588-596

DOI: 10.1016/j.cej.2010.08.083

A kinetic study of the preferential oxidation of CO in H-2 rich streams (CO-PrOx) over a cerium-copper oxide (CeCu) and a gold catalyst supported on cerium-iron oxide (Au/CeFe) is presented. The gold catalyst is very active but the CeCu oxide is more selective. A kinetic model describing the CO-PrOx system with CO2 and H2O in the feed has been formulated considering the oxidation of CO and H-2 and the reverse water-gas shift reaction. The rate equations have been implemented in computational fluid dynamics codes to study the influence of the operating variables on the CO-PrOx in microchannels and microslits. The CeCu catalyst is the only one capable of achieving final CO contents below 10-100 ppmv. Due to the opposite effect of temperature on activity and selectivity there is an optimal temperature at which the CO content is minimal over CeCu. This temperature varies between 170 and 200 degrees C as the GHSV increases from 10,000 to 50,000 h(-1). Simulations have evidenced the very good heat transfer performance of the microdevices showing that the CO-PrOx temperature can be controlled using air as cooling fluid although the inlet temperature and flow rate should be carefully controlled to avoid reaction extinction. Both microchannels and microslits behaved similarly. The fact that the microslits are much easier to fabricate may be an interesting advantage in favour of that geometry in this case.

Fischer-Tropsch synthesis in microchannels
Almeida, LC; Echave, FJ; Sanz, O; Centeno, MA; Arzamendi, G; Gandia, LM; Sousa-Aguiar, EF; Odriozola, JA; Montes, M
Chemical Engineering Journal, **167** (2011) 536-544
DOI: 10.1016/j.cej.2010.09.091

Different metallic supports (aluminum foams of 40 ppi, honeycomb monolith and micromonolith of 350 and 1180 cpsi, respectively) have been loaded with a 20%Co-0.5%Re/gamma-Al2O3 catalyst by the washcoating method. Layers of different thicknesses have been deposited onto the metallic supports. The catalytic coatings were characterized measuring their textural properties, adhesion and morphology. These structured catalysts have been tested in the Fischer-Tropsch synthesis (FTS) and compared with a microchannel block presenting perpendicular channels for reaction and cooling. The selectivity depends on the type of support used and mainly on the thickness of the layer deposited. In general, the C5+, selectivity decreased at increasing CO conversion for all of the systems (powder, monoliths, foams and microchannels block). On the other hand, the selectivity to methane increased with the thickness of the catalytic layer due to the higher effective H-2/CO ratio over the active sites resulting from the higher diffusivity of H-2 compared with CO in the liquid products filling the pores. The C5+. selectivity of the microchannels reactor is higher than that of the structured supports and the powder catalyst.

Design and testing of a microchannel reactor for the PROX reaction
Cruz, S; Sanz, O; Poyato, R; Laguna, OH; Echave, FJ; Almeida, LC; Centeno, MA; Arzamendi, G; Gandia, LM; Souza-Aguiar, EF; Montes, M; Odriozola, JA
Chemical Engineering Journal, **167** (2011) 634-642
DOI: 10.1016/j.cej.2010.08.088

The different steps for manufacturing a microchannel reactor for the PROX reaction are discussed. Transient Liquid Phase bonding (TLP) using a Ni-B-Si amorphous melt spun is used for joining micromilled Al-alloyed ferritic stainless steel plates followed by recrystallization at 1200 degrees C for 5 h. A CuOx-CeO2 catalyst synthesized by the coprecipitation method was washcoated on the microchannel block resulting in a homogenous 20-30 mu m thick layer. The catalytic activity for CO-PROX reaction is similar in both the powder catalyst and the microchannel coated reactor but the selectivity is higher in the microchannel reactor.

Ionic liquid protected heteropoly acids for methanol dehydration
Ivanova, S; Nitsch, X; Romero-Sarria, F; Louis, B; Centeno, MA; Roger, AC; Odriozola, JA
Catalysis Today, **171** (2011) 236-241
DOI: 10.1016/j.cattod.2011.03.077

We report herein the synthesis of an organic-inorganic hybrid composed by the ionic liquid protected Keggin structure, as a precursor for acid catalyst and its subsequent application in the methanol dehydration reaction. Special attention was paid to the thermal stability of the resulted hybrids as a function of the Keggin anion. The catalytic behaviour of these new materials are also studied and compared to the metal salt Cs(2)HPW(12)O(40). The prepared hybrids are less thermally stable than the metal salt, but their partial decomposition results in very active and selective catalysts for the dehydration of methanol to dimethyl ether.

Oxidation of CO over gold supported on Zn-modified ceria catalysts

Laguna, OH; Centeno, MA; Romero-Sarria, F; Odriozola, JA
Catalysis Today, **172** (2011) 118-123
DOI: 10.1016/j.cattod.2011.02.015

A series of Zn-modified ceria solids were prepared by thermal decomposition of the corresponding metal propionates. The formation of segregated ZnO particles on the ceria surface is evidenced for these solids using X-ray diffraction; in addition to this the characterization data may allow discarding the formation of a ZnO-CeO(2) solid solution. On modifying with Zn, the reducibility of the ceria support is enhanced, being the highest reducibility the one obtained for the ZnO-CeO(2) solid having a 1:9 Zn:Ce atomic ratio (CeZn10). The activity of this solid in the CO oxidation reaction was the highest among the tested Zn-modified ceria solids. Therefore, catalysts containing 1 wt.% gold, supported on pure ceria and CeZn solids, were prepared, characterized and their catalytic activities tested. The Zn-modified gold catalyst is more active than the un-modified Au/CeO(2) catalyst in the oxidation of CO; this behavior is related to the higher metallic dispersion of gold on the CeZn support surface. However, the number of oxygen vacancies acting as nucleation sites for gold, is hardly modified in the Zn-modified ceria support and, therefore, the higher gold dispersion must be related to high electron density sites on the catalyst surface as a result of Au-Ce-Zn interaction, this improved gold dispersion results in higher activities for CO oxidation.

Influence of the strong metal support interaction effect (SMSI) of Pt/TiO(2) and Pd/TiO(2) systems in the photocatalytic biohydrogen production from glucose solution

Colmenares, JC; Magdziarz, A; Aramendia, MA; Marinas, A; Marinas, JM; Urbano, FJ; Navio, JA
Catalysis Communications, **16** (2011) 1-6
DOI: 10.1016/j.catcom.2011.09.003

Two different catalysts consisting of Pt/TiO(2) and Pd/TiO(2) were submitted to diverse oxidative and reductive calcination treatments and tested for photocatalytic reforming of glucose water solution (as a model of biomass component) in H(2) production. Oxidation and reduction at 850 degrees C resulted in better photocatalysts for hydrogen production than Degussa P-25 and the ones prepared at 500 degrees C, despite the fact that the former consisted in very low surface area (6-8 m(2)/g) rutile titania specimens. The platinum-containing systems prepared at 850 degrees C give the most effective catalysts. XPS characterization of the systems showed that thermal treatment at 850 degrees C resulted in electron transfer from titania to metal particles through the so-called strong metal-support interaction (SMSI) effect. Furthermore, the greater the SMSI effect, the better the catalytic performance. Improvement in photocatalytic behavior is explained in terms of avoidance of electron-hole recombination through the electron transfer from titania to metal particles.

Gold Nanoparticles on Yttrium Modified Titania: Support Properties and Catalytic Activity

Plata, JJ; Marquez, AM; Sanz, JF; Avellaneda, RS; Romero-Sarria, F; Dominguez, MI; Centeno, MA; Odriozola, JA
Topics In Catalysis, **54** (2011) 219-228
DOI: 10.1007/s11244-011-9639-4

A series of titanium oxide catalysts modified with yttrium has been prepared by sol-gel method and their structural properties have been studied. The incorporation of yttrium in the titania lattice favors the formation of oxygen vacancies while at low Y loadings the anatase structure is preserved. The catalytic activity of these solids for CO oxidation is found to be significantly dependent on their physical properties. In particular the amount of dopant controls the number of surface oxygen vacancies created as well as the gold particle size, which directly affects the catalytic activity. Also, a linear relationship between the catalytic activity and the band gap values, which depend on the Y loading, is observed. Density functional theory based calculations show that Y atoms are incorporated at the TiO2 surface at substitutional positions only, while the preferred oxygen vacancies arise by removing the bridge surface oxygen atoms. These O-vacancies are the preferential adsorption sites for Au atoms and nanoparticles, acting as nucleation centers that favor the dispersion of the catalyst active phase over the support surface. In agreement with experiment, Y doping is found to decrease the band gap of the support due to a destabilization of the valence band of the oxide.

Structural and catalytic properties of lanthanide (La, Eu, Gd) doped ceria

Hernandez, WY; Laguna, OH; Centeno, MA; Odriozola, JA
Journal Of Solid State Chemistry, **184** (2011) 3014-3020
DOI: 10.1016/j.jssc.2011.09.018

Ce(0.9)M(0.1)O(2-delta) mixed oxides (M = La, Eu and Gd) were synthesized by coprecipitation. Independent of the dopant cation, the obtained solids maintain the F-type crystalline structure, characteristic of CeO(2) (fluorite structure) without phase segregation. The ceria lattice expands depending on the ionic radii of the dopant cation, as indicated by X-ray diffraction studies. This effect also agrees with the observed shift of the F(2g) Raman vibrational mode. The presence of the dopant cations in the ceria lattice increases the concentration of structural oxygen vacancies and the reducibility of the redox pair Ce(4+)/Ce(3+). All synthesized materials show higher catalytic activity for the CO oxidation reaction than that of bare CeO(2), being Eu-doped solid the one with the best catalytic performances despite of its lower surface area.

Photocatalytic coatings of silver-TiO(2) nanocomposites on foamed waste-glass prepared by sonochemical process

Lee, SW; Obregon-Alfaro, S; Rodriguez-Gonzalez, V
Journal Of Photochemistry And Photobiology A-Chemistry, **221** (2011) 71-76
DOI: 10.1016/j.jphotochem.2011.04.026

Silver-TiO(2) nanocomposite was prepared by photodeposition of silver nanoparticles on the surface of titanium dioxide. The sonochemical method was used for the deposition of Silver-

TiO(2) powder on commercial foamed waste-glass strips (FWGS). The Silver-TiO(2) and the coated FWGS was characterized by XRD, DRS, SEM, TEM and nitrogen adsorption. In order to enhance Silver-TiO(2) deposition, different parameters were evaluated such as the solvent effect and use of stabilizing agents. The best deposition was obtained with an aqueous solution of polyvinyl alcohol (PVA) and an ultrasound irradiation source of 23.3 kHz. The photocatalytic activity of the Silver-TiO(2) coated FWGS was evaluated in the UV photo-assisted destruction of the noxious microalgae, Tetraselmis suecica. It was found that after the photocatalytic irradiation, for 180 min, the algae cells were deformed, fragmented and annihilated, thereby avoiding its regeneration.

Comparative study of the photodeposition of Pt, Au and Pd on pre-sulphated TiO2 for the photocatalytic decomposition of phenol

Maicu, M; Hidalgo, MC; Colon, G; Navio, JA
Journal Of Photochemistry And Photobiology A-Chemistry, **217** (2011) 275-283
DOI: 10.1016/j.jphotochem.2010.10.020

A comparative study of the photodeposition of Pt, Au and Pd under the same experimental conditions onto pre-sulphated and non-sulphated TiO2 was performed. Morphological and surface characterisation of the samples as well as photocatalytic activity for phenol photooxidation was studied. The influence of sulphate pre-treatment on the deposits size and dispersion onto the TiO2 surface, and photodeposition yields with the different metals were also analysed. The photocatalytic activity of the doped materials was then investigated, observing that catalytic behaviour can be correlated to physical characteristics of the samples determined by (XRD) X-ray diffraction, (XPS) X-ray photoelectron spectroscopy, (XRF) X-ray fluorescence spectrometry and (TEM) transmission electron microscopy. Sulphate pre-treatment was found to influence both the level of dispersion and the size of metal clusters on the TiO2 surface. Sulphation and metallisation of samples was found to produce a synergistic enhancement in photoactivity for the degradation of phenol. The photoactivity of the catalysts with respect to the doped metal species was ordered Pt > Pd > Au.

Aluminum Anodization in Oxalic Acid: Controlling the Texture of Al2O3/Al Monoliths for Catalytic Aplications

Sanz, O; Echave, FJ; Odriozola, JA; Montes, M
Industrial & Engineering Chemistry Research, **50** (2011) 2117-2125
DOI: 10.1021/ie102122x

The anodization and postanodization processes of aluminum in order to prepare monoliths for catalytic applications have been studied in this work using oxalic acid as electrolyte. The effect of anodization variables (anodization time, current density, temperature, and electrolyte concentration) and postanodization processes on the surface morphology and textural properties of AAO (anodic aluminum oxide) films is analyzed. The anodization variables affect the two main processes taking part in the Al2O3 layer formation: alumina generation and its dissolution that are controlled by temperature, electrolyte concentration and time. The proper combination of both processes, as a result of the anodization variables choice, produces adherent alumina layers with tailored porosity and surface morphology that show excellent properties to be used as catalyst structured support. Larger pore sizes and the complete absence of sulfur that may poison reduced metal supported active phases are main differences with the classical, most often used, sulfuric acid anodization process.

High-Stable Mesoporous Ni-Ce/Clay Catalysts for Syngas Production
Daza, CE; Gamba, OA; Hernandez, Y; Centeno, MA; Mondragon, F; Moreno, S; Molina, R
Catalysis Letters, **141** (2011) 1037-1046
DOI: 10.1007/s10562-011-0579-1

A mesoporous-type catalytic support was synthesized through the modification of a smectite with polyvinyl alcohol (PVA) and microwaves. Texture and micro-morphology of the support was determined. Several techniques were employed in order to describe the chemical environment of active species on the surface. Ni(0) particle sizes were dependent on the structural site of reducible species. High stable Ni-Ce catalysts (calcined at 800 A degrees C) were evaluated in the CO(2) reforming of methane reaction at 700 A degrees C (WHSV = 96 L g(-1) h(-1), without dilution gas and pre-reduction). The catalysts have presented CH(4) conversions between 40 and 65%, CO(2) conversion between 35 and 65% and H(2)/CO ratios between 0.2 and 0.4.

Influence of Al_2O_3 reinforcement on precipitation kinetic of Cu-Cr nanocomposite
Sheibani, S; Ataie, A; Heshmati-Manesh, S; Caballero, A; Criado, JM
Thermochimica Acta, **526** (2011) 222-228
DOI: 10.1016/j.tca.2011.09.024

In this paper, the kinetic of precipitation process in mechanically alloyed Cu-1 wt.% Cr and Cu-1 wt.% Cr/3 wt.% Al(2)O(3) solid solution was compared using differential scanning calorimetry (DSC), X-ray diffraction (XRD) and transmission electron microscopy (TEM). The ageing kinetics in Cu-Cr and Cu-Cr/Al_2O_3 can be described using Johnson-Mehl-Avrami (JMA) and Sestak-Berggren (SB) models, respectively. These different behaviors have been discussed in details. It was found that in presence of Al_2O_3 reinforcement, the ageing activation energy is decreased and the overall ageing process is accelerated. This behavior is probably due to higher dislocation density previously obtained during ball milling and Al_2O_3-Cu interface. TEM observations confirm that Al_2O_3-Cu interface and structural defects act as a primary and secondary nucleation sites, respectively.

Modifying the Size of Nickel Metallic Particles by H-2/CO Treatment in Ni/ZrO2 Methane Dry Reforming Catalysts
Gonzalez-Delacruz, VM; Pereniguez, R; Temero, F; Holgado, JP; Caballero, A
ACS Catalysis, **1** (2011) 82-88
DOI: 10.1021/cs100116m

The effect of a reduction process with CO or H-2 on the Size of nickel particles in Ni/ZrO2 dry methane reforming catalysts have been studied by means of in situ X-ray Spectroscopy (XAS) and Diffuse Reflectance FTIR Spectroscopy (DRIFTS). Our results clearly indicate that a high temperature treatment with CO increases the dispersion of the nickel metallic phase. XAS results have shown a lower coordination number of Ni in the sample treated with CO than that reduced with H-2. From the DRIFTS results, it can he established that, under the CO treatment, the formation of Ni(CO)(4) complexes corrodes the nickel particles, decreasing their size. The formation of these gas molecules occurs without measurable losses of nickel from the catalyst which maintains the same nickel content after the hydrogen or the CO treatment at high temperature:Therefore, this airborne nickel compound, by colliding with the zirconia surface, must deposit the nickel metal metal atoms around onto the support. This behavior is evidence of an important interaction b etween nickel and zirconia surface as unlike other supports there is no losses of nickel during the dispersion process on zirconia. Although different effects of CO on nickel catalysts have been previously described, we have found for the first time several experimental evidences demonstrating the whole redispersion phenomenon.

ARTÍCULOS EN REVISTAS NO SCI / PAPERS IN NON-SCI JOURNALS

Gold Functionalized Supported Ionic Liquids Catalyst for CO Oxidation
S. Ivanova, L. Bobadilla, A. Penkova, F. Romero-Sarria, M.A. Centeno and J.A. Odriozola
Catalysts, **1** (2011) 52-68
DOI: 10.3390/catal1010052

CONGRESOS Y REUNIONES INTERNACIONALES / INTERNATIONAL CONGRESS AND MEETINGS

PARTICIPACIÓN EN LA ORGANIZACIÓN DE CONGRESOS Y REUNIONES / PARTICIPATION IN ORGANISING CONGRESSES AND MEETINGS

International conference "Nanostructured Catalysts and catalytic processes for the innovative energetic and sustainable development".
5 – 8 junio [Novosibirsk, Rusia]
José Antonio Odriozola Gordón [Miembro del Comité Científico]

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2011 AICHE Spring Meeting & 7 Global Congress on Process Safety
13 – 17 marzo [Chicago, Estados Unidos de América]

Role of support vacancies on the reactivity of gold catalysts in the CO-PROX reaction

Oscar H. Laguna, W.Y. Hernández, M. Isabel Domínguez Leal, Francisca Romero-Sarria, Svetlana Ivanova, Miguel Angel Centeno Gallego, Jose Antonio Odriozola Gordón
Comunicación oral

Methanol Reforming on structured catalysts and microchannel reactors
M.Montes, F.J. Echave, O.Sanz, B. Arhoun, Miguel Angel Centeno Gallego, José Antonio Odriozola Gordón, G. Arzamendi, L. Gandía
Comunicación oral

Effects of the characteristic dimension of catalytic wall microchannels and micromonoliths on the performances of microreactor coupling the methane steam reforming and combustion reactions: a CFD simulation study
G. Arzamendi, I. Uriz, P.M. Diéguez, M.Montes, Miguel Angel Centeno Gallego, José Antonio Odriozola Gordón, L. Gandía
Poster

XLIII Polish Annual Conference on Catalysis

16 – 18 marzo [Krakóv, Polonia]

Effect of redox calcination treatments of Pt/TiO_2 and Pd/TiO_2 systems on the photocatalytic reforming of biomass waste for biohydrogen production
J.C.Colmenares, A. Magdziarz, M.A.Aramendia, A.Marinas, J.M.Marinas, F.J.Urbano, José Antonio Navío Santos
Poster

SMALLWAT11 (3rd International Congress on Wastewater in Small Communities)

25 – 28 abril [Sevilla, España]

Rhodamine B degradation over Bi_2WO_6 coupled photocatalysts under sunlike irradiation
José Antonio Navio Santos, Sebastián Murcia López, M. Carmen Hidalgo López, Gerardo Colón Ibáñez
Poster

Phenol photodegradation over Au/TiO2 photocatalysts
José Antonio Navío Santos, Julie J. Murcia Mesa, M. Carmen Hidalgo López, Gerardo Colón Ibáñez
Poster

International Conference “Nanostructured catalysts and catalytic processes for the innovative energetics and sustainable development”, devoted to the year of Spain in Russia and of Russia in Spain

5 – 8 junio [Novosibirsk, Federación Rusa]

Hydrogen production in microchannel reactors
José Antonio Odriozola Gordón, Oscar H. Laguna, O. Sanz, Miguel Angel Centeno Gallego, G. Arzamendi, L.M. Gandía, F.J. Echave, M.Montes
Poster

XIX EUCOMC, 19th EUCHEMMS International Conference on Organometallic Chemistry

3 – 7 julio [Toulouse, Francia]

Olefin epoxidation in supported ionic-liquid-phase media catalyzed by oxoperoxo-molydenum complexes
F. Montilla, C.J. Carrasco, A. Galindo, Luis F. Bobadilla, José Antonio Odriozola Gordón
Poster

5th International FEZA Conference

3 – 7 julio [Valencia, España]

Influence of the silica source to the ionic liquid templated zeolite synthesis
Svetlana Ivanova, José María Martínez Blanes, Francisca Romero-Sarria, Miguel Angel Centeno, José Antonio Odriozola Gordón
Poster

Gold(III) stabilized over ionic liquid grafted in MCM-41 for highly efficient three-component coupling reactions
Luis F. Bobadilla, José Antonio Odriozola Gordón, T. Blasco
Poster

Photocatalytic and Advanced Oxidation Technologies for Treatment of Water, Air, Solids and Surfaces

4 – 8 julio [Gdansk, Polonia]

Oxydative dehyrogenation of ethanol over Au/TiO_2 photocatalysts
D.Sannino, V.Vaiano, P.Ciambelli, Mª.C. Hidalgo, J.J. Murcia Mesa, J.A.Navio
Oral

10º Congreso Europeo de Catálisis (EUROPACAT-X)

28 agosto – 2 septiembre [Glasgow, Reino Unido]

Study of supported vanadium oxide catalysts in the partial oxidation of H_2S by XAS and Raman in operando conditions
M.D. Soriano, Juan Pedro Holgado, J. Jiménez-Jiménez, P. Concepción, A. Jiménez-López, Alfonso Caballero Martínez, E. Rodríguez Castellón, J.M. López Nieto
Comunicación oral

Microchannel reactor for Steam Reforming of methanol
F.J. Echave, O. Sanz, I. Velasco, Miguel Angel Centeno, José Antonio Odriozola, G. Arzamendi, L.M. Gandía, M. Montes
Comunicación oral

"Operando" XAS and APPES experiments over $LaNi_{1-x}Co_xO_3$ (x=0, 0.5 y 1) perovskites as precursor for CH_4 reforming reactions
Rosa María Pereñíguez-Rodríguez, Victor Manuel Gonzalez-De La Cruz, Fátima Ternero-Fernández, Alfonso Caballero Martínez, Juan Pedro Holgado Vázquez
Poster

In situ XAS study of synergic effects on Ni-Co/ZrO_2 methane reforming catalysts
Víctor Manuel González-De La Cruz, Rosa María Pereñíguez-Rodríguez, Fátima Ternero-Fernández, Juan Pedro Holgado Vázquez, Alfonso Caballero Martínez
Poster

Low Cost Gold-Bimetallic Catalysts. Synergetic effect of the base metal
Fátima Ternero-Fernández, Víctor Manuel González-De La Cruz, Alfonso Caballero Martínez, Juan Pedro Holgado Vázquez
Poster

Improving the catalytic performance of Au-TiO_2 for low temperature CO Oxidation by control of the photodeposition parameters
Alfonso Caballero Martínez, Víctor Manuel González De la Cruz, Sergio Obregón, Fátima Ternero Fernández, Gerardo Colón Ibáñez
Poster

One template-three zeolites
Svetlana Ivanova, José María Martínez Blanes, Anna Penkova, Francisca Romero-Sarria, Miguel Angel Centeno Gallego, José Antonio Odriozola Gordón
Poster

Effect of the Co_3O_4 spinel morphology in the total CO oxidation
Andrea Álvarez Moreno, Svetlana Ivanova, Miguel Angel Centeno Gallego, José Antonio Odriozola Gordón
Poster

Surface acid-base properties of nickel tin catalysts for reforming of glyverol: in situ IR adsorption study
Anna Penkova, Luis F. Bobadilla, Francisca Romero-Sarria, Miguel Angel Centeno Gallego, José Antonio Odriozola Gordón
Poster

Gold supported on transition metal-doped ceria-alumina catalysts for total CO oxidation
Tomás R. Reina, Svetlana Ivanova, V. Idakiev, T. Tabakova, Miguel Angel Centeno Gallego, José Antonio Odriozola Gordón
Poster

Methanol steam reforming for hydrogen production over Ni and NiSn nanoparticles
Sandra Palma, Luis F. Bobadilla, Francisca Romero-Sarria, Miguel Angel Centeno Gallego, José Antonio Odriozola Gordón
Poster

Influence of H_2O and CO_2 during the preferential oxidation of CO (PROX) over a CuO_x/CeO_2-coated microchannel reactor
Oscar H. Laguna, S. Oraá, F.J. Echave, G. Arzamendi, L.M. Gandía, Miguel Angel Centeno Gallego, M. Montes, José Antonio Odriozola Gordón
Poster

International Conference on Materials and Technologies for Green Chemistry

5 – 9 septiembre [Tallinn, Estonia]

Ethanol partial photoxidation on Pt/TiO_2 catalysts as green route for acetaldehyde synthesis
Julie J. Murcia, D. Sannino, V. Vaiano, P. Ciambelli, M. Carmen Hidalgo López, José Antonio Navío Santos
Poster

European Symposium on Photocatalysis (JEP-2011)

29 – 30 septiembre [Bordeaux, Francia]

Synthesis, characterization and photocatalytic evaluation of Au-Bi_2WO_6
Sebastián Murcia López, José Antonio Navío Santos, M. Carmen Hidalgo López
Poster

Cyclohexane oxidation on Pt/TiO2 photocatalysts
Julie J. Murcia Mesa, M. Carmen Hidalgo, Sebastián Murcia López, José Antonio Navio Santos, D.Sannino, V.Vaiano, P. Ciambelli
Poster

Degradation of dimethyl phthalate using bare and Pt-doped photocatalysts
E. Pulido, O.González-Diaz, J.M.Doña, J. Pérez-Peña, José Antonio Navío Santos, Manuel Macias Azaña
Poster

1st International Congress on Catalysis for Biorefineries CatBior2011

2 – 5 octubre [Torremolinos, Málaga, España]

Preparation of Ru/GTDC for internal steam reforming anodes in solid oxide fuel cell
R.I. Vieira da Silva, Andrea Álvarez Moreno, Luis F. Bobadilla, W.Y. Hernández, Miguel Angenl Centeno Gallego, José Antonio Odriozola Gordón, M. Yuri Saeki
Poster

Comparison between conventional and structured catalyst in the steam reforming of glycerol
Luis F. Bobadilla, Andrea Álvarez Moreno, M. Isabel Domínguez Leal, Francisca Romero-Sarria, M. Montes, Miguel Angel Centeno Gallego, José Antonio Odriozola Gordón
Poster

CONGRESOS Y REUNIONES NACIONALES / NATIONAL CONGRESSES AND MEETINGS

COMUNICACIONES EN CONGRESOS Y REUNIONES / COMMUNICATIONS IN CONGRESS AND MEETINGS

NANOUCO III (Encuentro sobre Nanociencia y Nanotecnología de Investigadores y Tecnólogos Andaluces)

10 – 11 Febrero [Córdoba, España]

Fotooxidación selectiva de alcohol crotílico a crotonaldehido
F.J. López, M.Maicu, M.A. Aramendia, M. Carmen Hidalgo López, A.Marinas, José Antonio Navío Santos, F.J.Urbano
Poster

SECAT 2011 La Catálisis ante las crisis energética y medioambiental

29 junio – 1 julio [Zaragoza, España]

Fotooxidación selectiva de alcohol crotílico a crotonaldehido sobre sistemas basados en TiO_2
F.J.López-Tenllado, Mª.A. Aramendia, Julie J. Murcia Mesa, A. Marinas, J.M.Marinas, José Antonio Navío Santos, F.J.Urbano
Comunicación oral

Reactor de microcanales para la reacción de oxidación preferencial de CO en presencia de H_2 (PROX)
Oscar H. Laguna, S. Oraá, F.J. Echave, G. Arzamendi, Miguel Angel Centeno Gallego, L.M. Gandía, M. Montes y José Antonio Odriozola Gordón
Comunicación oral

Catalizadores de Au soportado en CeO_2-Al_2O_3 dopado con ZnO para la oxdación total y preferencial de CO
Tomás R. Reina, Svetlana Ivanova, Alicia Corrales Miralles, Miguel Angel Centeno Gallego y José Antonio Odriozola Gordón
Comunicación oral

Producción de hidrógeno a partir de reformado con vapor de metanol mediante catalizadores basados en nanopartículas de Ni y NiSn soportadas

Sandra Palma. Luis F. Bobadilla, Francisca Romero-Sarria, Miguel Angel Centeno Gallego y José Antonio Odriozola Gordón
Comunicación oral

Estabilidad de catalizadores de Pt y Ni en el reformado con vapor de etanol
R. Olivera, Luis F. Bobadilla, V. Cortés Corberán
Comunicación oral

Efecto térmico y catalítico en el reformado con vapor de glicerol. Influencia del metal y del carburo de silicio
L. Marcela Martínez Tejada, M. Araque, Miguel Angel Centeno Gallego, A.C. Roger
Poster

Efecto de la morfología de Co3O4 en la reacción de oxidación total de CO
Andrea Álvarez Moreno, Svetlana Ivanova, A. García-Sanchez, Miguel Angel Centeno Gallego, José Antonio Odriozola Gordón
Poster

Fotoactividad de catalizadores Pt/TiO_2 sintetizados por fotodeposición. Efecto de los parámetros de síntesis
Julie J. Murcia Mesa, José Antonio Navío Santos, M. Carmen Hidalgo López
Poster

Soportes catalíticos estructurados a partir de residuos industriales
S. Romero, M. Isabel Domínguez Leal, Ara Muñoz-Murillo, Miguel Angel Centeno Gallego y José Antonio Odriozola Gordón
Poster

Deposición de un catalizador Au/TiO_2 sobre acero inoxidable
M. Isabel Domínguez Leal, Alicia Corrales Miralles, Svetlana Ivanova, L.Marcela Martínez Tejada, Miguel Angel Centeno Gallego y José Antonio Odriozola Gordón
Poster

Producción de hidrógeno a partir de reformado con vapor de glicerol sobre catalizadores NiSn/MgO-Al_2O_3: efecto de la adición de MgO
Luis F. Bodadilla, Anna Penkova, Francisca Romero-Sarria, Miguel Angel Centeno Gallego y José Antonio Odriozola Gordón
Poster

Oro soportado en arcillas pilarizadas para la reacción de oxidación de CO: efecto del tamaño de agregado
Andrea Álvarez Moreno, R. Molina, Miguel Angel Centeno Gallego y José Antonio Odriozola Gordón
Poster

Monolitos metálicos para la combustión de CO: influencia del substrato
L. Marcela Martínez Tejada, Oihane Sanz, Miguel Angel Centeno Gallego y José Antonio Odriozola Gordón
Poster

Oxidación preferencial de CO en presencia de H2 (PROX) sobre catalizadores tipo Au/Ce1-x EuxO2-x/2
W.Y. Hernández, Francisca Romero-Sarria, Miguel Angel Centeno Gallego y José Antonio Odriozola Gordón
Poster

VI Reunión de Innovación Docente en Química, INDOQUIM 2011

19 – 22 julio [Alicante, España]

Aplicación de matrices de valoración (rúbricas) para la evaluación de competencias en la asignatura Operaciones Básicas de Laboratorio
M. Isabel Domínguez Leal, A. Palacios, Svetalana Ivanova, J. López, J.M. Jurado, F. Ortega, E. Díez, G. López, J. Hidalgo, E. Andreu
Poster

FORMACION / TRAINING

TESIS DOCTORALES/ DOCTOR DEGREE THESIS

Título:	**Diseño de nuevas aleaciones inoxidables superdúplex para aplicaciones avanzadas**
Autor:	Carlos Muñoz Luque
Directores:	José Antonio Odriozola, Miguel Angel Centeno, Francisco Javier García López
Calificación:	Sobresaliente “Cum Laude”
Centro:	Universidad de Sevilla

Título:	**Obtención de hidrógeno a partir de la biomasa. Reformado catalítico de glicerina**
Autor:	Luis Francisco Bobadilla Baladrón
Directores:	José Antonio Odriozola, Francisca Romero Sarria
Calificación:	Sobresaliente “Cum Laude”
Centro:	Universidad de Sevilla

Título: **Oxidación preferencial de CO en presencia de H_2: diseño de catalizadores basados en CeO_2 y aplicación a microrreactores**
Autor: Oscar Hernando Laguna Espitia
Directores: José Antonio Odriozola, Miguel Angel Centeno
Calificación: Sobresaliente “Cum Laude”
Centro: Universidad de Sevilla

FORMACIÓN DE GRADUADOS / MASTER DEGREE THESIS

Título: **Catalizadores de oro soportado para la reacción de oxidación CO**
Autor: Tomás Ramirez Reina
Directores: Svetlana Ivanova, José Antonio Odriozola
Grado: Trabajo Fin de Master
Centro: Universidad de Sevilla
Año Académico: 2010-2011

Título: **Limpieza de corrientes de hidrógeno mediante metanación selectiva de CO con catalizadores Ru/TiO_2**
Autor: Ara Muñoz Murillo
Directores: Miguel Angel Centeno, Oscar Hernando Laguna, José Antonio Odriozola
Grado: Trabajo Fin de Master
Centro: Universidad de Sevilla
Año Académico: 2010-2011

Título: **Catalizadores basados en la perovskita $NiLaO_3$ para el reformado de metano con vapor de agua**
Autor: Sandra Palma del Valle
Directores: Francisca Romero Sarria, José Antonio Odriozola
Grado: Trabajo Fin de Master
Centro: Universidad de Sevilla
Año Académico: 2010-2011

Título: **Microchannel reactors for CO preferential oxidation in presence of H_2: Effect of the catalytic layer thickness**
Autor: Badroudin Marecar
Directores: José Antonio Odriozola Gordón, Francisca Romero Sarriá
Grado: Trabajo de Investigación, Programa Erasmus, Escuela de Ingenieros
Centro: ENSICAEN, L'Ecole Nationale Supérieure d'Ingénieurs de Caen et Centre de Recherche, Caen (Francia)
Año Académico: 2010-2011

Título: **Effect of gold over $NiLaO_3$ perovskite catalysts for methane steam reforming**
Autor: Bastien Lorenzatti
Directores: José Antonio Odriozola Gordón, Francisca Romero Sarriá, Sandra Palma
Grado: Trabajo de Investigación, Programa Erasmus, Escuela de Ingenieros
Centro: ENSICAEN, L'Ecole Nationale Supérieure d'Ingénieurs de Caen et Centre de Recherche, Caen (Francia)
Año Académico: 2010-2011

EQUIPAMIENTO CIENTÍFICO AVAILABLE EQUIPMENT

- Molino de bolas de movimiento planetario PM100 de RETSCH
- Espectrofotómetro Infrarrojos: Thermo-Nicolet Nexus FT-IR; Thermo-Nicolet 380 FT-IR
- Accesorio DRIFTS, celdas de alta y baja temperatura
- Sistema de vacío cuarzo/vidrio para adsorción de moléculas sonda seguido por FT-IR
- Espectrómetro de masas: Balzers Thermostar
- Sistema TPR-TPO (con posibilidad de realizar pulsos) seguido de espectrómetro de masas (Balzers) y detector de conductividad térmica. PID Eng&Tech.
- Equipos comerciales de actividad catalítica Microactivity Reference PID Eng&Tech (4)
- Microscopio metalográfico: Leica DMIRM
- Rotavapor: Heidolph Hei-VAP Value
- Equipo de ultra-alto vacío para espectroscopía XPS y Auger equipado con cañón de argón para realizar devastado iónico.
- Estufas: P-Selecta; P-Selecta digiheat
- Ph-metros: Crison pH burette 24; Crison phMeter Basic 20; Crison micropH2000.
- Cromatógrafos (2): Agilent Technologies 7890 A GC System; Agilent Technologies 6890 N Network GC System.
- Micro-cromatógragos, microGC (2): Micro Gas Cromatograph CP-4900 Varian (2)
- HPLC: Varian 356-LC, Solvent Delivery Module Varian ProStar.
- Horno de soldadura: Microtest Máquina de ensayos EM2/200/FR
- Baño de ultrasonidos: P-Selecta Ultrasons Medi-II
- Horno Energon
- Horno para tratamiento de aceros a alta temperatura equipado con medidores de flujo e inyector de agua.
- Planta Piloto de Integración de reacciones catalíticas Reference PID Eng&Tech
- Espectrómetro Uv-Vis (Varian Cary 100, con esfera integradora para
- muestras sólidas)
- Analizador de Carbón Orgánico (TOC-V CHP Shimadzu 5000A)
- Cromatógrafo (HPLC Agilent Technologies 1200)
- Espectrómetro IR (Varian 660-IR FTIR Spectrometer)

- Dip-Coater con cámara de temperatura (SS-00 AB Table Dry Oven MTI
- Corporation)
- Espectrofotómetro FTIR con celdas DRIFTS y ATR.
- Sistema de análisis TPR/TPO con detector TCD y espectrómetro de masas.
- 6 reactores catalíticos de gases con detección por cromatografía de gases y espectrometría de masas.
- 2 reactores catalíticos de líquidos que permiten el seguimiento de hasta 8 reacciones de forma simultánea con control de temperatura y flujo de gases.
- 4 reactores catalíticos de líquidos de alta presión y temperatura con agitación interna y control de flujo de gases.
- Reactores fotocatalíticos con lámparas de Xe y Hg.
- Espectrofotómetros FTIR con accesorios DRIFTS, ATR y sistema de vacío en cuarzo/vidrio para adsorción de moléculas sonda
- Espectrómetros de masas
- Sistemas TPR-TPO (con posibilidad de realizar pulsos) seguido de espectrómetro de masas y detector de conductividad térmica.
- Microscopio metalográfico
- Rotavapor
- Estufas
- Ph-metros
- Cromatógrafos de Gases
- Micro-cromatógragos, microGC
- Cromatografos HPLC
- Horno de soldadura: Microtest Máquina de ensayos EM2/200/FR
- Baño de ultrasonidos
- Hornos
- Horno para tratamiento de aceros a alta temperatura equipado con medidores de flujo e inyector de agua.
- Planta Piloto de Integración de reacciones catalíticas Reference PID Eng&Tech
- Espectrómetro Uv-Vis, con esfera integradora para muestras sólidas)
- Analizador de Carbón Orgánico
- Dip-Coater con cámara de temperatura
- Reactores catalíticos de gases con detección por cromatografía de gases y espectrometría de masas.
- Reactores catalíticos de líquidos que permiten el seguimiento de hasta 8 reacciones de forma simultánea con control de temperatura y flujo de gases.
- Reactores catalíticos de líquidos de alta presión y temperatura con agitación interna y control de flujo de gases.
- Reactores fotocatalíticos con lámparas de Xe y Hg.

INGENIERÍA DE CERÁMICOS PARA AMBIENTES EXTREMOS

ENGINEERED CERAMICS FOR EXTREME ENVIRONMENTS

PROYECTOS DE INVESTIGACIÓN / RESEARCH PROJECTS

Unión Europea
Fondo Europeo de Desarrollo Regional
"Una manera de hacer Europa"
MINISTERIO DE CIENCIA E INNOVACIÓN

Microestructura y deformación plástica a alta temperatura de óxidos eutécticos basados en Al_2O_3

Código/Code:	MAT2009-13979-C03-01
Periodo/Period:	01-01-2010 / 31-12-2012
Organismo Financiador/Financial source:	Ministerio de Educación y Ciencia
Importe total/Total amount:	145.200 €
Investigador responsable/Research head:	Jiménez Melendo, M.
Componentes/Research group:	Martínez Fernández, J., De Arellano-López, A. R., Bravo León, A., Clauss Klamp, C., Varela Feria, F. M., Vaquero Aguilar, C.

RESUMEN / ABSTRACT

Se pretende desarrollar óxidos eutécticos binarios y ternarios basados en la alúmina – en concreto, Al_2O_3/ZrO_2, $Al_2O_3/Y_3Al_5O_{12}$(YAG), Al_2O_3/ZrO_2/YAG y $Al_2O_3/SiO_2/ZrO_2$, con la circona estabilizada con diferentes contenidos de Y_2O_3– con microestructuras controladas en el intervalo micro- a nanométrico, para su empleo en aplicaciones estructurales y térmicas de sistemas de generación y conversión más eficientes de la energía: soportes para pilas de combustible, reactores químicos, reactores enfriados por gas de alta temperatura, barreras térmicas sobre superaleaciones metálicas en turbinas y motores, etc.

Entre las altas prestaciones de estos materiales caben destacar: elevado punto de fusión, baja densidad, conductividad térmica, escasa reactividad química incluso a alta temperatura, y excelentes propiedades mecánicas tanto a bajas como a elevadas temperaturas: resistencia mecánica cercana a 5 GPa a temperatura ambiente, resistencia a la fluencia, al desgaste y a la erosión. Pero lo más novedoso y potencialmente interesante de estos materiales es su comportamiento superplástico, en microestructuras nanométricas, recientemente descubierto por el equipo investigador solicitante.Estos materiales se producirán por técnicas de procesamiento asistido por láser en tres configuraciones distintas: masivos, recubrimientos planos (capas individuales sobre soportes cerámicos y metálicos) y multicapas. En particular, para esta última configuración se diseñarán estructuras con campos de tensiones residuales favorables para unas prestaciones mecánicas y térmicas óptimas en función de las diferentes aplicaciones requeridas. Estas tensiones residuales se investigarán mediante técnicas de espectroscopía Raman y piezoespectroscopía, y se compararán con los resultados de simulaciones numéricas. Por otra parte, las técnicas de tratamiento por láser se emplearán también para alterar la microestructura de los recubrimientos cerámicos convencionales depositados por proyección térmica sobre las superaleaciones metálicas en componentes de motores así como para mecanizar los materiales producidos con objeto de conferirles una determinada geometría funcional, o con el fin de modificar su superficie de forma que mejore el comportamiento frente al desgaste.

Uno de los objetivos fundamentales de este proyecto será estudiar materiales con fases nanométricas que posibiliten un comportamiento superplástico a altas temperaturas (que

contrasta con la extraordinaria resistencia a la deformación de los materiales con fases micrométricas), de forma que abra la posibilidad de la unión y el conformado fácil con forma casi final de piezas complejas, recuperando su resistencia característica tras tratamientos térmicos.

Las propiedades mecánicas (resistencia a compresión y a flexión, módulo de elasticidad, dureza, tenacidad a fractura y desgaste) de los materiales se evaluarán desde temperatura ambiente hasta 1950 K mediante diferentes técnicas en aire, así como en otras atmósferas para determinar su influencia en el comportamiento mecánico o la degradación del material.

Una parte complementaria, pero fundamental, del proyecto es la caracterización estructural y microestructural de los materiales fabricados, así como su evolución con los ensayos mecánicos. De esta forma se podrán establecer las relaciones entre el comportamiento mecánico observado (propiedades necesarias para el diseño ingenieril) y sus parámetros microestructurales característicos. Con esta finalidad, se utilizarán técnicas de microscopía óptica convencional y confocal, electrónica con microanálisis y difracción, de fuerzas atómicas, así como difracción con textura por rayos X.

Del análisis de los resultados de los ensayos termo-mecánicos y de la caracterización microestructural se pretende llegar al entendimiento básico de la relación entre microestructura y propiedades. Esto permitirá retroalimentar el proceso de producción de los materiales eutécticos, para lograr microestructuras específicas para las diferentes aplicaciones con propiedades macroscópicas optimizadas.

This research addresses to produce binary and ternary oxide eutectics –specifically, Al_2O_3/ZrO_2, $Al_2O_3/Y_3Al_5O_{12}$(YAG), Al_2O_3/ZrO_2/YAG and $Al_2O_3/SiO_2/ZrO_2$, zirconia being stabilized with different amounts of Y_2O_3– with well-controlled microstructures in the micro- to nanometric range for structural and thermal applications in efficient-enhanced power generation and conversion systems: fuel cells, chemical and high-temperature gas cooled reactors, thermal barriers of steels and super alloys in gas turbines and diesel engine components, etc.

These materials are very attractive because of their excellent properties: high melting point, low density, thermal conductivity and chemical reactivity, and superior mechanical performance at both low and high temperature: mechanical strength close to 5 GPa at room temperature, and high creep, wear and erosion resistance. Very recently, superplasticity has been discovered in nanosized materials by the applicant team.

Oxide eutectics will be produced by laser-assisted processing techniques in three configurations: bulk, plates (on ceramic and metallic substrates) and multilaminates. For the later configuration, microarquitectures with optimized residual stresses will be designed for enhanced mechanical and thermal performance. The residual stresses will be investigated by using piezo- and Raman spectroscopy, and the data compared to numerical predictions. Laser techniques will be also used to modify the microstructure of conventional ceramic coatings deposited on metallic engine components by Air Plasma Spray, and for machining of ceramic components to obtain a given functional geometry or to modify the external surfaces for improved wear behavior.

One of the main goals of this Project is to produce materials with nanosized phases in order to achieve superplasticity (which contrasts with the superior creep resistance of microsized materials). This capability opens the possibility of using superplastic joining and forming as processing methods for complex pieces with near net shape, recovering back its characteristic resistance after thermal treatments.

The mechanical properties (flexural and compression resistance, elastic modulus, hardness, toughness and wear) will be evaluated from room temperature up to 1950 K in air as well as under other different environmental atmospheres in order to investigate their effect in the mechanical behavior or material degradation.

A significant part of the Project is the structural and microstructural characterization of the as-received materials, and their evolution during mechanical tests. Such an investigation is critical to establish relationships between the experimental mechanical behavior (necessary for engineering designs) and the microstructural and processing parameters. To this end, techniques of optical (particularly confocal), electron (image, microanalysis and diffraction) and atomic force microscopy, and X-ray diffraction with texture facilities will be used.

Mechanical and microstructural data will feedback the fabrication process in order to obtain materials with tailored properties for specific applications.

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MINISTERIO DE CIENCIA E INNOVACIÓN

Inmovilización de cationes en un espacio confinado de alta densidad de carga: gestión de residuos peligrosos

Immobilization of cations in high-density charge confined spaces: management of harmful cations wastes

Código/Code:	CTQ2010-14874/BQU (Plan Nacional)
Periodo/Period:	01-01-2011 / 31-12-2013
Organismo Financiador/Financial source:	MICINN
Importe total/Total amount:	82.280,00 €
Investigador responsable/Research head:	María Dolores Alba Carranza
Componentes/Research group:	Miguel Angel Castro Arroyo, Maria del Mar Orta Cuevas, Mery Carolina Pazos Zarama, Said ElMrabet, Esperanza Pavón González, Maria Villa Alfageme, Santiago Medina Carrasco, Ana Isabel Becerro Nieto, Alberto José Fernández Carrión

RESUMEN / ABSTRACT

El tema central del Proyecto aborda la exigencia tecnológica medioambiental de desarrollar metodologías avanzadas para la eliminación de agentes contaminantes. El interés y los esfuerzos encaminados al desarrollo de nuevas tecnologías orientadas a tratamientos más eficientes en la inmovilización y revalorización de los residuos peligrosos es crecientes en los planes de I + D + i de los últimos años. Es en este escenario donde debe encuadrarse la presente propuesta, circunscrita en dos hallazgos básicos experimentales: el diseño de silicatos laminares expansibles de alta carga con una distribución controlada de sus centros activos que le confieren especiales propiedades como precursores para el diseño de materiales eficaces en cuanto a la retención de residuos nocivos y radiactivos, y la obtención de fases disilicatos insolubles en condiciones suaves, apropiadas para la inmovilización de dichas especies. Dicho objetivo representa un cambio cualitativo en el trabajo que se viene desarrollando en cuanto a su aplicación a residuos radioactivos y tóxicos reales, de una parte, y en cuanto a la aplicación de la metodología desarrollada en sistemas modelos a silicatos de utilidad, de otra. Los objetivos se adecuan, en general, a las líneas prioritarias de Investigación básica de Química, en concre-

to en el área de Química Inorgánica (Química del Estado Sólido) y Química Medioambiental, pero a pesar de su carácter básico posee un carácter aplicado que se adecua a diversas líneas de investigación de Química Orientada y ha despertado el interés de diversas empresas observadoras (ENRESA, BEFESA y ALQUIMIA). Estos objetivos requieren el desarrollo de técnicas de análisis sofisticado como la Resonancia magnética Nuclear de Sólido, la Difracción de Rayos-X bajo atmósfera controlada o espectroscopia gamma de bajo recuento, teniendo en cuenta el objetivo particular de dicha área de usar la tecnología instrumental y experimental para el estudio de materiales, satisfaciendo además el objetivo O2.5 (Potenciar la disponibilidad de infraestructuras de uso interdisciplinar y de uso compartido por los distintos agentes del sistema) del plan nacional de I+D+i 2008-2011. La viabilidad de la propuesta se garantiza, en primer lugar, porque el EI ha publicado recientemente la síntesis de silicatos laminares hidratables de alta carga, donde describe un método a partir del cual se puede ajustar la carga deseada para el material; en segundo lugar, el EI posee una dilatada experiencia en el diseño de mecanismos de síntesis de silicatos, como se demuestra por los numerosos artículos publicados en esta área durante la última década y finalmente, el EI ha desarrollado metodología necesaria para el desarrollo de este experimento en colaboración con otros Grupos con los que mantiene una estrecha colaboración científica.

The central subject of this Project deals with the environmental technological exigency for development of advanced technologies for the elimination of polluting agents. The interest and the effort dedicated to the development of new technologies that allow more effective treatments of retention and new procedures of valorisation is increasing in numerous R&D plans in the last years. It is in this scene where the present proposal must be fitted and circumscribed into two experimental basic findings: designing expansible high layer charge silicates with a controlled distribution of active centres, which can be effective materials for the retention of hazardous and radioactive wastes, and obtaining insoluble disilicate phases in smooth conditions, appropriate for the immobilization of such species. This objective represents a qualitative change in the work that has been developed up to now in relation to the elimination of radioactive and toxic wastes as well as in the application of the methodology to silicate systems. The objectives are adapted, in general, to the high-priority lines of Basic Investigation of Chemistry, in the area of Inorganic Chemistry (Solid State Chemistry) and Environmental Chemistry in particular but, in spite of its basic character, the Project is adapted to diverse lines of investigation of Oriented Chemistry and it is supported by different EPOs (ENRESA, BEFESA and ALQUIMIA). These objectives, of eminent basic character, require the development of techniques of sophisticated analysis like advanced Solid State NMR, X-ray diffraction, under conditions of controlled pressure and temperature or gamma spectroscopy of low counts. This fact fits to the particular objective of the Chemistry Area of “using the instrumental and experimental technology for the study of materials” and with objective O2.5 (Enhance the availability of interdisciplinary infrastructures and sharing use of them) of the R+D+I National Plan 2008-2011. A guarantee of this proposal is that, in a first place, the Research Group (RG) has recently published the synthesis of expansible mica using a method that allows obtaining the desired layer charge in the material; secondly, the RG has a wide experience in the design of synthesis mechanisms of silicates as demonstrated by the number of papers published on this area during the last decade, and, finally, the RG has developed useful methodologies for the present Project in collaboration with other Groups with which it maintains a narrow scientific relationship.

Bioener: Aplicación de tecnologías biomiméticas a sistemas energéticos

Código/Code:	P09-TEP-5152 (Proyecto de Excelencia)
Periodo/Period:	02-02-2009 / 03-02-2014
Organismo Financiador/Financial source:	Junta de Andalucía
Importe total/Total amount:	311.167,68 €
Investigador responsable/Research head:	Julián Martínez Fernández
Componentes/Research group:	Antonio R. De Arellano-López, Alfonso Bravo León, Manuel Jiménez Melendo, F.M. Varela Feria, Joaquín Ramírez Rico, Antonio Gutiérrez Pardo

RESUMEN / ABSTRACT

Los avances tecnológicos han permitido diversificar y optimizar la producción de energía, lo que ha conducido al mismo tiempo, a desarrollar nuevas vías de almacenamiento de la misma. En particular, a medida que se diversifican los métodos de producción energética, es necesario desarrollar nuevos materiales para almacenamiento de energía, para su uso en dispositivos de consumo y transporte. Esto es especialmente importante para países que, como España, llevan años aumentando la presencia de las renovables en su carta de tecnologías de producción eléctrica y son actualmente líderes mundiales del sector. El Plan de Fomento de las Energías Renovables 2000-2010 tiene como objetivo para este año generar hasta el 30% de las necesidades de consumo energético nacionales a partir de energías renovables, mientras que en algunas comunidades autónomas la cuota de renovables supone ya más del 75% del consumo anual. La progresiva penetración de las renovables debe ir necesariamente acompañada del desarrollo de nuevas tecnologías de distribución y almacenamiento energético, teniendo en cuenta que la potencia suministrada por las renovables es intermitente y variable, al depender las condiciones meteorológicas.

Otra estrategia a corto plazo para reducir la dependencia de los combustibles fósiles es la mejora de la eficiencia los sistemas de generación de energía convencionales mediante el aumento de las temperaturas de operación, por ejemplo en turbinas de combustión de gas. El desarrollo de nuevos materiales para aplicaciones de alta temperatura ha ido tradicionalmente ligado a la demanda de mayores eficiencias. De entre ellos, los materiales cerámicos se postulan como candidatos para aplicaciones en entornos químicamente agresivos a temperaturas superiores a los 1000ºC. Carburos y nitruros en particular, con su elevado punto de fusión y excelentes propiedades termomecánicas, están siendo extensamente estudiados en la actualidad para este tipo de aplicaciones. Los cerámicos porosos también son de gran interés en aplicaciones energéticas, como intercambiadores de calor o sistemas de filtrado de gas de síntesis, entre otros.

De las líneas de investigación en nuevos materiales para almacenamiento energético, el desarrollo de nuevos sistemas de almacenamiento electroquímico tendrá un gran impacto a corto plazo, especialmente en el consumidor final: el desarrollo de baterías y condensadores electroquímicos de alta capacidad es clave para la viabilidad de tecnologías que, como los vehículos eléctricos, deberán implantarse en un corto plazo para reducir nuestra dependencia de los combustibles fósiles. Es por esta razón que los materiales para almacenamiento electro-

químico han recibido gran atención de la comunidad científica y constituyen uno de los grandes retos tecnológicos actuales.

El carburo de silicio biomórfico (bioSiC) es un material cerámico obtenido por infiltración reactiva de preformas de carbono obtenidas mediante pirólisis de precursores vegetales. El precursor, generalmente madera, se mecaniza en bruto y se carboniza mediante un proceso de pirólisis en atmósfera controlada a alta temperatura, obteniéndose un material de carbono macroporoso (bioC) cuya microestructura es similar a la del precursor vegetal. Este precursor se mecaniza hasta una forma cercana al producto final y se infiltra reactivamente con silicio líquido o gaseoso para obtener un material de SiC/Si que presenta unas excelentes propiedades termomecánicas, con una microestructura que mimetiza la microestructura de la madera original. Es posible seleccionar las propiedades del material resultante mediante la elección adecuada del precursor. El silicio residual puede eliminarse para obtener un material de SiC macroporoso. Es posible, por último, reinfiltrar el bioSiC poroso con otros materiales, por ejemplo metales para obtener cermets bioSiC/Al o bioSiC/Cu.

La posibilidad de producir materiales de carbono macroporosos con nanoporosidad controlada es interesante para su uso en aplicaciones electroquímicas, puesto que es posible infiltrar o recubrir los macroporos con una fase secundaria que proporcione funcionalidad adicional, por ejemplo en pilas de litio con arquitectura tridimensional o en supercondensadores oxido/carbono. En este sentido, el desarrollo de nuevos carbonos con porosidad y/o estructura controlada puede abrir una puerta hacia nuevas arquitecturas y diseños de dispositivo capaces de almacenar mayores densidades de energía.

La mayoría de materiales nanoporosos de carbono utilizados en la actualidad se obtienen mediante la activación de carbones obtenidos por pirólisis de precursores orgánicos sintéticos, aunque en los últimos años el carbono obtenido a partir de carburos ha sido objeto de gran interés. Es posible, mediante el tratamiento a alta temperatura de carburos metálicos en una atmósfera clorada, obtener carbonos nanoporosos de alta pureza que resultan idóneos para aplicaciones electroquímicas. En este sentido ya se ha demostrado la posibilidad de obtener carbono nanoporoso a partir de carburos obtenidos por infiltración reactiva de precursores vegetales.

El objetivo de este proyecto es doble: por un lado, se estudiará en detalle el procedimiento de obtención de materiales de carbono a partir de precursores vegetales, prestando atención a la posibilidad de introducir distintos gases (CO2, vapor de agua) durante el proceso de pirólisis para obtener carbones activos con nanoporosidad para su uso en sistemas de almacenamiento electroquímico. Se estudiará además el efecto de la temperatura de pirólisis en el grado de cristalinidad, nanoporosidad, tamaño de cristal y estructura del carbono resultante, y se explorará la posibilidad de promover la cristalización del carbono mediante el uso de distintos catalizadores. Se caracterizará la microestructura de los materiales resultantes, así como sus propiedades físicas y termo-mecánicas.

Technological advances have made possible to diversify and optimize energy production, which in turn has motivated the development of new ways to store energy. In particular, as production methods diversify, it is necessary to develop new materials for energy storage, both large scale and in consumer devices and transportation. This is especially important in the context of higher penetration of renewable energies, which often depend on climatological conditions and require ways to store excess energy at production peaks, so it can be used when production decreases.

In parallel to this strategy and to reduce the share of fossil fuels in the overall energy production, it is necessary to increase the efficiency of conventional power generation systems, for example by increasing material's life and operating temperatures, for example in gas turbine systems, among others. The development of materials for high temperature applications, especially ceramics, has been traditionally linked to the search for increased efficiency of power generation systems. Ceramic materials, due to their high melting point, good creep resistance and resistance to corrosion, are seen as candidates for application in chemically aggressive environments at temperatures over 1000 ºC. Carbides and nitrides in particular are being studied extensively for this kind of applications. Porous ceramics are also of great interest in energy applications, such as heat exchangers or syngas filtration systems, among others.

Among active research lines in the development of new materials for energy storage, electrochemical storage is expected to have the largest impact in the end consumer, as the design of high capacity batteries and electrochemical capacitors is key for the viability of technologies such as plug-in electric cars. For this reason, research into new materials for electrochemical storage has become a strong focal point among the scientific community and constitutes one to the great technological challenges of today.

Biomorphic silicon carbide (bioSiC) is a ceramic material obtained by reactive infiltration of carbon performs derived by pyrolysis of natural precursors. The precursor, usually wood, is rough-machined and then converted to carbon by pyrolysis in a controlled atmosphere at high temperatures. The result is a macroporous carbon material (bioC) with a microstructure that closely resembles that of the original precursor. This carbon template is then machined to near net shape and is melt reacted with silicon either in liquid or vapor phase to obtain a SiC composite with some residual Si that shows excellent thermomechanical properties and a microstructure that closely mimics that of the original wood precursor. Tailoring the material's properties is possible by adequate selection of the precursor, which determines the microstructure and thus the properties of the bioSiC. It is also possible to remove the remaining silicon through chemical etching to obtain a macroporous SiC material which can then be reinfiltrated to create novel composites and cermets, such as bioSiC/Al or bioSiC/Cu.

The prospect of producing macroporous carbon materials with controlled nanoporosity is interesting for electrochemical applications, as it would be possible to infiltrate or coat macropores with a second phase the provides additional function, for instance in three dimensional lithium batteries [3, 20] or carbon/oxide supercapacitors [4, 5]. In this way, the development of new carbon materials with controlled structure and porosity could open the door to novel architectures and designs for devices able to store larger amounts of energy.

Most nanoporous carbon materials used nowadays are obtained through activation of carbons made from pyrolysis of synthetic precursors [21], although in the last years carbide-derived carbons have been the subject of great interest [22, 23, 24]. It is possible to obtain high-purity nanoporous carbon through high temperature chlorination of metallic carbides, which rank among the best carbon materials for electrochemical applications. In this direction, is has already been shown that carbides obtained from natural precursors, such as bioSiC are viable precursors to carbide-derived carbons [25].

This proposal's aim is two-fold: on one side, the bioC processing will be studied in detail, paying special attention to precursor selection and to the possibility of introducing different atmospheres during the pyrolysis process, such as CO2 or water vapor, that promote nanoporosity in the material. The effect of processing parameter in the degree of crystallinity, nanoporosity, crystallite size and structure of the resulting carbon material will be assessed. The possibility of promoting carbon graphitization through the use of different catalysis in the pyrolysis process will be studied. The resulting carbon’s microstructure and physical properties will be studied and correlated to the processing parameters.

On the other side, the effect of the aforementioned treatments on the bioSiC material will be studied, and the possibility of obtaining novel cermets in-situ, such as bioSiC/Al, bioSiC/Ti, through melt infiltration, will be assessed. In a last step, the possibility of obtained carbon materials with enhanced structure from the ceramic carbides will be explored.

TRANSFERENCIA / TECHNOLOGICAL TRANSFER

CONVENIOS Y CONTRATOS / CONTRACTS AND AGREEMENTS

Valorización de materiales mediante oxidación catalítica

Periodo/Period:	01-01-2011 / 31-12-2011
Organismo Financiador/Financial source:	BEFESA
Importe total/Total amount:	20.279,01 €
Investigador responsable/Research head:	Miguel Angel Castro Arroyo
Componentes/Research group:	M. Dolores Alba Carranza, M. Mar Orta Cuevas, Santiago Medina, Esperanza Pavón

Caracterización de mecanismos de retención de actínidos en micas sintética: Aplicación de la retención de Cesio y Yodo

Periodo/Period:	01-10-2011 / 31-03-2013
Organismo Financiador/Financial source:	ENRESA
importe total/Total amount:	113.575,00 €
Investigador responsable/Research head:	Miguel Angel Castro Arroyo
Componentes/Research group:	M. Dolores Alba Carranza, M. Mar Orta Cuevas, Said ElMrabet, M. Carolina Pazos Zarama, Maria Villa Alfageme, Santiago Hurtado

PUBLICACIONES / PUBLICATIONS

ARTÍCULOS PUBLICADOS EN REVISTAS SCI / PAPERS IN SCI JOURNALS

Structure, Electrical Resistivity, and Thermal Conductivity of Beech Wood Biocarbon Produced at Carbonization Temperatures below 1000 degrees C
Parfen'eva, LS; Orlova, TS; Kartenko, NF; Smirnov, BI; Smirnov, IA; Misiorek, H; Jezowski, A; Muha, J; Vera, MC
Physics Of The Solid State, **53** (2011) 2398-2407
DOI: 10.1134/S1063783411110230

This paper reports on measurements of the thermal conductivity. and the electrical resistivity. in the temperature range 5-300 K, and, at 300 K, on X-ray diffraction studies of high-porosity (with a channel pore volume fraction of similar to 47 vol %) of the beech wood biocarbon prepared by pyrolysis (carbonization) of tree wood in an argon flow at the carbonization temperature T(carb) = 800 degrees C. It has been shown that the biocarbon template of the samples studied represents essentially a nanocomposite made up of amorphous carbon and nanocrystallites-"graphite fragments" and graphene layers. The sizes of the nanocrystallites forming these nanocomposites have been determined. The dependences rho(T) and kappa(T) have been measured for the samples cut along and perpendicular to the tree growth direction, thus permitting determination of the magnitude of the anisotropy of these parameters. The dependences rho(T) and kappa(T), which have been obtained for beech biocarbon samples prepared at T(carb) = 800 degrees C, are compared with the data amassed by us earlier for samples fabricated at T(carb) = 1000 and 2400 degrees C. The magnitude and temperature dependence of the phonon thermal conductivity of the nanocomposite making up the beech biocarbon template at T(carb) = 800 degrees C have been found.

Application of the solid state NMR to the study of the alcohol/alkane mixtures adsorption onto graphite
Alba, MD; Castro, MA; Clarke, SM; Medina, S; Messe, L; Millan, C
Solid State Nuclear Magnetic Resonance, **40** (2011) 138-143
DOI: 10.1016/j.ssnmr.2011.11.002

The mixing of molecules adsorbed from solution to different interfaces has both industrial and academic relevance and the mixing behaviour at the interface is a key to understanding for example, that the surface tension of a mixture of two surfactants is lower than either of the two pure materials and many other effects. In this paper, we report, for the first time, the application of Solid State NMR to the study of alkane/alcohol mixtures, in a range of relative size ratio between 0 and 0.35, adsorbed onto graphite at high, multilayer coverage. Moreover, this paper evaluated, for the first time, the utility of the combined used of H-1 and H-2 NMR for: (i) determining the surface composition and (ii) making a theoretical approach to the sorption isotherm. A variety of preferential adsorption behaviour is reported. Preferential adsorption of the longer molecule (decane vs. heptanol) from a mixture has been observed. However, if both components are of similar length, the alcohol is preferentially adsorbed (heptanol vs. octane and octanol vs. octane). Finally, a linear relation between the relative size ratio and the amount of alcohol at monolayer coverage is observed.

Monolayer structures of alkyl aldehydes: Odd-membered homologues
Phillips, TK; Clarke, SM; Bhinde, T; Castro, MA; Millan, C; Medina, S
Thin Solid Films, **519** (2011) 3123-3127
DOI: 10.1016/j.tsf.2010.12.084

Crystalline monolayers of three aldehydes with an odd number of carbon atoms in the alkyl chain (C-7, C-9 and C-11) at low coverages are observed by a combination of X-ray and neutron diffraction. Analysis of the diffraction data is discussed and possible monolayer crystal structures are proposed; although unique structures could not be ascertained for all molecules. We conclude that the structures are flat on the surface, with the molecules lying in the plane of the layer. The C-11 homologue is determined to have a plane group of either p2, pgb or pgg, and for the C-7 homologue the p2 plane group is preferred.

Preface: Directionally Solidified Eutectic and Advanced Ceramics Preface
Ramirez-Rico, J; Martinez-Fernandez, J; Llorca, J; Orera, VM; Sayir, A
Journal Of The European Ceramic Society, **31** (2011) 1189-1190
DOI: 10.1016/S0955-2219(11)00127-0

The effect of polymorphic structure on the structural and chemical stability of yttrium disilicates
Galunin, E; Vidal, M; Alba, MD
American Mineralogist, **96** (2011) 1512-1520
DOI: 10.2138/am.2011.3659

Under pressure and temperature conditions like those found in deep geological repositories (DGRs), rare-earth cations may react with silicates to form rare-earth disilicates. This study establishes the stability range of yttrium disilicates in response to changes in pH. The alpha, beta, gamma, and delta polymorphs of Y(2)Si(2)O(7) were synthesized by the sol-gel process at temperatures between 1100 and 1650 degrees C and subjected to pH(stat) leaching tests. By measuring the Y and Si leaching rates and monitoring the transformation of the crystalline and amorphous phases, we showed that yttrium disilicates were stable at pH > 5. At pH < 5, the pH stability sequence was consistent with the temperature-dependent stabilities of Y(2)Si(2)O(7) phases, with the delta polymorph showing the lowest leaching rates. Because rare-earth compounds can be used as a proxy for analogous actinide hosts, the results of this study can be used to predict the performance of engineered barriers in DGR.

Microstructural and mechanical evaluation of porous biomorphic silicon carbide for high temperature filtering applications
Bautista, MA; Cancapa, JQ; Fernandez, JM; Rodriguez, MA; Singh, M
Journal Of The European Ceramic Society, **31** (2011) 1325-1332
DOI: 10.1016/j.jeurceramsoc.2010.06.014

Biomorphic SiC (bioSiC) is a low cost SiC/Si composite obtained by melt infiltration of carbon preforms obtained from the pyrolysis of cellulose precursors. The porosity and pore size distribution of bioSiC can be tailored for specific applications by adequate selection of the wood precursor. Natural and artificial industrial woods were explored as possible bioSiC precursors. Silicon was removed by chemical etching. Relevant microstructural parameters such as pore size distribution, total porosity, and permeability were characterized. Since the filtration process involves large pressure gradients along the material at high temperatures, mechanical properties of porous bioSiC from the different precursors were evaluated at room temperature and 800 degrees C. The feasibility of porous bioSiC as a filtration material for high temperature gasification processes is discussed in terms of these properties. MDF-bioSiC is shown to be a promising material for such applications because of its good mechanical properties, interconnected porosity, pore sizes, and permeability.

Microstructural and mechanical evaluation of a Cu-based active braze alloy to join silicon nitride ceramics
Singh, M; Asthana, R; Varela, FM; Martinez-Fernandez, J
Journal Of The European Ceramic Society, **31** (2011) 1309-1316
DOI: 10.1016/j.jeurceramsoc.2010.07.022

Self-joining of St. Gobain Si3N4 (NT-154) using a ductile Cu-Al-Si-Ti active braze (Cu-ABA) was demonstrated. A reaction zone (similar to 2.5-3.5 mu m thick) developed at the interface after 30 min brazing at 1317 K. The interface was enriched in Ti and Si. The room temperature compressive shear strengths of Si3N4/Si3N4 and Inconel/Inconel joints (the latter created to access baseline data for use with the proposed Si3N4/Inconel joints) were 140 +/- 49 MPa and 207 +/- 12 MPa, respectively. High-temperature shear tests were performed at 1023 K and 1073 K, and the strength of the Si3N4/Si3N4 and Inconel/Inconel joints were determined. The joints were metallurgically well-bonded for temperatures above 2/3 of the braze solidus. Scanning and transmission electron microscopy studies revealed a fine grain microstructure in the reaction layer, and large grains in the inner part of the joint with interfaces being crack-free. The observed formation of Ti5Si3 and AlN at the joint interface during brazing is discussed.

High-temperature mechanical behavior of polycrystalline yttrium-doped barium cerate perovskite
Vaquero-Aguilar, C; Lopez-Robledo, MJ; Martinez-Fernandez, J; Real, C; Jimenez-Melendo, M
Journal Of The European Ceramic Society, **31** (2011) 1333-1338
DOI: 10.1016/j.jeurceramsoc.2010.05.023

The high-temperature mechanical properties of the mixed ionic-electronic conductor perovskite BaCe0.95Y0.05O3-delta with average grain size of 0.40 mu m have been studied in compression between 1100 and 1300 degrees C in air at different initial strain rates. The true stress-true strain curves display an initial stress drop, followed by an extended steady-state stage. As the temperature decreases and/or the strain rate increases, there is a transition to a damage-tolerant strain-softening stage and eventually to catastrophic failure. Analysis of mechanical and microstructural data revealed that grain boundary sliding is the primary deformation mechanism. The strength drop has been correlated with the growth of ultrafine grains during deformation, already present at grain boundaries and triple grain junctions in the as-fabricated material.

Electrical properties of biomorphic SiC ceramics and SiC/Si composites fabricated from medium density fiberboard

Orlova, TS; Popov, VV; Cancapa, JQ; Maldonado, DH; Magarino, EE; Feria, FMV; de Arellano, AR; Fernandez, JM

Journal Of The European Ceramic Society, **31** (2011) 1317-1323

DOI: 10.1016/j.jeurceramsoc.2010.06.015

A study has been made of the dependences of the electrical resistivity and the Hall coefficient on the temperature in the range 1.8-1300 K and on magnetic fields of up to 28 kOe for the biomorphic SiC/Si (MDF-SiC/Si) composite and biomorphic porous SiC (MDF-SiC) based upon artificial cellulosic precursor (MDF - medium density fiberboards). It has been shown that electric transport in MDF-SiC is effected by carriers of n-type with a high concentration of similar to 10(20) cm(-3) and a low mobility of similar to 0.4 cm(2) V-1 s(-1). The specific features in the conductivity of MDF-SiC are explained by quantum effects arising in disordered systems and requiring quantum corrections to conductivity. The TEM studies confirmed the presence of disordering structural features (nanocrystalline regions) in MDF-SiC. The conductivity of MDF-SiC/Si composite originates primarily from Si component in the temperature range 1.8-500 K and since similar to 500 to 600 K the contribution of MDF-SiC matrix becomes dominant.

Compressive strength degradation in ZrB2-based ultra-high temperature ceramic composites

Ramirez-Rico, J; Bautista, MA; Martinez-Fernandez, J; Singh, M

Journal Of The European Ceramic Society, **31** (2011) 1345-1352

DOI: 10.1016/j.jeurceramsoc.2010.05.020

The high temperature compressive strength behavior of zirconium diboride (ZrB2)-silicon carbide (SiC) particulate composites containing either carbon powder or SCS-9a silicon carbide fibers was evaluated in air. Constant strain rate compression tests have been performed on these materials at room temperature, 1400, and 1550 degrees C. The degradation of the mechanical properties as a result of atmospheric air exposure at high temperatures has also been studied as a function of exposure time. The ZrB2-SiC material shows excellent strength of 3.1 +/- 0.2 GPa at room temperature and 0.9 +/- 0.1 GPa at 1400 degrees C when external defects are eliminated by surface finishing. The presence of C is detrimental to the compressive strength of the ZrB2-SiC-C material, as carbon burns out at high temperatures in air. As-fabricated SCS-9a SiC fiber reinforced ZrB2-SiC composites contain significant matrix microcracking due to residual thermal stresses, and show poor mechanical properties and oxidation resistance. After exposure to air at high temperatures an external SiO2 layer is formed, beneath which ZrB2 oxidizes to ZrO2. A significant reduction in room temperature strength occurs after 16-24h of exposure to air at 1400 degrees C for the ZrB2-SiC material, while for the ZrB2-SiC-C composition this reduction is observed after less than 16 h. The thickness of the oxide layer was measured as a function of exposure time and temperatures and the details of oxidation process has been discussed.

Stability of Rare-Earth Disilicates: Ionic Radius Effect
Galunin, E; Alba, MD; Vidal, M
Journal Of The American Ceramic Society, **94** (2011) 1568-1574
DOI: 10.1111/j.1551-2916.2010.04272.x

Rare-earth (RE) disilicates, of general formula RE2Si2O7, are one of the products of the chemical reaction between RE (elements), which are actinide simulators, and the silicates used in the engineered barrier systems of deep geological repositories (DGPs). The aim of this paper is to establish the stability range of the disilicate phase as function of the nature of the RE (RE = Sc, Lu, or Y) and examine whether this phase would permit RE leaching under experimental conditions simulating those of the DGP. The beta-polymorphs of the RE disilicates were synthesized by the sol-gel method and subsequently submitted to a pH(stat) leaching test. The rates of RE and Si leaching were measured and the transformation of the crystalline and amorphous phases was examined by X-ray powder diffraction and nuclear magnetic resonance techniques. The results indicate that the disilicate phases were stable within a wide range of pH, their stability being related to the hydrated ratio of the RE. Disilicate stability increased with the ionic radius of the RE. As a result, the Sc disilicate was stable throughout the pH range tested, whereas Y and Lu disilicate leaching was only observed at pH < 4. Thus, it was confirmed that the formation of the disilicate phases could contribute to the confinement of radioactive wastes in engineered barriers.

Interaction of Eu-isotopes with saponite as a component of the engineered barrier
Alba, MD; Castro, MA; Chain, P; Hurtado, S; Orta, MM; Pazos, MC; Villa, M
Applied Clay Science, **52** (2011) 253-257
DOI: 10.1016/j.clay.2011.02.027

Bentonite is accepted as the best clay material in the engineered barrier of deep geological repositories (DGRs) for radioactive waste disposal. In recent years, the interactions between a wide range of rare-earth (REE) cations and smectites have been studied. A combined study of stable europium and radioactive isotopes is reported here. Saponite was subjected to hydrothermal reactions with stable and radioactive (Eu-152) europium ions under subcritical conditions. The structural changes of saponite were evaluated by XRD and SEM. The effect of temperature and reaction time on the changes was quantified by measuring Eu-152 through gamma spectrometry. The reaction between europium and saponite was a first-order reaction. The presence of Eu in the precipitate in an amount much higher than the cation exchange capacity of saponite confirmed participation of chemical reactions or surface adsorption in the europium immobilization, even at temperatures as low as 150 degrees C. The reaction rate constant indicated that an 8- to 9-month period was needed for the completion, without significant changes, of the europium/saponite chemical reaction under the subcritical conditions of 200 degrees C and 350 degrees C. (C) 2011 Elsevier B.V. All rights reserved.

Blocking of grain reorientation in self-doped alumina materials

Suarez, M; Fernandez, A; Menendez, JL; Ramirez-Rico, J; Torrecillas, R
Scripta Materialia, **64** (2011) 517-520
DOI: 10.1016/j.scriptamat.2010.11.031

Alumina nanoparticles 10-20 nm in diameter were nucleated on alumina particles, 150 nm average diameter, by a colloidal route followed by calcination. It is shown that after sintering, the final grain size is up to 20% smaller due to the addition of the alumina nanoparticles. Electron backscattered diffraction analysis shows that whereas a correlation in the relative crystalline orientations between neighbouring grains exists in the pure materials, the addition of alumina nanoparticles results in a random crystalline orientation.

Remediation of metal-contaminated soils with the addition of materials - Part I: Characterization and viability studies for the selection of non-hazardous waste materials and silicates

Gonzalez-Nunez, R; Alba, MD; Orta, MM; Vidal, M; Rigol, A
CHEMOSPHERE, **85** (2011) 1511-1517
DOI: 10.1016/j.chemosphere.2011.09.042

Contamination episodes in soils require interventions to attenuate their impact. These actions are often based on the addition of materials to increase contaminant retention in the soil and to dilute the contaminant concentration. Here, non-hazardous wastes (such as sugar foam, fly ash and a material produced by the zeolitization of fly ash) and silicates (including bentonites) were tested and fully characterized in the laboratory to select suitable materials for remediating metal-contaminated soils. Data from X-ray fluorescence (XRF), N(2) adsorption/desorption isotherms, X-ray diffraction (XRD) and scanning electron microscopy/energy-dispersive X-ray spectroscopy (SEM-EDX) analyses revealed the chemical composition, specific surface area and the phases appearing in the materials. A pH titration test allowed the calculation of their acid neutralization capacity (ANC). The metal sorption and desorption capacities of the waste materials and silicates were also estimated. Sugar foam, fly ash and the zeolitic material were the best candidate materials. Sugar foam was selected because of its high ANC (17000 meq kg(-1)), and the others were selected because of their larger distribution coefficients and lower sorption reversibilities than those predicted in the contaminated soils.

Evolution of Phases and Al-Si Distribution during Na-4-Mica Synthesis

Alba, MD; Castro, MA; Naranjo, M; Orta, MM; Pavon, E; Pazos, MC
JOURNAL OF PHYSICAL CHEMISTRY C, **115** (2011) 20084-20090
DOI: 10.1021/jp207408h

Na-4-mica, a highly charged fluorophlogopite, has recently attracted much attention because of its unique combination of high charge (four charges per unit cell) and its swelling and cation-exchange properties. The ability to improve the properties of this mica depends on gaining knowledge about its phase evolution during the calcination process. For the synthesis, the stoichiometric powder mixture (4SiO(2)/2Al(2)O(3)/6MgF(2)/8NaCl) was heated to 900 degrees C for 0-600 h. The obtained solids were characterized by X-ray fluorescence (XRF); X-ray diffraction (XRD); scanning electron microscopy/energy-dispersive X-ray (SEM/EDX) analysis; (29)Si, (27)Al, and (23)Na magic-angle-spinning MAS NMR spectroscopy; and thermogravimetric/differential thermal analysis (TG/DTA). The results showed that the precursors are rapidly (t < 3 h) transformed into sodalite, Al(6)Na(8)(SiO(4))(6)Cl(2), and a 2:1 phyllosilicate. For t <= 7.5 h, the amount of 2:1 phyllosilicate increased as a result of the decomposition of sodalite, with a progressive incorporation of aluminum in the 2:1 phyllosilicate being observed. For t = 7.5 h, synthesis of Na-4-mica was considered to be complete, as the material remained essentially unaltered for the next 15 h. For t = 30 h, the mica started to decompose, and for very long reaction times (t >= 300 h), only forsterite and a carnegierite phase were present.

Examination of competitive lanthanide sorption onto smectites and its significance in the management of radioactive waste

Galunin, E; Alba, MD; Santos, MJ; Abrao, T; Vidal, M

Journal Of Hazardous Materials, **186** (2011) 1930-1941

DOI: 10.1016/j.jhazmat.2010.12.098

The competitive effect of La and Lu (analogues of radionuclides appearing in radioactive waste) in the sorption in four smectites was examined. Sorption and desorption distribution coefficients (K-d; K-d,K-des), and desorption rates (R-des) were determined from batch tests in two media: deionized water and, to consider the influence of cement leachates, 0.02 mol L-1 Ca. The competitive effect was lower when high-affinity sites were available, as in the water medium at the lowest range of initial lanthanide concentration, with high Kd for La and for Lu (5-63 x 10(4) L kg(-1)). Lower K-d was measured at higher initial concentrations and in the Ca medium, where Lu showed a stronger competitive effect. This was confirmed by fitting the sorption data to a two-solute Langmuir isotherm. The desorption data indicated that sorption was virtually irreversible for the scenarios with high sorption, with an excellent correlation between K-d and K-d,K-des (R-2 around 0.9 for the two lanthanides). Assuming that radioactive waste is a mixture of radionuclides, and that Ca ions will be provided by the cement leachates, this would reduce the retention capacity of clay engineered barriers.

Formation of Organo-Highly Charged Mica

Alba, Maria D.; Castro, Miguel A.; Mar Orta, M.; Pavon, Esperanza; Carolina Pazos, M.; Valencia Rios, Jesus S.

Langmuir, **27** (2010) 9711-9718

DOI: 10.1021/la200942u

The interlayer space of the highly charged synthetic Na-Mica-4 can be modified by ion-exchange reactions involving the exchange of inorganic Na(+) cations by surfactant molecules, which results in the formation of an organophilic interlayer space. The swelling and structural properties of this highly charged mica upon intercalation with n-alkylammonium (RNH(3))(+) cations with varying alkyl chain lengths (R = C12, C14, C16, and C18) have been reported. The stability, fine structure, and evolution of gaseous species from alkylammonium Mica-4 are investigated in detail by conventional thermogravimetric analysis (TGA), Fourier transform infrared spectroscopy (FTIR), in situ X-ray diffraction (XRD), and solid-state nuclear magnetic resonance (MAS NMR) techniques. The results clearly show the total adsorption of n-alkylammonium cations in the interlayer space which expands as needed to accommodate intercalated surfactants. The surfactant packing is quite ordered at room temperature, mainly involving a paraffin-type bilayer with an all-trans conformation, in agreement with the high density of the organic compounds in the interlayer space. At temperatures above 160 degrees C, the surfactant molecules undergo a transformation that leads to a liquid-like conformation, which results in a more disordered phase and expansion of the interlayer space.

Bulk and Adsorbed Monolayer Phase Behavior of Binary Mixtures of Undecanoic Acid and Undecylamine: Catanionic Monolayers
Sun, C; Bojdys, MJ; Clarke, SM; Harper, LD; Jefferson, A; Castro, MA; Medina, S
Langmuir, **27** (2011) 3626-3637
DOI: 10.1021/la1048198

Differential scanning calorimetry (DSC) and X-ray powder diffraction (PXRD) have been used to determine the phase behavior of the binary mixtures of undecanoic acid (A) and undecylamine (B) in the bulk. In addition, we report DSC data that indicates very similar behavior for the solid monolayers of these materials adsorbed on the surface of graphite. The two species are found to form a series of stoichiometric complexes of the type AB, A(2)B, and A(3)B on the acid rich side of the phase diagram. Interestingly, no similar series of complexes is evident on the amine rich side. As a result of this complexation, the solid monolayers of the binary mixtures exhibit a very pronounced enhancement in stability relative to the pure adsorbates.

CONGRESOS Y REUNIONES INTERNACIONALES / INTERNATIONAL CONGRESS AND MEETINGS

COMUNICACIONES EN CONGRESOS Y REUNIONES / COMMUNICATIONS IN CONGRESS AND MEETINGS

XVII Congreso Argentino de FisicoQuímica y Química Inorgánica
3 – 6 mayo [Córdoba, Argentina]

Análisis por ATD, determinación de superficie y RMN de sólidos, de la influencia del catión interlaminar en los cambios estructurales de montmorillonitas y sus productos de tratamientos térmicos y mecánicos
MA. Fernandez, Maria Dolores Alba, R. Torres
Poster

SMARTER-2. 2nd Structure elucidation by combining magnetic resonance, computation modelling and diffraction

23 - 27 mayo [Aveiro, Portugal]

Getting more out of Rare Earth Silicates: X-Ray Diffraction vs Nuclear Magnetic Resonance
M. Dolores Alba Carranza, Miguel Angel Castro Arroyo, P. Chain, A. Cota, Said El Mrabet, M. Mar Orta Cuevas, E. Pavón, M. Carolina Pazos Zarama
Comunicación oral

4th International Congress on Energy and Environment Engineering and Management

26 - 27 mayo [Mérida, España]

High-temperature mechanical behavior of nickel oxide/zirconia composites
M. Oliva-Ramírez, F.A. Huaman-Mamani, C. Vaquero-Aguilar, Manuel Jiménez-Melendo
Comunicación oral

ICRER-2011. International Conference on Radioecology & Environmental Radioactivity. Environment & Nuclear Renaissance

19 - 24 junio [Ontario, Canadá]

Advances on the Chemicals interaction of stable and radioactive isotopes with Bentonite FEBEX and MX80
M. Villa, S. Hurtado, Carolina Pazos Zarama, M. Mar Orta Cuevas, Miguel Angel Castro Arroyo, P Chaín, E Pavón, María Dolores Alba Carranza
Poster

18th International Symposium on Metastable, Amorphous and Nanostructured Materials

26 junio – 1 julio [Gijón, España]

Characterization of the high-temperature mechanical properties of nickel oxide/tetragonal zirconia composites
M. Oliva-Ramirez; F.A. Huaman-Mamani, C. Vaquero-Aguilar and Manuel Jimenez-Melendo
Comunicación oral

18th International Conference on Solid State Ionics

3 – 8 julio [Varsovia, Polonia]

Fabrication and high-temperature mechanical properties of doped barium cerate perovskite proton conductor
Manuel Jiménez-Melendo, C. Vaquero-Aguilar, M. Oliva-Ramirez, F.A. Huaman-Mamani
Comunicación oral

Journee d´etude sur “etude des argiles et des zeolithes: Applications environnementales

26 octubre [Fez, Marruecos]

Clay minerals: Management of harmful cation waste

Maria Dolores Alba Carranza, Miguel Angel Castro Arroyo, P. Chain, A. Cota, Said El Mrabet, P. Fernández, S. Hurtado, S. Medina, M. Mar Orta Cuevas, E. Pavon, MC Pazos, M. Villa

Comunicación oral

Aplicación de la RMN de sólidos al estudio de la interfase sólido-líquido

María Dolores Alba Carranza

Conferencia Invitada

CONGRESOS Y REUNIONES NACIONALES / NATIONAL CONGRESSES AND MEETINGS

COMUNICACIONES EN CONGRESOS Y REUNIONES / COMMUNICATIONS IN CONGRESS AND MEETINGS

I Jornada Ingeniería de Cerámicos para Ambientes Extremos

10 junio [Sevilla, España]

Formación de nanogalerías organofílicas en micas de alta carga: agentes eliminadores de NOCs

Mery Carolina Pazos Zarama

Comunicación oral

Capacidad de retención de residuos tóxicos en micas de alta carga: estudio del espacio interlaminar

Esperanza Pavón González

Comunicación oral

Efecto competitivo bentonitas-contenedor metálico en la retención del elemento radioactivo Eu^{3+}

Said El Mrabet

Comunicación oral

Simposium de Resonancia Magnética Nuclear de Estado Sólido

9 septiembre [Sevilla, España]

Aplicación de la RMN de sólidos al estudio de la interfase sólido-líquido

María Dolores Alba Carranza

Conferencia Invitada

FORMACION / TRAINING

TESIS DOCTORALES/ DOCTOR DEGREE THESIS

Título: **Mecanismos de interacción de cationes inorgánicos en el espacio interlaminar de micas expansibles de alta carga**
Autor: Esperanza Pavón González
Directores: Miguel Angel Castro Arroyo
Calificación: Apto “Cum Laude” por unanimidad
Centro: Universidad de Sevilla

FORMACIÓN DE GRADUADOS / MASTER DEGREE THESIS

Título: **Solubilidad de Hf en la matriz ZrSiO4: efecto en el orden estructural a largo y corto alcance**
Autor: Agustín Cota Reguero
Directores: María Dolores Alba Carranza
Grado: Trabajo Fin de Master
Centro: Universidad de Sevilla
Año Académico: 2010-2011

Título: **Microestructura, resistencia a la oxidación y propiedades mecánicas de cerámicos monolíticos fibrosos de SiC**
Autor: María Carmen Vera García
Directores: Julian Martínez Fernández y Joaquín Ramírez Rico
Grado: Trabajo Fin de Master
Centro: Universidad de Sevilla
Año Académico: 2010-2011

Título: **Materiales carbonosos para aplicaciones energéticas obtenidos a partir de precursoles vegetales**
Autor: Antonio Gutiérrez Pardo
Directores: Julian Martínez Fernández y Joaquín Ramírez Rico
Grado: Trabajo Fin de Master
Centro: Universidad de Sevilla
Año Académico: 2010-2011

Título: **Comportamiento mecánico a alta temperatura de compuestos de óxido de niquel-circona tetragonal**
Autor: Manuel Oliva Ramírez
Directores: Manuel Jiménez Melendo
Grado: Trabajo Fin de Master
Centro: Universidad de Sevilla
Año Académico: 2010-2011

Título: **Microestructura y comportamiento mecánico a alta temperatura del compuesto eutéctico ternario Al_2O_3-$Er_3Al_5O_{12}$-ZrO_2**
Autor: Fredy Huaman Mamani
Directores: Manuel Jiménez Melendo
Grado: Trabajo Fin de Master
Centro: Universidad de Sevilla
Año Académico: 2010-2011

EQUIPAMIENTO CIENTÍFICO AVAILABLE EQUIPMENT

- Horno tubular hasta 1200º C
- Horno tubular en atmósfera controlada hasta 1700º C
- Horno de Cámara hasta 1650º C
- Horno de Cámara hasta 1200 ºC
- Estufa hasta 400º C
- Estufa hasta 200º C
- Caja de guantes
- Reactores hidrotermales
- Línea de vacío

MECANOQUÍMICA Y REACTIVIDAD DE MATERIALES
MECHANO-CHEMISTRY AND REACTIVITY OF MATERIALS

Proyectos de Investigación / Research Projects

Unión Europea
Fondo Europeo de Desarrollo Regional
"Una manera de hacer Europa"
MINISTERIO DE CIENCIA E INNOVACIÓN

Estudio de los procesos de degradación de los materiales utilizados en la construcción de Órganos Históricos

Study of the degradation processes on the materials used in the manufacture of historical organs

Código/Code: MAT2010-20660 (Plan Nacional)
Periodo/Period: 2010 / 2013
Organismo Financiador/Financial source: Ministerio de Ciencia e Innovación
Importe total/Total amount: 48.400 €
Investigador responsable/Research head: Angel Justo Erbez
Componentes/Research group: Adolfo Iñigo Iñigo, Juan Poyato Ferrera, José Luis Pérez Rodríguez, Liz Karen Herrera Quintero, Angel Justo Estebaranz, Adrián Durán Benito, M. Carmen Jiménez de Haro, Belinda Sigüenza Carballo

RESUMEN / ABSTRACT

El principal objetivo del proyecto es conocer la composición, microestructura y propiedades mecánicas de las aleaciones estaño-plomo de tubos de órganos históricos españoles. Además se estudiarán los procesos de degradación y corrosión sobre los tubos, así como los productos generados por dichos procesos. Los análisis se realizarán en diferentes Institutos Científicos y Tecnológicos españoles (ICMSE, AIMEN, IRNASA) y grandes instalaciones europeas (ESRF, C2RMF). Se persigue conocer los vectores que provocan los procesos de corrosión, como son los compuestos volátiles desprendidos de las maderas y otros materiales orgánicos utilizados en la construcción de órganos, vapor de agua y/o anhídrido carbónico.

Los trabajos se realizarán en materiales con diferentes grados de corrosión tomados en los propios instrumentos, incluyendo principalmente aleaciones metálicas y maderas. Además, se prepararán aleaciones en el taller de organería Grenzing con distintas proporciones estaño-plomo, y con trazas de otros elementos como As o Bi. Estas aleaciones se someterán a ensayos de corrosión acelerada y se correlacionarán los resultados de la composición y los ensayos de resistencia a la tracción y de fluencia con la velocidad de corrosión.

Se compararán los resultados obtenidos en el laboratorio (aleaciones preparadas) con las muestras procedentes de los órganos y se sacarán conclusiones acerca de las posibles causas de alteración, las composiciones idóneas para las restauraciones y las aleaciones más resistentes a la corrosión para aplicarlas a la construcción de órganos nuevos.

The main objective of the project is to know the composition, microstructure and mechanical properties of tin-lead alloys from Spanish historical pipe organs. Also, we will study the degradation and corrosion processes on the pipe organs and the products of corrosion produced by these processes. Analyses will be performed in Spanish research and technological institutes (ICMSE, AIMEN, IRNASA) and European facilities (ESRF, C2RMF). This objective

pursues to know the vectors that produce the corrosion, like the volatile compounds from the wood and other organic materials used in the construction of pipe organs, water vapour and/or carbon dioxide.

The work will be carried out in materials with different grades of corrosion taken in the organs, including alloys and woods. Also, alloys with different tin-lead ratios, and with traces of other elements (As, Bi) will be prepared and will be undergone to corrosion tests. Results from the composition and results of tensile and creep tests will be correlated with the corrosion rate.

The results obtained in the laboratory will be compared with the samples coming from the organs, and conclusions will be reached about the possible alteration causes, the suitable compositions for the restorations, and the most resistant alloys to the corrosion, to apply them to the construction of new organs.

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Preparación de materiales multiferroicos por métodos mecano-químicos y térmicos con control inteligente de temperatura

Preparation of multiferroic materials by mechanical alloying and termal methods with smart temperatura control

Código/Code: MAT2008-06619
Periodo/Period: 01-01-2009 / 31-12-2011
Organismo Financiador/Financial source: Ministerio de Ciencia e Innovación
Importe total/Total amount: 60.500 €
Investigador responsable/Research head: Pérez Maqueda, Luis A.
Componentes/Research group: Diánez Millán, M.J., Criado Luque, J.M.

RESUMEN / ABSTRACT

Los materiales multiferroicos, aquellos que presentan simultaneamente dos o mas propiedades ferroicas, tienen un gran interés en la actualidad debido al gran número de aplicaciones que pueden derivarse de sus propiedades. A pesar del interés suscitado por estos materiales, Su dificultad de preparación por métodos convencionales como fases puras de estequiometria controlada y pureza adecuada limita sus aplicaciones. En este proyecto se propone el uso de dos métodos alternativos para la preparación de materiales multiferroicos con composición, estructura y microestructura controlada: a) la síntesis mecanoquímica directa y b) la descomposici6n de precursores mediante métodos térmicos con control inteligente de la temperatura. El primer método implica la utilización de un molino planetario de alta energía de molienda, diseñado por nosotros en colaboración con la empresa MC2, Ingeniería y Sistemas, que permite controlar la atmósfera durante la mecanosíntesis hasta presiones de 20 atmósferas de cualquier gas inerte o reactivo seleccionado. El método alternativo al propuesto anteriormente implica la preparación de diversos precursores y su posterior descomposición mediante el método de control inteligente de la temperatura. En este método, el propio proceso es quien determina, automáticamente, la progresión de la temperatura según una función de evolución del grado de avance del proceso con el tiempo, a diferencia de los convencionales, donde el operador predetermina una función temperatura-tiempo. En publicaciones previas hemos puesto de manifiesto que este método permite un control muy preciso de la textura y microestructura del producto, que no es posible empleando métodos convencionales de calentamiento. Las muestras preparadas se caracterizaran en cuanto al estado de oxidaci6n de las especies, estructura, microestructura y propiedades.

Multiferroic materials are those with two or more ferroic properties. There is a significant interest in those materials due to the large number of possible applications due to their properties. It has been claim in literature that the lack of reliable preparation methods for stoichiometric defect-free compounds hinders the development of applications of these compounds in devices. In this project, we propose the use of two alternative procedures for the preparation of multiferroic compounds: mechanical alloying and thermal decomposition of precursors under smart temperature conditions. The first procedure implies the use of a high-energy mill designed in cooperation with MC2 firm. The mill is connected to the gas system during operation. Thus, it is possible to control pressures up to 20 atm of any reactive or inert gas. The alternative proposed procedure implies the preparation of several precursors and their decomposition under smart temperature conditions. In the smart temperature control methods, the process itself determines the temperature evolution according to a function of the process evolution with time. These methods differ from the conventional ones in the control procedure, thus, in the conventional ones the function temperature-time is fixed while in the smart temperature control methods the process itself determines the evolution of temperature. In previous publications, we have observed that by using the smart temperature procedure, microestructure of samples could be tailored, while by using conventional heating procedures such control could not be achieved. Prepared samples will be characterized in terms of the oxidation state of the different cations, structure, microstructure and properties.

Mecanosíntesis de materiales de interés tecnológico

Mechanosynthesis of technological materials

Código/Code: MAT2010-17046
Periodo/Period: 01-01-2011 / 31-12-2011
Organismo Financiador/Financial source: Ministerio de Ciencia e Innovación
Importe total/Total amount: 14.520 €
Investigador responsable/Research head: Francisco J. Gotor Martínez
Componentes/Research group: M. Jesús Sayagués de Vega, Concepción Real Pérez, M. Dolores Alcalá González, José Manuel Córdoba Gallego, Ernesto Chicardi Augusto

RESUMEN / ABSTRACT

Los molinos de bolas de alta energía, planetarios, vibratorios y en menor medida los de atrición, son capaces de transferir a un sólido (ó una mezcla) cantidades importantes de energía mecánica. Los efectos de esta acción mecánica no se reducen sólo a una gradual disminución del tamaño de las partículas, sino que es posible inducir reacciones químicas en estado sólido. Como los procesos repetidos de fractura y soldadura de las partículas aumentan el área de contacto de los reactivos y se generan sin cesar superficies frescas, los procesos continuados de interdifusión hacen que la reacción ocurra a temperatura ambiente. La nueva fase formada posee, en general, un carácter nanoestructurado y presenta un gran número de defectos, lo que incide positivamente en la posterior etapa (si fuera necesaria) de sinterización. Estos procesos denominados mecanoquímicos constituyen una vía atractiva y alternativa en la síntesis de materiales nanocristalinos. Se trata de un método muy versátil que permite obtener un gran número de materiales en forma masiva, a temperatura ambiente y con un equipamiento relativamente sencillo. Este tipo de procesos es muy competitivo en término de costes y no genera ningún tipo de residuo, lo que le confiere un extraordinario valor añadido. Es un método especialmente prometedor en la obtención de soluciones sólidas complejas y de materiales compuestos tanto por su preparación con un carácter nanométrico como por la excelente homogeneidad y dispersión de los distintos constituyentes.

En el presente proyecto, se pretende demostrar con ejemplos concretos que la aplicación de los procesos mecanoquímicos al campo de la síntesis de materiales permite desarrollar productos de manera más simple o que no serían posible de obtener por otros procedimientos. Los sistemas seleccionados como objeto de estudio son los siguientes: (i) carburos, nitruros y boruros de metales de transición, y (ii) óxidos mixtos con estructura perovskita de fórmula general (A1-xA'x)(B1-yB'y)O3-z (A/A'=La, Sr; B/B'=Mn, Cr, Mg, Ga). En el primer caso, se pretenden desarrollar materiales compuestos para fines estructurales basados en soluciones sólidas complejas de los compuestos refractarios especificados. En el segundo caso, se pretenden desarrollar los distintos componentes de las pilas cerámicas de combustible de forma que todos tengan la misma estructura perovskita y gran similitud composicional. Por último, indicar que se intentarán estudiar y modelizar los procesos mecanoquímicos de alta energía con el fin de realizar con mayor garantía de éxito su posible escalado.

High-energy ball milling devices, such as planetary, vibratory and attritor mills, introduce into the starting powders increasing amounts of energy. Collisions and friction between the balls and between the balls and the wall of the vial result not only in a steadily reduction of particle size, but also induce solid state chemical reactions. During high-energy milling, intimate mixing of reactants takes place and fresh surfaces are continually created, which make possible that solid-state reactions progress gradually at room temperature. The new phase has frequently a nanometric character and a great amount of defects, which favours a subsequent sintering process. The mechanochemistry method represents an attractive and alternative route in the synthesis of nanocrystalline materials. Mechanochemical techniques are simple, flexible, and able to prepare a large variety of materials in a bulk-manner at room temperature. Mechanochemistry has been revealed as a practical way to obtain cost-effective materials and more convenient than other synthesis methods because of avoiding the use of heat and solvents can reduce environmental contamination. Due to an almost infinite compositional flexibility, mechanochemistry is suitable for the production of complex solid solutions and composites because of excellent powder homogeneity can be achieved at the same time as the nanostructure.

In this project, the ability of mechanochemistry to produce easily and in a reproducible manner different materials that sometimes cannot be synthesized via conventional routes is explored. The following systems have been selected: (i) carbides, nitrides, and borides of transition metals, and (ii) oxides with a perovskite structure and general formula (A1-xA'x)(B1-yB'y)O3-z (A/A'=La, Sr; B/B'=Mn, Cr, Mg, Ga). In the first case, the aim is to develop composite materials based on complex solid solutions of the after-mentioned refractory compounds for structural applications. In the second case, the final goal is to design solid oxide fuel cells where all the components possess the same perovskite structure and similar chemical composition. In addition, the study and modelling of high-energy ball milling processes will be intended in order to permit more easily the scaling-up of the process.

Mecanosíntesis de hidruros metálicos y perowskitas multiferróicas en un molino planetario de alta energía de molienda bajo presiónes elevadas

Mechanosynthesis of metallic hydrides and multiferroic perowskites in a high energy mil under high pressure

Código/Code:	TEP-03002 (Proyecto de Excelencia)
Periodo/Period:	01-02-2008 / 31-03-2011
Organismo Financiador/Financial source:	Junta de Andalucía
Importe total/Total amount:	197.668 €
Investigador responsable/Research head:	Pérez Maqueda, L.A.
Componentes/Research group:	Gotor, F.J., Diánez, M.J., Criado, J.M., Alcalá, M.D., Poyato, J., Pérez Rodríguez, J.L., Sánchez Jiménez, P.E.

RESUMEN / ABSTRACT

El objetivo principal del proyecto implica la utilización de un molino planetario de alta energía de molienda, diseñado en colaboración con la empresa andaluza MC2, Ingeniería y Sistemas, S.L., que permite controlar la atmósfera durante la mecanosíntesis hasta presiones de 20 atmósferas de cualquier gas inerte o reactivo seleccionado, para la síntesis mecanoquímica directa de dos tipos de materiales: hidruros de magnesio modificados de interés en el almacenamiento de hidrógeno y cerámicas multiferróicas. En este proyecto se propone por primera vez la preparación de cerámicas multiferróicas con estructura perowskita mediante molienda reactiva en atmósfera controlada a temperatura ambiente. Proponer nuevos métodos de síntesis para estos materiales es de gran interés pues su uso está limitado por sus dificultades de preparación, que requieren el uso de temperaturas relativamente elevadas y presiones de varios GPa. Las cerámicas preparadas se caracterizarán mediante la medida de sus propiedades eléctricas y magnéticas, correlacionándolas con su estructura y microestructura. Los hidruros de magnesio modificados se prepararán por reacción mecanoquímica directa sólido-gas bajo elevadas presiones de hidrógeno. Los materiales obtenidos se caracterizarán en cuanto a su estructura, microestructura y comportamiento como sistemas para el almacenamiento de hidrógeno; realizando una evaluación de las cinéticas de deshidrogenación e hi-

drogenación. También se propone el uso de los métodos de control inteligente de temperatura para optimizar el intercambio de hidrógeno.

The main objective of the Project is the use of a high energy mil, developed in cooperation with the firm MC2, ingeniería y sistemas, S.L., that allows controlling the atmosphere during the treatment at pressure of up to 20 bar of any inert or reactive gas, for the preparation of two kinds of materials: modified magnesium hydrides for hydrogen storage and multiferroic ceramics. In this project we propose for the first time the preparation of multiferroic ceramics by mechanical alloying at room temperature. This is a challenging topic because the preparation of such materials requires pressure of up to several GPa. The prepared materials will be characterized in terms of their properties. Metallic hydrides will be prepared by mechanical alloying under high pressure of hydrogen. The prepared materials will be characterized in terms of their structure, microstructure and hydrogen storage behavior, including the kinetics of hydrogenation and dehydrogenation.

COOPERACIÓN INTERNACIONAL Y OTROS INTERNATIONAL COOPERATION AND OTHERS

Síntesis mecanoquímica y propiedades de materiales nanoestructurados

Código/Code: 2009SK0002
Periodo/Period: 1-01-2010 / 31-12-2011
Organismo Financiador/Financial source: Proyecto conjunto con instituciones extranjeras CSIC-Academia Eslovaca de Ciencias
Importe total/Total amount: 10.600 €
Investigador responsable/Research head: Francisco J. Gotor Martínez
Componentes/Research group: José Manuel Criado Luque, M. Jesús Sayagués de Vega, Concepción Real Pérez, M. Dolores Alcalá González, José Manuel Córdoba Gallego

Microstructural characterization and properties of copper base alloys hardened by metallurgical transformations

Periodo/Period: 1-01-2009 / 31-12-2011
Entidad Financiadora/Financial source: FONDECYT/CONYCIT. Ministerio de Tecnología Chileno
Investigador responsable/Research head: E. Donoso Catalán
Componentes/Research group: José Manuel Criado Luque, Maria Jesús Diánez Millán

Phase transformations and strengthening during aging of Cu-Ni-X alloys

Periodo/Period: 01-01-2011 / 31-12-2012
Entidad Financiadora/Financial source: FONDECYT/CONYCIT. Ministerio de Tecnología Chileno

Investigador responsable/Research head:	E. Donoso Catalán
Componentes/Research group:	José Manuel Criado Luque, Maria Jesús Diánez Millán

TRANSFERENCIA / TECHNOLOGICAL TRANSFER

PATENTES / PATENTS

Procedimiento de obtención de nanopartículas metálicas funcionalizadas con moléculas orgánicas fluorescentes
Inventores: Ana Paula Zaderenko Partida, Carlos Caro Salazar, José Antonio Mejías Romero, María Jesús Sayagués de Vega
Ámbito Geográfico: Nacional
PATENTE SOLICITADA. N. de solicitud: P201130447
Fecha Solicitud/Licencia: 25 marzo 2011
Entidades Titulares: Universidad Pablo Olavide y CSIC

Procedimiento de obtención de un material compuesto a base de diboruro de titanio con contenidos variables de partículas nanométricas y/o submicrométricas de monoboruro, nitruro, carburo o carbonitruro de titanio mediante reacción autosostenible inducida por molienda
Inventores: Francisco J. Gotor Martínez, María Jesús Sayagués de Vega, Pedro José Sánchez Soto, Miguel Angel Áviles Escaño, José Manuel Córdoba Gallego, Ernesto Chicardi Augusto
Ámbito Geográfico: Nacional
PATENTE SOLICITADA. N. de solicitud: P201131835
Fecha Solicitud/Licencia: 15 noviembre 2011
Entidades Titulares: CSIC

PUBLICACIONES / PUBLICATIONS

ARTÍCULOS PUBLICADOS EN REVISTAS SCI / PAPERS IN SCI JOURNALS

Compositional and Quantitative Microtextural Characterization of Historic Paintings by Micro-X-ray Diffraction and Raman Microscopy
Romero-Pastor, J; Duran, A; Rodriguez-Navarro, AB; Van Grieken, R; Cardell, C
Analytical Chemistry, **83** (2011) 8420-8428

DOI: 10.1021/ac201159e

This work shows the benefits of characterizing historic paintings via compositional and microtextural data from micro-X-ray diffraction (mu-XRD) combined with molecular information acquired with Raman microscopy (RM) along depth profiles in paint stratigraphies. The novel approach was applied to identify inorganic and organic components from paintings placed at the 14th century Islamic University-Madrasah Yusufiyya-in Granada (Spain), the only Islamic University still standing from the time of Al-Andalus (Islamic Spain). The use of mu-XRD to obtain quantitative micro textural information of crystalline phases provided by two-dimensional diffraction patterns to recognize pigments nature and manufacture, and decay processes in complex paint cross sections, has not been reported yet. A simple Nasrid (14th century) palette made of gypsum, vermilion, and azurite mixed with glue was identified in polychromed stuccos. Here also a Christian intervention was found via the use of smalt, barite, hematite, Brunswick green and gold; oil was the binding media employed. On mural paintings and wood ceilings, more complex palettes dated to the 19th century were found, made of gypsum, anhydrite, barite, dolomite, calcite, lead white, hematite, minium, synthetic ultramarine blue, and black carbon. The identified binders were glue, egg yolk, and oil.

Kinetic Analysis of Complex Solid-State Reactions. A New Deconvolution Procedure
Perejon, A; Sanchez-Jimenez, PE; Criado, JM; Perez-Maqueda, LA
Journal Of Physical Chemistry B, **115** (2011) 1780-1791
DOI: 10.1021/jp110895z

The kinetic analysis of complex solid-state reactions that involve simultaneous overlapping processes is challenging. A method that involves the deconvolution of the individual processes from the overall differential kinetic curves obtained under linear heating rate conditions, followed by the kinetic analysis of the discrete processes using combined kinetic analysis, is proposed. Different conventional mathematical fitting functions have been tested for deconvolution, paying special attention to the shape analysis of the kinetic curves. It has been shown that many conventional mathematical curves such as the Gaussian and Lorentzian ones fit kinetic curves inaccurately and the subsequent kinetic analysis yields incorrect kinetic parameters. Alternatively, other fitting functions such as the Fraser-Suzuki one property fit the kinetic curves independently of the kinetic model followed by the reaction and their kinetic parameters, and moreover, the subsequent kinetic analysis yields the correct kinetic parameters. The method has been tested with the kinetic analysis of complex processes, both simulated and experimental.

Forgery detection on an Arabic illuminated manuscript by micro-Raman and X-ray fluorescence spectroscopy
Duran, A; Franquelo, ML; Centeno, MA; Espejo, T; Perez-Rodriguez, JL
Journal Of Raman Spectroscopy, **42** (2011) 48-55
DOI: 10.1002/jrs.2644

An Arabic manuscript, supposed to be from the 14th century, was investigated and its components (pigments and dyestuffs) characterised using micro-Raman and X-ray fluorescence (XRF) spectroscopy, the latter employing a portable XRF/X-ray diffraction (XRD) system. The presence of anatase, rutile, calcite, barite, zinc oxide, carbon black, vermilion, hematite, goethite, beta-naphthol, copper phthalocyanine, pigmosol green and a brass-based pigment was detected in the different zones of the illuminated manuscript. The detection of titanium oxides, barite and organic synthetic colourants such as beta-naphthol and copper phthalocyanine and derived compounds provides indisputable indication of forging, repainting or retouching after the 19th century in the image of the manuscript.

An improved model for the kinetic description of the thermal degradation of cellulose

Sanchez-Jimenez, PE; Perez-Maqueda, LA; Perejon, A; Pascual-Cosp, J; Benitez-Guerrero, M; Criado, JM

Cellulose, **18** (2011) 1487-1498

DOI: 10.1007/s10570-011-9602-3

In spite of the large amount of work performed by many investigators during last decade, the actual understanding of the kinetics of thermal degradation of cellulose is still largely unexplained. In this paper, recent findings suggesting a nucleation and growth of nuclei mechanism as the main step of cellulose degradation have been reassessed and a more appropriate model involving chain scission and volatilization of fragments has been proposed instead. The kinetics of cellulose pyrolysis have been revisited by making use of a novel kinetic method that, without any previous assumptions regarding the kinetic model, allows performing the kinetic analysis of a set of experimental curves recorded under different heating schedules. The kinetic parameters and kinetic model obtained allows for the reconstruction of the whole set of experimental TG curves.

Constant rate thermal analysis for thermal stability studies of polymers

Sanchez-Jimenez, PE; Perez-Maqueda, LA; Perejon, A; Criado, JM

Polymer Degradation And Stability, **96** (2011) 974-981

DOI: 10.1016/j.polymdegradstab.2011.01.027

This paper explores the relationship between the shapes of temperature time curves obtained from experimental data recorded by means of constant rate thermal analysis (CRTA) and the kinetic model followed by the thermal degradation reaction. A detailed shape analysis of CRTA curves has been performed as a function of the most common kinetic models. The analysis has been validated with simulated data, and with experimental data recorded from the thermal degradation of polytetrafluoroethylene (PTFE), poly(1,4-butylene terephthalate) (PBT), polyethylene (PE) and poly(vinyl chloride) (PVC). The resulting temperature time profiles indicate that the studied polymers decompose through phase boundary, random scission, diffusion and nucleation mechanisms respectively. The results here presented demonstrate that the strong dependence of the temperature time profile on the reaction mechanism would allow the real kinetic model obeyed by a reaction to be discerned from a single CRTA curve.

Creep behavior of TiC_xN_{1}-x-CoTi cermets synthesized by mechanically induced self-sustaining reaction

Morales-Rodriguez, A; Gallardo-Lopez, A; Dominguez-Rodriguez, A; Cordoba, JM; Aviles, MA; Gotor, FJ
Journal Of The European Ceramic Society, **31** (2011) 299-302
DOI: 10.1016/j.jeurceramsoc.2010.10.007

The plastic flow of TiCxN1-x-CoTi cermets has been investigated by uniaxial compression tests carried out in argon atmosphere at temperatures between 1100 and 1200 degrees C. Two different cermets, with 5 wt.% W or WC content as sintering additives, have been explored to assess the influence of the sintering additives on creep. The microstructural observations of deformed samples and the mechanical results indicate that the hard phase (ceramic grains) controls the plastic deformation. The stress exponent changes from 1 to 2 with increasing strain rate, suggesting a transition in the deformation mechanism from diffusional creep to grain boundary sliding; both with similar activation energy values of about 400 kJ/mol. This value of activation energy agrees with C diffusion in the carbonitride grains as the strain rate controlling mechanism.

Formation of the complete range of Ti(5)Si(3-x)Ge(x) solid solutions via mechanically induced self-sustained reactions
Cordoba, JM; Chicardi, E; Aviles, MA; Gotor, FJ
Intermetallics, **19** (2011) 1688-1692
DOI: 10.1016/j.intermet.2011.07.005

The complete range of Ti(5)Si(3)-Ti(5)Ge(3) solid solutions was synthesised from elemental mixtures of Ti, Si, and Ge under an inert atmosphere via mechanically induced self-sustaining reactions (MSR). The stoichiometry of Ti(5)Si(3-x)Ge(x) solid solutions was controlled by adjusting the Si/Ge ratio of the initial mixture. The chemical composition and lattice parameters of the materials confirmed that Ti(5)Si(3)-Ti(5)Ge(3) solid solutions with good chemical homogeneity could be produced via MSR.

Study of ground and unground leached vermiculite II. Thermal behaviour of ground acid-treated vermiculite
Perez-Rodriguez, JL; Maqueda, C; Murafa, N; Subrt, J; Balek, V; Pulisova, P; Lancok, A
Applied Clay Science, **51** (2011) 274-282
DOI: 10.1016/j.clay.2010.11.031

In this study, we examined the annealing effect on the material obtained after acid treatment of ground vermiculite which constituted amorphous silica and beta-FeOOH. The XRD patterns of the starting sample measured at temperatures from 30 to 1200 degrees C showed that the crystalline phase was present until similar to 300 degrees C; whereas the sample heated between 300 and 800 degrees C was practically amorphous. This is in agreement with previous observations that beta-FeOOH decomposes to amorphous or poorly crystalline phase, beta-Fe2O3, and transforms only slowly to crystalline alpha-Fe2O3. At 850 degrees C the sample showed the first signs of a crystalline phase which was fully developed at 1050 degrees C. The XRD, HRTEM and Mossbauer spectroscopy showed, after heating at 1050 degrees C, the presence of crystalline phase, consisting of quartz, cristobalite, alpha-Fe2O3 and epsilon-

Fe2O3. This effect showed in fact that well crystallized iron oxide nanoparticles embedded into the silica matrix are usually formed at relative high temperatures (similar to 1000 degrees C), which is in contrast to silica-free material. Element mapping of one particle of the composite obtained by annealing the sample at the highest temperature showed well-separated Fe2O3 and SiO2 particles in a composite material. Impurities of Al and Mg (from the original vermiculite) accompanied the silica components and TiO2 associated with Fe2O3 grains was also detected.

Intercalation and dynamics of hydrated Fe2+ in the vermiculites from Santa Olalla and Ojen
Lerf, A; Wagner, FE; Poyato, J; Perez-Rodriguez, JL
Journal Of Solid State Electrochemistry, **15** (2011) 223-229
DOI: 10.1007/s10008-010-1171-0

Although the intercalation of Fe3+ into layered phyllosicilicates-especially into smectites-attracted much attention in the past two decades, the information about Fe2+ loaded phyllosilicates is sparse. Here we present an investigation of the Fe2+ exchanged vermiculites from Santa Olalla and Ojén (Andalusia, Spain) by means of Mossbauer spectroscopy. The room temperature Mossbauer spectra are very similar to those of the starting compounds (Na forms) except for a decrease of the contribution of structural Fe3+ and a concomitant increase of the contribution of Fe2+ sites, indicating an internal redox process. The extent of this redox reaction is different for the two vermiculites. Thus, the intercalated Fe2+ acts as an electron mediator from the external medium to the structural Fe3+ ions. A new component attributable to intercalated Fe2+ is practically invisible in the room temperature Mossbauer spectra, but increases strongly and continuously during cooling to 4.2 K, where it is the dominant feature of the Mossbauer patterns. At 4.2 K, its quadruple splitting amounts to 3.31 mm/s, which is in excellent agreement with the quadrupole slitting of Fe2+ coordinated to six water molecules in a highly symmetric octahedral arrangement. The strong decrease of the Mossbauer-Lamb factor of this component with increasing temperature indicates a weak bonding of the Fe2+ in the interlayer space.

Influence of Al_2O_3 reinforcement on precipitation kinetic of Cu-Cr nanocomposite
Sheibani, S; Ataie, A; Heshmati-Manesh, S; Caballero, A; Criado, JM
Thermochimica Acta, **526** (2011) 222-228
DOI: 10.1016/j.tca.2011.09.024

In this paper, the kinetic of precipitation process in mechanically alloyed Cu-1 wt.% Cr and Cu-1 wt.% Cr/3 wt.% Al(2)O(3) solid solution was compared using differential scanning calorimetry (DSC), X-ray diffraction (XRD) and transmission electron microscopy (TEM). The ageing kinetics in Cu-Cr and Cu-Cr/Al_2O_3 can be described using Johnson-Mehl-Avrami (JMA) and Sestak-Berggren (SB) models, respectively. These different behaviors have been discussed in details. It was found that in presence of Al_2O_3 reinforcement, the ageing activation energy is decreased and the overall ageing process is accelerated. This behavior is probably due to higher dislocation density previously obtained during ball milling and Al_2O_3-Cu interface. TEM observations confirm that Al_2O_3-Cu interface and structural defects act as a primary and secondary nucleation sites, respectively.

ICTAC Kinetics Committee recommendations for performing kinetic computations on thermal analysis data

Vyazovkin, S; Burnham, AK; Criado, JM; Perez-Maqueda, LA; Popescu, C; Sbirrazzuoli, N
Thermochimica Acta, **520** (2011) 1-19
DOI: 10.1016/j.tca.2011.03.034

The present recommendations have been developed by the Kinetics Committee of the International Confederation for Thermal Analysis and Calorimetry (ICTAC). The recommendations offer guidance for reliable evaluation of kinetic parameters (the activation energy, the pre-exponential factor, and the reaction model) from the data obtained by means of thermal analysis methods such as thermogravimetry (TGA), differential scanning calorimetry (DSC), and differential thermal analysis (DTA). The recommendations cover the most common kinetic methods, model-free (isoconversional) as well as model-fitting. The focus is on the problems faced by various kinetic methods and on the ways how these problems can be resolved. Recommendations on making reliable kinetic predictions are also provided. The objective of these recommendations is to help a non-expert with efficiently performing analysis and interpreting its results.

Thermal analysis of monument patina containing hydrated calcium oxalates

Perez-Rodriguez, JL; Duran, A; Centeno, MA; Martinez-Blanes, JM; Robador, MD
Thermochimica Acta, **512** (2011) 5-12
DOI: 10.1016/j.tca.2010.08.015

This work describes the thermal transformation of patina samples formed on the surface of dolomitic rocks used to build the Romanesque Torme's Church (Burgos, Spain). Analyses were performed using a combination of high-temperature XRD, simultaneous TG/DTA and gas mass spectrometry. The XRD analysis revealed the presence of hydrated calcium oxalates. The following three steps were proposed for the thermal transformation of the raw material: dehydration of weddellite/whewellite to form calcium oxalate, transformation of calcium oxalate to calcium carbonate, and formation of calcium oxide produced via decomposition of the calcite. DTA/TG and mass spectrometry analyses confirmed this mechanism. In addition, a high proportion of organic compounds was detected and was possibly formed via degradation of products applied for the building's conservation by the action of microorganisms attack. Mass spectrometry analysis revealed CO (and CO_2) gas evolved during the transformation of CaC_2O_4 to $CaCO_3$. The CO_2 gas also appears at 765 degrees C due to the decomposition of calcium carbonate, and it appears over a large range of temperatures due to the decomposition of organic compounds. The TG analyses performed in a CO_2 atmosphere were used to determine the percentages of Ca and Mg contained in dolomite, and the calcium carbonate formed by oxalate decomposition. DRIFTS and mass spectrometry results revealed the presence of several aliphatic and/or aromatic compounds containing C=O groups.

Thermal study of unaltered and altered dolomitic rock samples from ancient monuments The case of Villarcayo de Merindad de Castilla la Vieja (Burgos, Spain)

Perez-Rodriguez, JL; Duran, A; Perez-Maqueda, LA
Journal Of Thermal Analysis And Calorimetry, **104** (2011) 467-474
DOI: 10.1007/s10973-011-1348-5

In this study, the decomposition behaviour of unaltered and altered dolomitic rock samples used in Cultural Heritage buildings was studied by simultaneous TG-DTA experiments at different atmospheres, X-ray diffraction in a high-temperature chamber, and evolved gas analysis. The components of dolomite rock samples and hydrated calcium oxalate formed during the alteration processes of the rocks were characterized, and the decomposition mechanisms of these components were determined. The TG-DTA experiments carried out at CO2 atmosphere were used to determine the carbonate compounds in the rock samples. The TG-DTA study characterized the presence of organic compounds formed during the biological degradation of the rock samples, possibly responsible of the hydrated calcium oxalate formation.

Analytical study of Roman and Arabic wall paintings in the Patio De Banderas of Reales Alcazares' Palace using non-destructive XRD/XRF and complementary techniques
Duran, A; Perez-Rodriguez, JL; de Haro, MCJ; Franquelo, ML; Robador, MD
Journal Of Archaeological Science, **38** (2011) 2366-2377
DOI: 10.1016/j.jas.2011.04.021

A portable XRD/XRF system and complementary laboratory techniques were employed to improve the knowledge of the procedures used to create Roman and Arabic wall paintings. Integrated physicochemical investigations were conducted on fragments of artworks collected from the archaeological excavation of the Patio de Banderas in the Reales Alcazares' Palace of Seville (Spain), and a comparative study on the pigments from both historical periods was performed. As a result, pigments such as vermilion, red ochre, yellow ochre, green earth, Egyptian blue, carbon and phosphor-based black pigments were detected in Roman samples; however, in the Arabic fragments, only haematite was observed. In addition, the size and shape of the particles of the wall paintings were studied with an XRD 2-dimensional detector and SEM-EDX.

Mechanochemical synthesis of $Ti_{1-x}Zr_xB_2$ and $Ti_{1-x}Hf_xB_2$ solid solutions
Aviles, MA; Cordoba, JM; Sayagues, MJ; Gotor, FJ
CERAMICS INTERNATIONAL, **37** (2011) 1895-1904
DOI: 10.1016/j.ceramint.2011.02.004

Solid solutions of TiB_2-ZrB_2 and TiB_2-HfB_2 were obtained under an inert atmosphere by high-energy ball-milling mixtures of Ti/Zr/B and Ti/Hf/B, respectively. Milling promoted mechanically induced self-sustaining reactions (MSR), and the ignition time was dependent on the initial composition of the mixture. The stoichiometry of $Ti_{1-x}ZrxB_2$ and $Ti_{1-x}Hf_xB_2$ solid solutions was controlled by adjusting the atomic ratio of the reactants. The solid solutions were characterised by X-ray diffraction, transmission electron microscopy, electron diffraction, and energy dispersive X-ray spectroscopy. The results revealed that TiB_2-ZrB_2 possessed a nanometric microstructure and good chemical homogeneity. However, in the TiB_2-HfB_2

system, an inhomogeneous solid solution was obtained when a Ti-rich mixture was employed. The solid solutions showed good thermal stability; thus, can be used as raw materials for the development of technological materials for structural applications.

Mechanochemical Synthesis of Visible Light Sensitive Titanium Dioxide Photocatalyst

Subrt, J; Criado, JM; Szatmary, L; Dianez, MJ; Murafa, N; Perez-Maqueda, LA; Brezova, V
International Journal Of Photoenergy, (2011) 156941
DOI: 10.1155/2011/156941

Phase transition of anatase nanoparticles into the phases TiO(2)-II and rutile under grinding was studied. The addition of ammonium carbamate to the reaction mixture inhibits the phase conversion and the cold welding of particles. The UV-visible absorption spectrum showed narrowing the band gap width after grinding with an ammonium carbamate additive resulting in shift of the light absorption of the ground sample towards the visible region. By EPR, intensive formation of OH(center dot) radical at irradiation of the sample with both UV (lambda > 300 nm) and visible (lambda > 435 nm) light was observed. High photocatalytic activity of the ground sample in visible light region was demonstrated also by measurement of kinetics of the photocatalytic decomposition of 4-chlorophenol.

Natural Earth Pigments From Roman and Arabic Wall Paintings Revealed by Spectroscopic Techniques

Garofano, I; Duran, A; Perez-Rodriguez, JL; Robador, MD
Spectroscopy Letters, **44** (2011) 560-565
DOI: 10.1080/00387010.2011.610655

Full identification of pigments used in wall paintings by Romans and Arabs that were recently discovered was achieved by the combined application of several spectroscopy methods. Identification of pigments was provided by the use of micro-Raman and FT-IR spectroscopy, while UV-Visible spectroscopy and chromatic studies permitted the authors to identify slight variations of hue attributed to mixtures of pigments. Natural earths and minerals were detected as the main pigments employed by both civilizations, although some differences were found between them. Red ochre, vermilion, yellow ochre, Egyptian blue, green earth, calcite, carbon, and possibly ivory blacks were identified in the Roman paintings. Only hematite and calcite were observed in the Arabic fragments.

Old and Modern Pigments Identification from a 14th Century Sculpture by Micro-Raman

Franquelo, ML; Duran, A; Arquillo, D; Perez-Rodriguez, JL
Spectroscopy Letters, **44** (2011) 464-468
DOI: 10.1080/00387010.2011.610401

The chromatic characterization of the external part of the sculpture showed homogeneity values in the majority of the colored zones. The optical microscopy study showed different layers in the painting cross-sections. The complex polychromy was attributed to several restoration processes carried out along the time. The composition of the different layers of painting cross-sections was studied using the micro-Raman technique. The micro-Raman technique was very useful in characterizing some pigments that are difficult to determine by other experimental techniques. The study showed the presence of several pigments that had been applied in ancient and recent times.

Synthesis and characterization of titanium-vanadium ternary nitride (TixV1-xN).
Roldan, MA; Alcala, MD; Ortega, A; Real, C
BOLETIN DE LA SOCIEDAD ESPANOLA DE CERAMICA Y VIDRIO, **50** (2011) 31-40
DOI: 10.3989/cyv.052011

Titanium-Vanadium nitride (TiVN) has been prepared from carbothermal reduction of corresponding oxides and also by direct nitridation of a mix of two metals employing the ATVC method. The characterization of the final product by X-ray diffraction, scanning electron microscopy, electron energy loss (EELS), and X-ray absorption spectroscopy (XAS) is presented. The synthesis of the ternary nitride has been possible in all range of composition and the final product is obtained with nanometric particle size and a high microhardness after sintering.

Characterization Of Materials And Conservation Proces Of The Colection Of Arabic Manuscript Documents Of Granada Archivo Historico-Provincial
Arias, TE; Stoytcheva, IL; Garcia, DC; Benito, AD; de Haro, MCJ
AL-QANTARA, **32** (2011) 519-532

This paper presents the main conclusions of our study of the Arabic documents preserved in the Archivo Historico Provincial of Granada. The analysis of the contents of each document, the materials and inks used in their support, and also the similarities of the page layout reveals the use of identical production protocols. Furthermore, this research also enables us to establish important similarities between the paper production processes in the latter stages of the Islamic rule in the Iberian Peninsula and the earlier stages of its incorporation in the Crown of Castilla - in particular in relation to how the archival documents were issued, both externally and internally.

ARTÍCULOS PUBLICADOS EN REVISTAS NO-SCI / PAPERS IN NON-SCI JOURNALS

Differences and similarities in the materials and techniques of medieval mural painting in the coastal region of Slovenia
A. Kriznar, A. Ruiz-Conde and P.J. Sánchez-Soto
e-Preservation Science (e-PS), 8 (2011) 62-67
ISSN: 1581-9280 (web edition) ISSN: 1854-3928 (print edition)

Premios Real Maestranza de Caballería y Real Academia Sevillana de Ciencias a investigadores jóvenes en su convocatoria de 2010
P.J. Sánchez-Soto
Químicos del Sur, 30 (2011) 18

Synchrotron radiation experiments in Spanish cultural heritage baroque materials: an overwiew
L.K. Herrera, A. Duran, A. Justo
Coalition, 21 (2011) 1579-8410

100 Preguntas, 100 Respuestas
Antonio Luis Agüí Palomo, Manuel María Domínguez Pérez, Rafael Marín Galvín, Fernando Muriel Azuaga, Rafael Pacheco Reyes, Juan Luis Pérez Bernal, Francisco Pérez Viguera, Concepción Real Pérez, Fernando Romero Guzmán, Joan Antoni Bas Carbonell, Josep María Fernández Novell
Andalucia Innova Especial Química, Febrero (2011) 1-39

De la Arcilla a la Cerámica: homenaje a Guillermo García Ramos, docente en Química e Investigador en Cerámica
Pedro José Sánchez Soto
Ed. Excmo. Ayuntamiento de Dos Hermanas, Delegación Municipal de Fiestas Mayores (Coordinación y Notas: P.S. Núñez), Editorial Mirte S.L.
Dos Hermanas Revista Cultural 2011, num. 68, (2011) 216-220
ISBN: 978-84-95591-41-8581-9280 (web edition) ISSN: 1854-3928 (print edition)

LIBROS Y OTRAS PUBLICACIONES / BOOKS AND OTHER PUBLICATIONS

Study of European ancient mirrors using micro diffraction techniques and Mössbauer spectroscopy
L.K. Herrera, A. Justo, A. Muñoz-Páez, J.L. Pérez-Rodríguez, A. Lerf, F.E. Wagner
En: Glass Science in Art and Conservation 2011, Fraunhofer Verlag (Eds. Sabrina Rota and Katrin Wittstadt) pp. 83-85
ISBN: 978-3-8396-0255-3

Las filitas: caracterización y aplicaciones
I.G. García Rodríguez
En: Las filitas: caracterización y aplicaciones, Universidd de Almería (Eds. P.J. Sánchez Soto y E. Garzón Garzón) 120 páginas
ISBN: 978-84-694-8485-2

Reconstrucción experimental de los procesos degradantes derivados de eflorescencias salinas en Cerámica
Lupión J.J., Arjonilla Mª, González J., Ruiz-Conde A., and Sánchez-Soto P.J.
En: Proceedings Book of 18th International Meeting on Heritage Conservation, Granada, Ed. Universidad de Granada, Sección Estudio Científico y Documentación, volumen 1, pp. 219-222
ISBN: 978-84-338-5339-4

Nuevas aportaciones al conocimiento de la loza dorada en Al-Andalus
Pascual Cosp J., Fernández de Miguel S., Díaz Monsalve J.A., Sánchez-Soto P.J.
En: Proceedings Book of 18th International Meeting on Heritage Conservation, Granada, Ed. Universidad de Granada, Sección Estudio Científico y Documentación, volumen 1, pp. 614-615
ISBN: 978-84-338-5339-4

CONGRESOS Y REUNIONES INTERNACIONALES / INTERNATIONAL CONGRESS AND MEETINGS

PARTICIPACIÓN EN LA ORGANIZACIÓN DE CONGRESOS Y REUNIONES / PARTICIPATION IN ORGANISING CONGRESSES AND MEETINGS

1st Central and Eastern European Conference on Thermal Analysis and Calorimetry
7 - 10 septiembre [Craiova, Rumania]
José Manuel Criado Luque [Miembro del “Honorific Committee”]

VII International Conference on Mechanochemistry and Mechanical Alloying
19 - 23 junio [Herzeg-Novi, Montenegro]
José Manuel Criado Luque [Miembro del “International Advisory Committee”]

COMUNICACIONES EN CONGRESOS Y REUNIONES / COMMUNICATIONS IN CONGRESS AND MEETINGS

I Congreso Internacional El Patrimonio Cultural y Natural como motor de desarrollo: investigación e innovación

26 – 28 enero [Jaén, España]

Interdisciplinary research on mural paintings (15-16th centuries) in the church ‘Nuestra Señora de Las Nieves (La Rinconada, Sevilla)’: Conservation state, cleaning and restoration
Antonio Ruiz Conde, G. Durán, María Arjonilla, J. Pascual, J.J. Lupión, M.A. González, Pedro J. Sánchez-Soto

Comunicación oral

TECHNART 2011

26 – 29 abril [Berlin, Alemania]

µ-XRD and µ-Raman Techniques for revealing the polychrome of a Spanish Gothic Sculpture
José Luis Pérez Rodriguez, Marisa Franquelo, Adrián Durán, D. Arquillo, J. Castaing
Comunicación oral

Glass Science in Art and Conservation GLASSAC11

10 - 12 mayo [Bronnbach Monastery, Alemania]

Study of European ancient mirrors using micro diffraction techniques and Mössbauer spectroscopy
L.K. Herrera, Angel Justo, Adela Muñoz-Paez, José Luis Perez-Rodriguez, A. Lerf, F.E. Wagner
Comunicación oral

4th International Congress of Energy and Environment Engineering and Management

26 - 27 mayo [Mérida, España]

Reuse of flyash from cogeneration of biomass for the production of new geopolymers
L. Pérez-Villarejo, S. Martínez, F.J. Iglesias, D. Eliche, Pedro J. Sánchez-Soto, Antonio Ruiz Conde
Poster

12th Conference of the European Ceramic Society

19 - 23 junio [Estocolmo, Suecia]

Preparation of Multiferroic $BiFeO_3$ perovskite by a direct mechanochemical process
Antonio Perejón, Pedro E. Sánchez-Jimenez, Luis A. Pérez-Maqueda, José Manuel Criado
Poster

9th International Conference in Preparation of Ceramic Materials

14 - 16 agosto [Herlany, República Eslovaca]

Nanocrystalline BaTiO3 prepared by high-energy ball milling
M. Fabian, K. L. da Silva, María Jesús Sayagues, Concepción Real Pérez, Francisco J. Gotor, J. Veres, L. Oroszova, J. Briancin
Poster

VII International Conference On Mechanochemical Alloying

31 agosto - 3 septiembre [Herzeg-Novi, Montenegro]

Synthesis of ZnSe by a mechanically-induced self-sustaining reaction: A case study for the ignition time dependence on milling parameters
M. Achimovicova, P. Balaz, Concepción Real Pérez, Francisco J. Gotor
Comunicación oral

Development of $Ti_xTa_{1-x}C_yN_{1-y}$ based cermets via a mechanically induced self sustaining reaction
Ernesto Chicardi, José Manuel Córdoba, Miguel Angel Avilés, María Jesús Sayagués, Francisco J. Gotor
Poster

Development of Cathodes ($La_{1-x}Sr_xMnO3_{\pm\delta}$) for solid oxide fuel cells by mechanosynthesis
María Jesús Sayagués, José Manuel Córdoba, Francisco J. Gotor
Poster

Properties of Machanochemically synthesized Bi_2S_3 nanoparticles
E. Dutkova, L.T akaccs, P. Baláz, J. Briancin, Concepción Real Pérez, María Jesús Sayagués
Poster

Proposal of a new mechanochemical phase diagram for the binary system Cu-Zn
Maria Jesús Diánez, José Manuel Criado, E. Donoso, Luis A. Pérez-Maqueda
Poster

Multiferroic Perowskite Materials obtained by reactive grinding
Antonio Perejón, Pedro E. Sánchez-Jiménez, María Jesús Diánez, José Manuel Criado, Luis A. Pérez Maqueda
Poster

Thirteenth Annual Conference YUCOMAT 2011

5 - 9 septiembre [Herzeg-Novi, Montenegro]

Mechanochemical synthesis and characterization of II-IV nanocrystals: challenge for cytoxicity issues
P. Balaž, R. Jardin, G. Mojžišova, J. Mojžiš, E. Dutkova, María Jesús Sayagués, E. Turianicova, Balaž
Poster

Mechanochemical Synthesis and Characterisation of Nanocrystalline Bismuth Selenides (BiSe, Bi_2Se_3)
M. Achimovicova, Concepción Real Pérez, Francisco J. Gotor, N. Daneu
Poster

1st Central and Eastern European Conference on Thermal Analysis and Calorimetry

7 - 10 septiembre [Craiova, Rumania]

New experimental methods and analysis procedure for kinetic analysis of solid state processes
Luis A. Pérez-Maqueda, José M. Criado, Antonio Perejón, Pedro E. Sánchez-Jiménez, María Jesús Diánez
Conferencia Invitada

Development of several thermoanalytical devices for the synthesis of materials by means of the Sample Controlled Thermal Analysis
J.M. Criado, M.J. Diánez, L.A. Pérez-Maqueda, A. Perejón, P.E. Sánchez-Jiménez
Comunicación oral
Advanced linear local kinetic methods for the in-depth characterization of heterogeneous processes
A. Rotaru, M. Gosa, Luis A. Pérez-Maqueda, José M. Criado
Comunicación oral

A new point of view for approaching the Arrhenius integral leading to accurate values of the activation energy from a linear plot of ln p(x) as a function of 1/T
José M. Criado Luis A. Pérez-Maqueda, Antonio Perejón, Pedro E. Sánchez-Jiménez
Poster

11th Inter-American Congress on Microscopy. CIASEM 2011

25 - 29 septiembre [Mérica Yucatán, México]

Influence of Aging on the structure and mechanical properties of a Cu10Ni5,5Sn alloy
E. Donoso, María Jesús Diánez, José Manuel Criado, Antonio Perejón, María Jesús Sayagués, Luis A. Pérez Maqueda
Poster

VI Congreso Latinoamericano de Biología, Física y Química Ambiental

11 - 15 octubre [Perú]

Formulaciones de Liberación Lenta del Herbicida Metribuzina Basadas en Geles de Minerales de la Arcilla
Celia Maqueda, E. Morillo, José Luis Pérez-Rodriguez
Poster

VI Iberian Congress of Agricultural Engineering, VI Congreso Ibérico de Agro-Engenharia, VI Congreso Ibérico de Agroingeniería

18 - 20 octubre [Evora, Portugal]

Procedimiento de planificación de recogida y flujo de los residuos de construcción y demolición
E. Garzón, A. Sabio, Pedro J. Sánchez-Soto
Poster

2nd Joint Congress of the Portuguse and Spanish Microscopy Societies: Micros copy at the frontiers of science

18 - 21 octubre [Aveiro, Portugal]

Microstructural analysis of components for SOFCs based on $La1-xSrxMnO3\pm\delta$ ($0\leq x\leq 1$) system obtained by mechanochemistry
María Jesús Sayagués, José Manuel Córdoba, F. J. Gotor
Poster

Microstructural characterization of silver nanoparticles for biomedical applications
A. P. Zaderenko, P.M. Castillo, M. de la Mata, Maria Jesús Sayagués, J.A. Sánchez
Poster

Microstructural characterization of silver nanoparticles for bioimaging applications
A.P. Zaderenko, C. Caro, M. de la Mata, J.A. Sánchez, María Jesús Sayagués
Poster

18th International Meeting on Heritage Conservation

9 - 11 noviembre [Granada, España]

Reconstrucción experimental de los procesos degradantes derivados de eflorescencias salinas en Cerámica
J.J. Lupión Alvarez, María Arjonilla Alvarez, J. González, Antonio Ruiz Conde, Pedro J. Sánchez-Soto
Poster

Nuevas aportaciones al conocimiento de la loza dorada en el Al-Andalus
J. Pascual Cosp., S. Fernández de Miguel, J.A. Diaz-Monsalve, Pedro J. Sánchez-Soto
Poster

IV Spanish-Portuguese Glass and Ceramic Congress, IV Congreso Luso-Espanhol de Cerâmica e Vidro y LI Congreso de la Sociedad Española de Cerámica y Vidrio

16 - 18 noviembre [Aveiro, Portugal]

Development of multicomponent-multiphase materials based on (Ti, Ta, Nb)$CxN1-x$ carbonitride solid solutions
José Manuel Córdoba, Enersto Chicardi, María Jesús Sayagués, Francisco J. Gotor
Comunicación oral

Síntesis de materiales compuestos del sistema Ti-B-C-N de interés para aplicaciones en ambientes extremos
Francisco J. Gotor, María Jesús Sayagués, Miguel Angel Avilés, José Manuel Córdoba, Ernesto Chicardi, Pedro J. Sánchez-Soto
Poster

Consolidation of $Ti_yTa_{1-y}C_{0.5}N_{0.5}$ based cermets by spark plasma sintering
José Manuel Córdoba, Ernesto Chicardi, María Jesús Sayagués, Rosalía Poyato, Francisco J. Gotor Martínez
Poster

Effect of sintering time on the microstructure and mechanical properties of (Ti, Ta) (C, N) based cermets
Ernesto Chicardi, Y. Torres, José Manuel Córdoba, J. A. Rodríguez, María Jesús Sayagués, Francisco J. Gotor
Poster

Effect of the binder content, additives and sintering time on the solubility of (Ti) (C, N) based cermets
José Manuel Córdoba, Ernesto Chicardi, María Jesús. Sayagués, Francisco J. Gotor
Poster

Azul egipcio vs. Azul esmalte. La influencia de su manufactura
M.T. Rodríguez García, Pedro J. Sánchez-Soto
Poster

Caracterización de pigmentos cerámicos y soportes en obras del Patrimonio
Antonio Ruiz Conde, M.A. González, Pedro J. Sánchez-Soto
Poster

Planificación de recogida y flujo de residuos sólidos de construcción y demolición, hormigón, cerámica y otros, mediante utilización de una herramienta informatizada para su gestión sostenible
A. Sabio, E. Garzón, Pedro J. Sánchez-Soto
Poster

Estudio del ensanchamiento preferencial de los perfiles de difracción de rayos X en pigmentos de hematites obtenidos a partir de limonita
Juan Carlos González, A. Bustamante, Antonio Ruiz Conde, Pedro J. Sánchez-Soto
Poster

Materiales cerámicos y refractarios de forsterita: una revisión sobre procedimientos de preparación
Pedro J. Sánchez-Soto, Antonio Ruiz Conde, Francisco J. Gotor, E. Garzón, J. Pascual
Poster

Congresos y Reuniones Nacionales / National Congress and Meetings

VII Congreso "la investigación ante la sociedad del conocimiento" Sostenibilidad y medioambiente

9 - 11 noviembre [Alcoy, Alicante, España]

Nuevos métodos eficientes de calentamiento en tecnología de materiales
Luis A. Pérez Maqueda
Conferencia Invitada

VI Congreso Nacional del Órgano Hispano

2 - 6 diciembre [Valladolid, España]

El Órgano de la Seo de Zaragoza: Notas sobre su historia, restauración y composición material
A. Justo-Estebaranz, O. Laguna, L. K. Herrera, A. Durán, B. Sigüenza, M.C. Jiménez de Haro, y A. Justo
Comunicación oral

Formacion / Training

Tesis Doctorales/ Doctor Degree Thesis

Título: **Conservación-Restauración de los materiales cerámicos aplicados en Arquitectura. Factores, mecanismos e indicadores de alteración: degradación por sistemas salinos**
Autor: Juan José Lupión Alvarez
Directores: Mª Arjonilla Alvarez y Pedro J. Sánchez Soto
Calificación: Apto "Cum Laude" por unanimidad
Centro: Universidad de Sevilla

Título: **Prospección, caracterización y mejora de las propiedades de las filitas**
Autor: Isabel Gádor García Rodríguez
Directores: Pedro J. Sánchez Soto y E. Garzón Garzón
Calificación: Apto "Cum Laude" por unanimidad
Centro: Universidad de Almería

Título: **Metodología microanalítica integrada para estudios científicos no invasivos en Patrimonio Histórico Andaluz**
Autor: María Luisa Franquelo Zoffmann
Directores: José Luis Pérez Rodríguez, Adrián Durán Benito
Calificación: Apto “Cum Laude” por unanimidad
Centro: Universidad de Sevilla

Formación de Graduados / Master Degree Thesis

Título: **Síntesis de materiales cerámicos no oxídicos a partir de la descomposición de precursores poliméricos**
Autor: Cristina García Garrido
Directore: Luis A. Pérez Maqueda y Pedro E. Sánchez Jiménez
Grado: Trabajo Fin de Master
Centro: Universidad de Sevilla
Año Académico: 2010-2011

Equipamiento Científico Available Equipment

- Microdurómetro FM700 Future-Tech
- Máquina de ensayo universal AGS-J, Shimadzu
- 3 Termobalanzas CI Electronics
- Dilatómetro diferencial ADAMEL LHOMARGY DI-24
- 2 molinos planetarios PULVERISETTE 7 (Fritsch)
- 1 molino planetario PULVERISETTE 7 Premium Line (Fritsch)
- 1 molino planetario PULVERISETTE 4 (Fritsch)
- 1 molino planetario PM100 (Retsch)
- 1 molino vibratorio MM301 (Retsch)
- 1 molino vibratorio SPEX 8000
- 1 molino centrífugo PULVERISETTE (Fritsch)
- 1 molino de atrición O1HD (Union Process)
- Calorímetro SETARAM differential scanning DSC 111
- Horno horizontal alta temperatura 1800ºC AGNI
- Horno horizontal alta temperatura 1600ºC Carbolite
- Horno horizontal 1200ºC Carbolite
- Microcortadora metalográfica manual EVOLUTION (REMET)
- Microcortadora metalográfica MICROMET (REMET)
- Prensa automática metalográfica IPA30 (REMET)
- Pulidora automática LS2 (REMET)
- Analizador Termomecánico TMA 1000 (Linseis)
- Calorímetro diferencial de barrido DSC (TA instruments Q200)

MATERIALES FUNCIONALES NANOESTRUCTURADOS
NANOSTRUCTURED FUNCTIONAL MATERIALS

PROYECTOS DE INVESTIGACIÓN / RESEARCH PROJECTS

El destino del material subducido
Crust to core: The fate of subducted material

Código/Code:	MRTN-CT-2006-035957
Periodo/Period:	01-7-2006 / 31-01-2011
Organismo Financiador/Financial source:	Unión Europea
Importe total/Total amount:	219.122 €
Investigador responsable/Research head:	Ana Isabel Becerro Nieto
Componentes/Research group:	Universidad de Bayreuth (Alemania), Universidad de Milán (Italia), University College London (Reino Unido), Geological Survey of Norway (Noruega), Universidad Pierre et Marie Curie, París (Francia), Friedrich Schiller Universitat Jena (Alemania), UniverzitaKarlova V Praga (República Checa)

RESUMEN / ABSTRACT

Uno de los procesos más interesantes y determinantes de la dinámica y la química de la Tierra es el transporte de material desde su superficie hacia el interior. Este fenómeno, que tiene lugar en los límites de placas convergentes, se encuentra relacionado no sólo con la tectónica de placas sino también con la formación de terremotos y volcanes, así como con la evolución química de la atmósfera terrestre. A pesar de la importancia del fenómeno de la subducción, existen muchos aspectos de la misma escasamente estudiados hasta la fecha, de manera que el avance en su comprensión requiere la integración de varias subdisciplinas de la Geología, así como la integración de campos científicos próximos. Para solucionar dicha fragmentación y avanzar en el conocimiento básico del proceso de subducción, hemos formado una red europea que combina los recursos y experiencia en petrología, mineralogía experimental y teórica, y el análisis, síntesis y estudios dinámicos del interior de la Tierra.

At convergent plate boundaries material is transported from the Earth's surface to its interior; this is one of the central processes in the solid Earth, determining its dynamic, chemical, and thermal evolution. It is linked to a wide range of surface features, ranging from plate tectonics to earthquakes and volcanoes to the chemical evolution of the Earth's atmosphere.Despite this importance many aspects of the subduction process and associated material fluxes are poorly understood to date, and advances in understanding require the integrated efforts of many sub-disciplines in the Earth sciences as well as integration of neighbouring fields. To overcome the fragmentation and advance the basic understanding of the subduction process we form a European network which combines unique facilities and expertise in petrology, experimental and computational mineralogy, analysis, synthesis, and dynamic studies of the Earth's interior.

Unión Europea
Fondo Europeo de Desarrollo Regional
"Una manera de hacer Europa"
MINISTERIO DE CIENCIA E INNOVACIÓN

Estudio de Materiales modificados superficialmente mediante Reflexafs SURCOXAFS

Study of Surface modified materials and coatings by ReflEXAFS SURCOXAFS

Código/Code:	MAT2008-06652
Periodo/Period:	01-01-2009 / 31-12-2011
Organismo Financiador/Financial source:	Ministerio de Ciencia e Innovación
Importe total/Total amount:	54.450 €
Investigador responsable/Research head:	Muñoz Páez, Adela

RESUMEN / ABSTRACT

La espectroscopia de Absorción de Rayos X en modo reflexión, ReflEXAFS, es una técnica novedosa que proporciona la información característica del EXAFS, estructura del entorno local del elemento absorbente, junto con la obtenida por medidas de reflectometría, tales como rugosidad, espesor de capa o densidad. Todo ello focalizado en la zona próxima a la superficie, proporcionando además la posibilidad de controlar el espesor analizado en función del ángulo de incidencia del haz, en el rango de 20 a 200 Å. Asimismo, y a diferencia de otras espectroscopias superficiales como XPS, permite acceder a capas "enterradas". Por ello es muy útil para el estudio de materiales con propiedades singulares en su superficie, tales como los modificados superficialmente y los obtenidos por deposición de capas finas. Habiendo desarrollando los protocolos de medida en proyectos previos, se propone la aplicación de la técnica a sistemas reales de dos tipos: aceros modificados superficialmente mediante nitruración y materiales formados por capas finas mixtas con propiedades ópticas y magnéticas singulares. Aparte del interés intrínseco de la técnica y de los sistemas objeto de estudio, este proyecto tiene relevancia en el marco del desarrollo de la espectroscopia XAS en relación con la línea española del ESRF, SPLINE, y de la nueva fuente española de radiación sincrotrón ALBA.

X-ray Absorption spectroscopy in reflection mode, ReflEXAFS, is a novel technique yielding the typical information from EXAFS, local structure around de absorbing atom, together with that obtained from reflectometry, such as roughness, layer thickness or density within the near surface region. The technique has also the capability of controlling the thickness of the region probed simply by changing the incidence angle, within a rather interesting range, 20-200 Å. Moreover, in contrast with other surface spectroscopic techniques, such as XPS, it allows the study of buried layers. For all these reasons, it is a useful tool to provide structural information of surface materials, such as those with thin layer structure, coatings and surface modified bulk materials. In previous projects we developed measurement protocols for this technique at using model sample. Herewith we propose to apply the technique to real systems of two types: surface modified steels by nitriding treatments and materials made of mixed thin layers with optic and magnetic properties. Apart form the intrinsic interest of the technique itself and the systems which are going to be prepared and studied, this project is relevant in the framework of the development of XAS-based techniques of potential application in the Spanish beamline at the ESRF, SPLINE, as well as in the new Spanish synchrotron source, ALBA.

Unión Europea
Fondo Europeo de Desarrollo Regional
"Una manera de hacer Europa"
MINISTERIO DE CIENCIA E INNOVACIÓN

Láminas delgadas porosas funcionales y nanoestructuras 1D soportadas de óxidos para el desarrollo de microfluídica en lámina delgada, válvulas fotónicas y micro plasmas (POROUSFILMS) Functional porous thin films and 1D supported oxide nanostructures for the development of thin film microfluidics, photonic, valves, and microplasmas (POROUSFILMS)

Código/Code:	MAT2010-18447
Periodo/Period:	01-01-2011 / 31-12-2013
Organismo Financiador/Financial source:	Ministerio de Ciencia e Innovación
Importe total/Total amount:	278.300 €
Investigador responsable/Research head:	Francisco Yubero Valencia
Componentes/Research group:	Agustín R. González-Elipe, Juan Pedro Espinós Manzorro, Alberto Palmero Acebedo, Rafael Alvarez Molina, Juan Carlos González González, Victor J. Rico Gavira, Jorge Gil Rostra, Ana Isabel Borrás Martos, Lola González García, José Cotrino Bautista

RESUMEN / ABSTRACT

En este proyecto se prepararán láminas delgadas de TiO_2, ZnO, SiO_2 y SnO_2 dopado, así como nanostructruras de fibras soportadas de estos óxidos mediante deposition por plasma y por evaporación a ángulo rasante (GLAD). Se controlará la nano- y micro-estructura de las capas y fibras mediante la selección de las condiciones adecuadas de deposición usando GLAD y, en el caso de la deposición mediante plasma, tras ajustar y modelizar el plasma y sus principales parámetros de operación, así como los fenómenos ligados a la vaina del plasma y su influencia en el desarrollo de la nanoestructura de las capas y fibras. El primer objetivo del proyecto es conseguir controlar la porosidad y otras propiedades críticas (ópticas, conductividad eléctrica, comportameinto frente al mojado, etc.) de los materiales sintetizados para propiciar el desarrollo de nuevos métodos de manejo de fluidos (líquidos y gases) a escalas micro y, posiblemente, nanométricas de manera de inventar y desarrollar aplicaciones en los campos de microfuídica y microplasmas.

Un objetivo adicional es el procesado de estas estructuras tanto en una aproximación 2D (procesado litográfico) como 3D mediante el uso de técnicas basadas en láser, el apilamiento en multicpas de diferentes estrucuras de capas finas porosas y/o la deposición selectiva de zonas hidrofóbicas de otros materiales tales como polímeros, siliconas, etc. A partir de estas estructuras se desarrollarán dispositivos microfluídicos basados en láminas delgadas porosas de TiO2 y ZnO activadas con luz (válvulas fotónicas). Estos materiales se vuelven superhidrofílicos cuando se iluminan con luz de $\lambda<390$ nm que, usada para iluminar ciertas áreas pequeñas del material (canales, circuitos micrométricos, etc.) usando lámparas adecuadas o un láser, permitirá activar selectivamente esas zonas. El desarrollo de microfiltración controlada por luz es otra nueva aplicación en este campo que debe permitir la difusión/filtración preferente de

líquidos polares a través de las zonas iluminadas (válvula abierta). Conseguir una rápida reversión de este proceso (válvula cerrada) is otro reto que se abordará dentro del proyecto.

Un objetivo final de carácter exploratorio es el modelado, diseño y desarrollo de microplasmas basados en las estrucutras porosas en forma de capa delgada desarrolladas durante las etapas iniciales del trabajo. Estos prototipos de microplasmas estarán formados por electrodos de capas porosas de SnO_2 dopadas permeables a gases y capas aislantes porosas de SiO2 que actuarán como barreras de separación. La evaluación de las caracterísitcas del plasma en estos dispositivos prototipo será una acción addicional que se abordará en el proyecto.

Functional TiO_2, ZnO, SiO_2 and doped SnO_2 in the form of porous thin films and other supported fiber-like nanostructures will be prepared by plasma deposition and evaporation at glancing angles (GLAD). Precise control of the nano and microstructure of the films and fibers will be attained by selecting appropriate GLAD deposition conditions and, in the case of plasma deposition, by adjusting the principal plasma parameters after modelling the plasma processes and sheath-related phenomena that control the development of the film/fibers nanostructure. The primary objective of the project is to successfully tailor the porosity and other key properties (optical, electrical conductivity, wetting behaviour etc.) of the synthetized materials to enable novel methods of fluid handling (liquids and gases) at the micro and, possibly, nanoscales so as to invent and develop applications in the fields of microfluidic and microplasmas.

A further objective is the processing of these structures in both 2D (i.e., lithographic processsing) and 3D by use of laser-based techniques, multilayer stacking of different porous thin film structures and/or selected plasma deposition of hydrophobic patches of other materials such as polymers, silicones, etc. Microfluidic thin film-based devices controlled by light (i.e., photonic valves) will then be developed by employing appropriately designed TiO_2 and ZnO porous structures. These materials become superhydrophilic when illuminated with light of $\lambda<390$ nm which will be used to selectively illuminate very small areas (channels, micrometer circuits, etc.) by either a suitable lamp or a laser. Light-controlled microfiltration is envisaged as another new application in this field, whereby preferential diffusion/filtration of polar liquids through the illuminated zones may be induced (i.e. valve open). Achieving prompt reversal of this process (i.e. valve closed) is another challenge that will be addressed by the project.

A final, exploratory objective is the modelling, design and development of microplasmas based on the most promising thin film porous structures developed during the earlier phases of the work. These prototype microplasma devices will consist of porous doped SnO_2 thin film electrodes permeable to gases with porous insulator layers (SiO_2) acting as separation barriers. Evaluation of the plasma characteristics of these prototype devices will be another distinct task undertaken by the project.

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Control del la Absorción y la Emisión Ópticas de Nanomateriales en Cristales Fotónicos Control of Optical Emission and Absorption Properties of Nanomaterials in Photonic Crystals

Código/Code:	MAT2008-02166
Periodo/Period:	01-01-2009 / 31-12-2011
Organismo Financiador/Financial source:	Ministerio de Ciencia e Innovación
Importe total/Total amount:	242.000 €
Investigador responsable/Research head:	Míguez García, Hernán R.
Componentes/Research group:	Ocaña, M., Calvo, M., Nuñez, N., Mihi, A., Lozano, G., Colodrero, S., Hidalgo, N., Sánchez, O.

RESUMEN / ABSTRACT

En este proyecto se estudiarán las modificaciones que tienen lugar tanto en la absorción como en la emisión ópticas de nanomateriales de diverso tipo (nanopartículas dopadas con tierras raras, nanopartículas semiconductoras, films de colorantes organicos de grosor nanométrico) por el hecho de encontrarse éstos formando parte de una estructura de cristal fotónico. El estudio se realizará tanto desde el punto de vista fundamental como aplicado, centrándose en materiales que tengan interés en distintos campos de la tecnología actual. La motivación principal de este proyecto desde el punto de vista aplicado radica en la posibilidad de modificar controladamente estos procesos de absorción y emisión, de tal modo que puedan inhibirse o amplificarse según convenga a un fin determinado. En concreto, se pretende poner en práctica estos nuevos fenómenos para el diseño de células solares más eficientes, capaces de recolectar una mayor cantidad de la radiación incidente, y en el desarrollo de films para sensores sensibles a modificaciones de distinto tipo en su entorno, tales como presencia de analitos de distinto tipo, variaciones en la presión del vapor ambiente, etc.... En su aspecto más fundamental, nuestra propuesta ahonda en el análisis de la interacción entre luz y materia en sistemas en los que existe una fuerte dispersión y anisotropía de la constante dieléctrica, y en los que es posible obtener bajas velocidades de propagación de fotones. Para este análisis se emplearán cristales fotónicos con orden tridimensional como matrices en los que se infiltrará una gran variedad de nanomateriales tanto orgánicos como inorgánicos en diferentes configuraciones y cuya absorción y emisión serán estudiadas.

In this project the modifications of both optical emission and absorption of nanomateriales of different sort (rare earth doped nanoparticles, semiconductor quantum dots, and films of organic dyes of nanometer dimensions) that occur when they are embedded in a photonic crystal structure. Both fundamental and applied aspects of the subject will be analysed, efforts being focused on materials of current technological interest. From the applied point of view, this project finds its motivation in the possibility that photonic crystal offer of modifying those absorption and emission processes in a controlled manner so that they can be inhibited or amplified depending on the specific goal pursued. Particularly, we seek to put into practice these concepts to generate new designs of more efficient solar cells, capable of harvesting a larger amount of the incident radiation, and in the development of films for sensing devices sensitive to modifcations of different kind, such as presence of targeted molecules,

variations of ambient gas pressure, etc... In its more fundamental aspect, our project aims at deepening our knowledge of the interaction between light and matter in systems in which there exists a strong dispersion and anisotropy of the dielectric constant, and in which it is possible to attain very low photon propagation speeds. For this analysis, we will employ photonic crystals with three dimensional order as hosts in which a wide range of organic and inorganic nanomaterials will be integrated in different configurations and whose absorption and emission will be experimentally and theoretically studied.

Funcionalización superficial de materiales para aplicaciones de alto valor añadido (FUNCOAT) Surface functionalisation of materials for high added value applications (FUNCOAT)

Código/Code: CSD2008-00023 (Consolider)
Periodo/Period: 15-12-2008 / 15-12- 2013
Organismo Financiador/Financial source: Ministerio de Ciencia e Innovación
Importe total/Total amount: 420.000 €
Investigador responsable/Research head: González-Elipe, A.R.
Componentes/Research group: Fernández Camacho, A., Espinós, J.P., Yubero, F., Cotrino, J., Sánchez López, J.C., Barranco, A., Palmero, A., Rojas, C., A. Borrás

RESUMEN / ABSTRACT

FUNCOAT es un proyecto integrado dentro de la convocatoria CONSOLIDER-INGENIO 2010 que persigue explotar las sinergias existentes entre la comunidad científica española en materiales, teniendo como objetivo general el desarrollo de nuevos métodos y la optimización de procedimientos de funcionalización superficial de materiales para la mejora de sus propiedades. El proyecto integra a 14 centros de investigación diferentes, que cubren desde aspectos básicos y teóricos hasta diversas aplicaciones finales. Esta integración de esfuerzos es crítica para lograr avances sustanciales en este campo, más allá que la mera acumulación de resultados. Los grupos de investigación pertenecen a diversas Universidades, CSIC (organismo que actúa como gestor del proyecto) y centros tecnológicos, y presentan relaciones científicas que, en algunos casos, se remontan hasta hace 15 años. Objetivos científico-técnicos parciales son: la comprensión de los fenómenos fundamentales que rigen la modificación de superficies y crecimiento de capas, el control micro y nanoestructural de superficies y capas delgadas, la optimización de los procesos de crecimiento de las capas, la obtención de superficies modificadas con características multifuncionales con aplicaciones en diversos campos (protección mecánica, óptica, magnetismo, biomateriales, energía, etc) y, finalmente, el desarrollo de nuevos dispositivos y aplicaciones de los materiales funcionales en sectores tecnológicos clave. Otros objetivos horizontales, relacionados con los anteriores, son la formación de investigadores en técnicas y métodos de funcionalización y el desarrollo de una transferencia tecnológica eficaz a los sectores productivos. Sectores estratégicos clave en los que las actividades de FUNCOAT inciden con mayor impacto son la metalurgia, vidrio, plásticos, sensores, salud y

energía. El proyecto se estructura en torno a los ejes de actividad siguientes que deben permitir la mejor coordinación de los esfuerzos y la integración de las distintas actividades de los grupos. A) Fenómenos básicos de superficies, intercaras y láminas delgadas, B) Nuevos procesos para el control de la micro- y nano- estructura superficiales, C) Recubrimientos mecánicos y metalúrgicos para protección superficial, D) Funcionalización química de superficies y aplicaciones biomédicas, E) Recubrimientos para aplicaciones ópticas y control eficiente de captación energía solar, F) Nuevos fenómenos magnéticos en superficies e interfases.

FUNCOAT is an integrated project within the application call CONSOLIDER-INGENIO 2010 aiming at the exploitation of synergies existing in the Spanish scientific community, with the general objective of developing principles, processes and devices related to the surface functionalisation of materials. The project integrates 14 well-accredited research centres covering from fundamental and theoretical aspects to final applications. This large effort of integration is critical to achieve substantial advances in this broad field, which go beyond the mere accumulation of results. The research teams belong to different institutions: University, CSIC (responsible for the management of the project) and Technological centres. They maintain scientific relationships among them that extend over the last 15 years. Specific scientific and technological objectives are: understanding of fundamental phenomena driving the modification of surfaces and interfaces, control of the micro- and nano- structure of surfaces and thin films, optimization of thin film deposition methods, process development of multifunctional surfaces for novel applications (mechanical and metallurgical, optical, magnetic, energy, biomaterials, etc) and, finally, the production of new devices based on functionalised surfaces. Other important objectives include the technological transfer of the scientific results to the productive sectors as well as the education and training of scientists, young researchers and engineers. Strategic sectors of our modern society where the activities of FUNCOAT find a direct impact are material processing, energy, environment, health care, agriculture, etc. In order to accomplish an efficient coordination of efforts and the integration of the activities of all the groups, the project is structured around six workpackages: A) Fundamental phenomena in surfaces, interfaces and thin films, B) New processes for the control of the micro- and nano-structure of films and surfaces, C) Mechanical and metallurgical coatings for surface protection, D) Chemical functionalisation and biomedical applications, E) Coatings for optical control, photonic applications and solar energy collection and F) Novel magnetic phenomena in surfaces/interfaces.

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Síntesis mediante plasma CVD de nuevos materiales orgánicos nanoestructurados integrado en dispositivos planares para aplicaciones como sensores fotónicos y de marcaje de seguridad NANOPLASMA

Plasma CVD synthesis of novel organic nanostructured materials integrated in planar devices for photonic sensing and security applications NANOPLASMA

Código/Code: MAT2010-21228 (Plan Nacional)

Periodo/Period: 01-01-2011 / 31-12-2013
Organismo Financiador/Financial source: Ministerio de Ciencia e Innovación. Programa Fondos FEDER Unión Europea.
Importe total/Total amount: 169.4000 €
Investigador responsable/Research head: Angel Barranco Quero
Componentes/Research group: Ana Borrás Martos, Agustín R. González-Elipe, Juan Pedro Espinós, José Cotrino, Carmen Ruiz, M. Carmen López-Santos, Ricardo Molina

RESUMEN / ABSTRACT

En NANOPLASMA se propone el desarrollo de nuevas técnicas basadas en plasmas para la síntesis y procesado de nuevos materiales funcionales orgánicos. La tecnología de plasma para síntesis de materiales actualmente en uso, como el CVD activado por plasma (PECVD) o los procesos de polimerización por plasma, implica siempre la fragmentación completa de un precursor volátil. En contraste NANOPLASMA persigue la síntesis de una nueva familia de materiales luminiscentes en forma de película delgada o nanocables 1D soportados, mediante el control químico y del proceso de fragmentación en la zona remota de una descarga de plasma. La investigación se centrará en la síntesis de matrices orgánicas con microestructura nanométrica controlada que incorporan moléculas orgánicas luminiscentes (por ejemplo perilenos, rodaminas, ftalocianinas y porfirinas) y nanocables orgánicos 1D a partir del mismo tipo de moléculas.

El proyecto también contempla el desarrollo de metodologías basadas en procesos de etching por plasma y ablación láser, para la fabricación de patrones litográficos 2D a partir de las láminas delgadas y las nanoestructuras soportadas. La investigación se contempla con estudios básicos encaminados al desarrollo de procesos de “patterning químico” basados en procesos de funcionalización superficial mediante plasmas y de derivatización química de monocapas autoensambladas. Tanto la metodología sintética mediante plasmas remotos como los procesos de microstructuración son totalmente compatibles con la tecnología optoelectrónica actual y la tecnología microelectrónica. Ambos procesos, por tanto, pueden llevarse a cabo a escala de oblea de silicio (wafer scale) y escalarse a procesos de fabricación industrial efectivos.

Estos materiales y procesos se emplearán en la fabricación de dos tipos de dispositivos a escala de prototipo como son: los sensores de gases fotónicos y las microestructuras luminiscentes para aplicaciones de marcado inteligente. Los sensores de gases consistirán en una lámina o estructura luminiscente integrada en un cristal fotónico 1D diseñados de acuerdo a las propiedades ópticas y la longitud de onda de la emisión luminiscente de la capa sensora correspondiente. Los dispositivos de marcado inteligente consistirán en patrones litográficos complejos construidos a partir de láminas o multicapas luminiscentes con funcionalidades específicas e, incluso, respuesta ambiental o sensora no desarrollada por ninguna otra tecnología hasta la fecha.

NANOPLASMA proposes the development of novel techniques based on plasma for the synthesis and processing of new organic functional materials. In contrast with the established plasma technology used in plasma enhanced CVD and plasma polymerization that implies the complete fragmentation of volatile precursor molecules, NANOPLASMA processes achieve the synthesis of new families of fluorescent thin films and supported 1D nanomaterials by control-

ling the chemistry and fragmentation degree at the boundaries of plasma discharge. The research focuses in the synthesis of organic matrices with a well controlled nanometric microstructure incorporating luminescent dye molecules (i.e. perylenes, rhodamines, phtalocyanines y porphirins) and 1D luminescent organic nanowires formed by similar molecules.

The project also contemplates the development of methodologies based on the plasma etching and laser ablation for the production of 2D lithographic patterns of the luminescent thin films and nanostructures. The research in this line will be completed with basic studies aiming the development of a “chemical patterning” process based on the plasma surface functionalization and chemical derivatization of self-assembled monolayers. Both the synthetic methodologies and the patterning strategies of NANOPLASMA are fully compatible with the present optoelectronic and silicon technologies and can be adapted to wafer scale integration for mass scale production.

These materials and processes will be used for the fabrication of two types of prototype devices: photonic gas sensors and luminescent microstructures for intelligent labelling applications. The gas sensing devices consist of a luminescence film and/or structure integrated onto a 1D photonic crystal with a stacking defect designed and constructed to couple the luminescent signal of the sensor layer. The intelligent labelling devices are patterned lithographic structures made on single or multilayer structures of luminescence films with specific functionalities and environmental responses not achieved by any available technology.

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Materiales mesoporosos (HA-SBA-15) funcionalizados con una proteína rhBMP-2 con afinidad por colágeno y sus estructuras híbridas con colágeno para ingeniería del tejido óseo

Mesoporous materials (HA-SBA-15) functionalized with a collagen-targeted rhBMP-2 and their related collagen hybrid composites for bone tissue engineering

Código/Code:	BIO2009-13903-C02-02 (Plan Nacional)
Periodo/Period:	01-01-2010 / 31-12- 2012
Organismo Financiador/Financial source:	Ministerio de Ciencia e Innovación
Importe total/Total amount:	77.440 €
Investigador responsable/Research head:	M. Aránzazu Díaz Cuenca
Componentes/Research group:	M. Lourdes Ramiro Gutiérrez

RESUMEN / ABSTRACT

Los materiales soporte denominados biomateriales, matrices, armazones, andamiajes tisulares o scaffold son uno de los elementos básicos para la fabricación de nuevos tejidos artificiales. El biomaterial sirve de soporte para las interacciones celulares y para la formación de matriz extracelular (ECM). Entre los distintos tipos de materiales que se emplean naturales o sintéticos, las cerámicas bioactivas con base de sílice en el sistema ternario SiO2-CaO-P2O5

han mostrado excelente propiedades para su aplicación en cirugía ortopédica reparadora y regeneradora. Por otra parte el desarrollo de nuevas rutas de síntesis que combinan la química sol-gel y el autoensamblado de moléculas (polímeros) directoras o formadoras de estructura ofrece grandes posibilidades para la síntesis de de nuevos materiales bioactivos organizados a escala nanométrica con alta superficie y reactividades mejoradas. Trabajo previo de la IP de esta solicitud ha resultado en la síntesis de un nuevo biomaterial nanocomposite (HA-SBA-15) biocompatible constituido por nanopartículas de hidroxiapatito de calcio en asociación con la matriz de sílice mesoestructurada. Además de la biocompatibilidad, la alta superficie y la distribución de poros con un tamaño homogéneo hacen que este material sea un candidato muy interesante para su utilización como matriz para la adsorción de moléculas terapéuticas, medicamentos o factores de crecimiento que requieran su liberación de forma controlada. Las proteínas morfogenéticas de hueso (BMPs) han sido utilizadas ampliamente debido a sus propiedades osteoinductoras. Las proteínas recombinantes BMP-2 y BMP-7 han sido aprobadas por la FDA para su uso en cirugía ortopédica, sin embargo, el uso de estos factores de crecimiento no está muy extendido debido al alto costo de estos tratamientos y al miedo a posibles efectos secundarios como consecuencia de su utilización en altas concentraciones sin un sistema de liberación adecuado. Por otra parte resultados recientes del equipo coordinador de esta solicitud (subproyecto 2) ha producido y patentado una proteína recombinante BMP (rh-BMP-2) con un dominio de unión al colágeno tipo I (CBD). Esta proteína de fusión ha mostrado ventajas respecto a la proteína nativa BMP-2 y su uso combinado con colágeno puede representar una alternativa terapéutica mejor y más segura en la reparación del tejido óseo. En este subproyecto se propone el estudio de nuevas rutas de síntesis para producir un material nano-organizado (HA-SBA-15) con variaciones en los parámetros texturales y las nanopartículas de HA con el objetivo de optimizar las propiedades de adsorción y posterior liberación de la proteína rhBMP-2 con afinidad por colágeno. Un objetivo paralelo será determinar las variables y condiciones experimentales adecuadas para incorporar la proteína rhBMP-2-CBD al material nano-organizado. El estudio analizará la cantidad de biomolécula, la cinética de desorción y su integridad. Una segunda tarea de esta propuesta es la consolidación del material particulado nano-organizado en piezas tridimensionales híbridas de material cerámico-colágeno biocompatibles, macroporosas y con una estabilidad mecánica mínima que permita su utilización en los experimentos in vivo que se proponen llevar a cabo como parte de las tareas del Subproyecto 2. Se ensayaran métodos para obtener piezas tridimensionales que conserven sus características nanoestructuradas. Se abordará la integración del material sin funcionalizar y funcionalizado con rhBMP-2-CBD.

A key component in tissue engineered materials for bone repair and regeneration is the scaffold that serves as a template for cell interactions and the formation on bone-extracellular matrix. This scaffold material also provides structural support to the newly formed tissue. Materials in the ternary system SiO_2-CaO-P_2O_5 have demostrated excellent bioactivity for their use in orthopaedic repair and regeneration. The development of new synthesis routes which combine sol-gel chemistry and Block Copolymer (BCPs) self-assembly procedures have potential to be used as interesting methods to produce mesoporous organised SiO_2-CaO-P_2O_5 materials with improved surface area and reactivity. Previous work carried out by the PI of this application has resulted in the synthesis of a biocompatible material (HA-SBA-15) consisting of calcium phosphate hydroxyapatite (HA) nanoparticles growth within a mesoporous (nano-sized-pore-organised) silica SBA-15 structure. Among their biocompatibility, the high surface area and the ordered distribution of pores with very homogeneous size confers to this material very interesting properties for their application as a matrix material for the adsorption of therapeutic agents, drugs or growth factors with requires their application in a controlled and prolonged release. The bone morphogenetic proteins (BMPs) have been widely used because their potent osteinductive properties and certain recombinant proteins BMP-2 and BMP-7 have been approved by the FDA for their use in orthopaedic surgery. Nevertheless, the use of these growth factors is not very extended due to the very high costs of these treatments and the fear to possible undesired side effects due to the use of high concentrations without any controlled delivery system. On the other hand, recent achievements of the team coordinator of this project application (Subproject 2) has produced and patented a recombinant BMP (rhBMP-2) with an additional decapeptidic collagen type I binding domain (CBD) which has shown that this fusion protein has advantages over native BMP-2, and that its combination with collagen may be better and safer alternative for bone repair. In this SubProject application we propose to work in new synthesis routes to produce a nanostructured composite material (HA-SBA-15) with variations in the textural and HA nanoparticle parameters to optimise improved collagen targeted BMP-2 protein adsorption capacities and delivery properties capacities and kinetics. A related objective will be to find and asses the experimental conditions and variables to incorporate successfully a collagen targeted BMP-2 protein to the nano-organised material. The study will cover the analysis of the biomolecule loading, desorption kinetics and final integrity. A second task of the proposed project will be the consolidation of the nano organised powder precursors in 3D ceramic-collagen hybrids composite scaffolds structures which fulfil requirements of biocompatibility, macroporosity and minimal mechanical stability for be using in the in the vivo experimental models which will be carried out as part of the working plan of the other SubProject (Subproyect 2). Work will be carried out to develop fabrication methods of the nanostructured materials into 3D scaffolds while retaining their nanostructural features. The integration of both the protein free HA-SBA-15 and also the fuctionalised collagen targeted BMP-2 material will be considered.

Aplicaciones de cristales fotónicos en células solares: aumento de la eficiencia de conversión de potencia mediante la amplificación de la absorpción óptica

Applications of photonic crystals in solar cells: power conversion efficiency enhancement though optical absorption amplification

Código/Code:	P08-FQM-03579 (Proyecto de Excelencia)
Periodo/Period:	14-01-2009 / 13-01- 2012
Organismo Financiador/Financial source:	Junta de Andalucía
Importe total/Total amount:	291.923 €
Investigador responsable/Research head:	Míguez García, Hernán R.
Componentes/Research group:	Ocaña, M., Calvo, M., Nuñez, N., Mihi, A., Lozano, G., Colodrero, S., Hidalgo, N., Sánchez Sobrado, O.

RESUMEN / ABSTRACT

El concepto central en el que se basa esta propuesta es que los cristales fotónicos, adecuadamente implementados en una célula solar, permiten obtener mejoras sustanciales de su eficiencia. Más concretamente, el presente proyecto pretende estudiar el efecto de la propagación anómala de la radiación electromagnética que tiene lugar en materiales fotónicos sobre la eficiencia y operatividad de células fotovoltaicas de colorante de diverso tipo. El proyecto propone la fabricación de láminas delgadas de partículas coloidales (diámetro comprendido entre 0.010 µm y 1 µm) de óxidos de distinto tipo (óxido de titanio, óxido de estaño, óxido de zinc, óxido de silicio, etc…), pudiendo estas partículas encontrarse tanto en una red ordenada (cristal coloidal) como en forma desordenada pero formando parte de una superestructura que presente orden en una escala de longitud mayor (estructuras multicapas de nanopartículas). Se ha demostrado recientemente que este tipo de estructuras, cuando se acoplan siguiendo un diseño preciso a un electrodo de una célula solar, dan lugar a un aumento extraordinario de la absorción óptica como consecuencia de la localización de luz en la lámina absorbente. Este aumento de la absorción se traduce en un aumento de la fotocorriente que da lugar a su vez a un aumento de la conversión de potencia de la celda. Algunos de los trabajos pioneros a escala mundial en la comprensión del efecto y la aplicación de cristales fotónicos en células solares han sido realizados en el Instituto de Ciencia de materiales de Sevilla y el objetivo primordial de este proyecto es establecer una línea experimental sólida en esta temática que ya ha dado resultados de gran impacto y extraordinariamente prometedores. El presente proyecto se enmarca dentro de la subárea de Nanociencias, Nanotecnología y Materiales dedicada a Nuevos Materiales Fotónicos para Células Solares y Pantallas, según establece en la convocatoria la Consejería de Innovación, Ciencia y Empresa de la Junta de Andalucía.

Porous photonic crystals introduced in heterojunction solar cells allow to enhance significantly their photovoltaic performance by increasing the light harvested by the device. This concept, pioneered by the multifunctional optical materials group, have lead to highly efficient and transparent dye solar cells that preserve their potential application as window modules, one of their main added values. The concepts proposed in this project are not only interesting from a fundamental point of view in photonics and energy conversion, but also of clear relevance for building integrated photovoltaics.

Materiales poliméricos y nanocomposites híbridos en forma de lámina delgada para aplicaciones fotónicas y fotovoltaicas (NANOPHOTON)

Polymeric and hybrid nanocomposite thin films for photonic and photovoltaic applications

Código/Code: P09-TEP-5283 (Proyecto de Excelencia)
Periodo/Period: 01-01-2010 / 31-12-2012
Organismo Financiador/Financial source: Junta de Andalucía
Importe total/Total amount: 257.923,68 €
Investigador responsable/Research head: Barranco Quero, Angel
Componentes/Research group: Juan Pedro Espinós, Francisco Yubero, Ana Borrás, Fabián Frutos, Lola González-García, Said Hamad, S. Lago, Alberto Palmero, Carmen

Ruiz-Herrero, Juan R. Sánchez-Valencia, Johan Toudert, Santiago Lago Aranda, Said Hamad, Victor Rico Gavira

RESUMEN / ABSTRACT

El proyecto NANOPHOTON persigue el desarrollo de una nueva familia de materiales, estructuras y prototipos de dispositivos con aplicación en campos tales como el aprovechamiento de energía solar, el análisis medioambiental y la tecnología espacial. El punto de partida del proyecto es la investigación en nuevos materiales ópticamente activos en forma de película delgada nanométrica de carácter polimérico e híbrido. Estas láminas delgadas activas se procesarán e integrarán usando diferentes técnicas para formar estructuras ópticas de uso como sensores fotónicos ambientales, filtros fotónicos insensibles al ángulo de incidencia para comunicaciones en satélites y celdas fotovoltaicas. Un aspecto muy interesante del proyecto es su completa compatibilidad con los métodos sintéticos de uso común en tecnología microelectrónica y optoelectrónica siendo fácilmente transferibles a la industria. NANOPHOTON integra desde estudios fundamentales de simulación molecular a procesos de fabricación de estructuras nanométricas con actividad fotónica pasando por la fabricación de estructuras y prototipos para llegar a test de validación de prototipos en condiciones reales.

The Nanophoton project aims the development of a novel family of materials, structures and device prototypes for application in solar energy, environmental sensing and space communication technology. The starting point of the project is the research in the photonic properties of hybrid nanometric films. These functional thin films will be processed and integrated in optical structures. The project encompasses fundamental molecular simulation studies, the development of novel nanometric functional structures, the study of suitable processing/integration procedures and the validation of prototype devices. These devices will be of three kinds: photonic gas sensors, detectors insensitive to the angle of detection for diffuse optical communications and photovoltaic cells. An interesting characteristic of the Nanophoton technology will be its fully compatibility with the current optoelectronic and microelectronic industrial manufacturing processes.

Plasmas de nitrógeno para funcionalización superficial de materiales (PLASNITRO)
Nitrogen Plasmas for the superficial functionalization of materials

Código/Code:	P07-FQM-03298 (Proyecto de Excelencia)
Periodo/Period:	01-02-2008 / 31-01- 2011
Organismo Financiador/Financial source:	Junta de Andalucía
Importe total/Total amount:	96.200 €
Investigador responsable/Research head:	José Cotrino Bautista
Componentes/Research group:	Agustín R. Gónzalez-Elipe, Francisco Yubero

RESUMEN / ABSTRACT

En el proyecto PlasNitro se aborda la caracterización de plasmas de nitrógeno en diversas aplicaciones tecnológicas relacionadas con técnicas de deposición y funcionalización de materiales, reformado y procesos de esterilización que involucran a la Tecnología de Plasma. Se pondrán a punto diferentes procedimientos para medir propiedades de los plasmas, usados en dopado, deposición, funcionalización y modificación de materiales, que contienen nitrógeno usando técnicas de diagnosis basadas en la detección de especies de nitrógeno. El nitrógeno es hoy día un componente usual, sólo o en mezclas con otros gases, en muchos procesos usados en tecnología de plasma. Su caracterización experimental y/o teórica permitirá obtener propiedades fundamentales del plasma (densidad electrónica, temperatura electrónica, temperatura del gas, especies reactivas, etc.) y conocer la contribución a las reacciones homogéneas (en fase plasma) y heterogéneas (interacción plasma-superficie) de los componentes procedentes del nitrógeno. En el proyecto se elaborarán códigos numéricos para obtener la función de distribución electrónica en el plasma. Para este fin será necesaria previamente la evaluación de la distribución vibracional del nitrógeno. Este paso implica tener en cuenta múltiples procesos vibracionales-vibracionales, vibracionales-traslacionales y vibracionales-rotacionales. A partir de la función de distribución electrónica se podrán construir modelos de fluido del plasma en los que intervienen las especies más importantes. Los cálculos teóricos se complementarán con medidas experimentales usando sonda electrostática de Langmuir, que permitirán medir la función de distribución electrónica, así como densidad y temperatura de los electrones. Mediante un analizador de gases residuales se controlará la presión parcial de nitrógeno en cada aplicación y los componentes neutros del plasma. Los modelos cinéticos del plasma de nitrógeno permitirá en muchos casos la interpretación de medidas en el plasma alejado del equilibrio termodinámico y las técnicas de escalado dinámico y simulación Monte Carlo permitirán el control de la nano/microestructura de los materiales depositados/modificados. Se tendrán, de esta forma, técnicas que permitirán controlar y mejorar los procedimientos de trabajo y las propiedades deseadas en los materiales.

The project PlasNitro discusses the characterization of nitrogen plasmas in various technological related applications with techniques of deposition and functionalization of materials, reforming and processes of sterilization. Different procedures to measure properties of plasmas will go down to point, plasma that can be used in doping, deposition, functionalization and modification of materials and that contain nitrogen. In all cases by using techniques of diagnosis based in the detection of nitrogen species. Nitrogen is a usual component nowadays, only or in mixtures with other gases, in a lot of processes used in technology of plasma. Its experimental characterization and/or the modeling will allow getting fundamental properties from plasma (electron density, electron temperature, temperature of the gas, reactive species, etc.) and knowing the contribution to the homogenous (in phase plasma) and heterogeneous (in the surface-material interaction) reactions of the appropriate components of nitrogen. Numerical codes to get out the electron energy distribution function in plasma will become elaborate in the project. To this end the evaluation of the vibrational distribution of nitrogen will be necessary previously. This step implies taking into account multiple vibrational-vibrational processes, vibrational-translactional and vibrational-rotational processes. In the project we will be able to obtain models of fluid of the nitrogen plasma with the contributions of the most important species of the plasma. The theoretical calculations will be complemented with experimental measurements using electrostatic Langmuir's probe, this will allow measuring the electron energy distribution function, as well as density and temperature of the electrons. The partial nitrogen pressure in each application and the plasma's neutral components will be controlled by means of an analysis of residual gases. The kinetic modeling of the nitrogen plasma will enable the interpretation of measurements in the plasma out of the thermodynamic equilibrium and by using the Monte Carlo technique of simulation that enable the control of deposition/modification and the nano/microstructure of the materials. We will have, in this way, techniques that they will enable to control themselves and improving the procedures of work and the properties desired in the materials.

Desarrollo de recubrimientos y andamios bioactivos de material cerámico nanoestructurado para la regeneración ósea (BIOCEREG) Development of Nanostructured Ceramic Coatings and Scaffolds for Bone Regeneration (BIOCEREG)

Código/Code:	CTS-661 (Proyecto de Excelencia)
Periodo/Period:	06-07-2011 / 05-06-2015
Organismo Financiador/Financial source:	Junta de Andalucía
Importe total/Total amount:	240.497 €
Investigador responsable/Research head:	M. Aránzazu Díaz Cuenca
Componentes/Research group:	M. Lourdes Ramiro Gutiérrez, Sara Borrego González

RESUMEN / ABSTRACT

Este Proyecto pretende contribuir al avance en el desarrollo de nuevos biomateriales con bioactividad mejorada para su aplicación en la reparación y regeneración ósea. Se propone la preparación de nuevos recubrimientos y andamios cerámicos mediante técnicas de procesado láser a partir de materiales cerámicos particulados, nanoestructurados de composición bioactiva en el sistema SiO2-CaO-P2O5 sintetizados en el ICMS por la Dra. Díaz (IP de esta solicitud). La hipótesis de partida es que las características nanoestructurales y texturales del material cerámico particulado en combinación con la fuente láser tiene un gran potencial para resultar en deposiciones con microestructura y nanoestructura controlada. Se plantea procesar dos tipos de pieza prototipo: i) piezas de sustrato metálico (de titanio) con recubrimiento cerámico de composición bioactiva y ii) piezas monolito (andamio) solo cerámica bioactiva con geometría controlada. Hay que distinguir por tanto la persecución de dos hitos. Un primer Hito es la obtención de materiales prototipo (recubrimientos y andamios) con unos requerimientos de micro y nanoestructura, superficie, propiedades mecánicas, homogeneidad y reproducibilidad mínimas. Y un segundo Hito consistente en la verificación de sus propiedades biológicas in vitro e in vivo. El éxito en ambos hitos es lo que finalmente denominaremos biomaterial prototipo. La obtención de los recubrimientos tendría una translación muy directa para implementarse en distintas partes de los componentes de implantes ortopédicos. En este sentido el equipo de investigación integra a biólogos de regeneración esquelética y clínicos de cirugía

ortopédica y traumatología que van a estudiar la bioactividad y biocompatibilidad de estos recubrimientos sobre sustratos de titanio suministrados por Synthes, empresa líder en fabricación y comercialización de implantes para ortopedia, que participa en esta propuesta como EPO. Por otra parte y desde el punto de vista del procesado de materiales, la aplicación del procesado láser a los materiales cerámicos nanoestructurados SiO2-CaO-P2O5 es totalmente novedoso y creemos que puede optimizarse para obtener recubrimientos y también andamios tridimensionales, conformados con macroporosidad interconectada pero a su vez con microestructura fina y nanoestructura, que culminen en la obtención de piezas prototipo con alta reproducibilidad y de calidad e innovación tecnológica elevada. El Proyecto se encuadra en áreas de investigación fuertemente innovadoras y pujantes como son la nanotecnología y la medicina regenerativa ambas con un carácter multidisciplinar intrínseco donde la frontera entre las distintas disciplinas científicas tradicionales aparece difuminada. El Proyecto aúna esfuerzos de investigadores con formación básica en las disciplinas de química (ICMS), física e ingeniería (Empresa Subcontratada AIMEN), biología (UMA-CIBER-BBN) y medicina clínica y traslacional (HCS). Creemos que la integración de estos tres pilares i) síntesis, procesado y caracterización de materiales, ii) biología de la regeneración e ingeniería tisular y iii) práctica clínica ofrece una propuesta con capacidad para aportar resultados de impacto trasferibles a la industria y que puede por tanto ayudar al desarrollo de productos para aplicaciones en la reparación y regeneración esquelética en Andalucía.

The aim of this Project is to advance in the development of new biomaterials with improved bioactivity for their application in bone repair and regeneration. The goal is the preparation of new coatings and scaffolds of ceramic materials using laser processing techniques from nanostructured ceramic particulates in the SiO2-CaO-P2O5 system which will be synthesised at the ICMS. The hypothesis is the compositional properties and the textural parameters of the particulates in combination with the laser source have potential for processing depositions with controlled macro-nanostructure. It is programmed to prepare two types of prototype pieces: i) Titanium metallic substrates with bioactive ceramic coatings and ii) monolith scaffolds of bioactive ceramic with controlled geometry. There are two milestones to highlight. The first one is the fabrication of prototype pieces (coatings and scaffolds) with reproducibility, homogeneity, micro-nanostructural features, and surface and mechanical properties requirements. A second milestone will be the evaluation of their in vitro an in vivo biological properties. The achievement of both mentioned milestones will lead to the final biomaterial prototype. Bone regeneration biologists and orthopaedic surgeons will study the bioactivity and biocompatibility of the coatings on titanium substrates provided by Synthes which is a leader Company in orthopaedic trauma devices for internal and external fixation and is included in the proposal as EPO. The application of the laser processing to the SiO2-CaO-P2O5 nanostructured ceramic materials is completely new and we believe that it could be optimised for obtaining coatings and reticulated scaffolds while keeping their nanostructural features. The Project integrates material scientist, laser engineers, biologists and orthopaedic surgeons. We believe that this multidisciplinary approach with work in the i) synthesis, processing and characterisation of materials, ii) regeneration biology and tissue engineering and iii) medical practise could achieve results with potential to be transferred to the industry to promote the orthopaedic products to improve Andalusian bone repair and regeneration therapies.

Desarrollo de membranas de regeneración ósea guiada modificadas a escala nanométrica (OSTEOMEM)

Development of bones regeneration membranes modified at nanometric scale (OSTEOMEM)

Código/Code:	P09-CTS-5189 (Proyecto de Excelencia)
Periodo/Period:	01-01-2010 / 31-12-2012
Organismo Financiador/Financial source:	Junta de Andalucía
Importe total/Total amount:	221.673,68 €
Investigador responsable/Research head:	R. González-Elipe, Agustín
Componentes/Research group:	Cotrino, J., Alvarez Molina, R., López Santos, C., Gil Rostra, J., Terriza Fernández, A.

RESUMEN / ABSTRACT

OSTEOMEM persigue el desarrollo de membranas de regeneración ósea reabsorbibles y biodegradables de base polimérica para su uso en cirugía oral y maxilofacial para el tratamiento de defectos óseos. Durante la curación de estos, las membranas deben preservar la aparición de tejidos blandos en los mismos propiciando que la regeneración del hueso ocupe el defecto, dejando tras la reabsorción de la membrana una estructura de tejidos análoga a la que existía antes de la intervención quirúrgica. Este efecto se basa fundamentalmente en un mecanismo de barrera con membranas que se degradan en el interior del cuerpo en un periodo de cuatro a seis meses, evitando la segunda cirugía que generalmente se requiere para retirar membranas no biodegradables. Se espera que las membranas desarrolladas en el proyecto permitan alcanzar los resultados clínicos de las membranas de regeneración animal evitando los problemas asociados a su origen.

OSTEOMEM aims at developing disposable and biodegradable membranes for bone regeneration to be use in chirurgic oral and maxillofacial implants for the treatment of defects. During the healing of the bone defects, membranes must simultaneously preserve the formation of soft tissues and promote the filling of the hole by the new bone, so that, after the reabsorption of the membrane, the structure of tissues would be similar to that prior to the chirurgical intervention. To achieve that, the membranes should degrade within the body in a period of four-six months, thus avoiding the need of a second intervention required to remove non-biodegradable membranes. It is expected that the membranes developed in the project are comparable to that of animal membranes and avoid the problems associated with the use of these latter.

Control de procesos en plasmas para la síntesis de materiales nanoestructurados en forma de láminas delgadas (PLASMATER)

Process-control in plasmas for the synthesis of nanostructured thin films (PLASMATER)

Código/Code:	P09-FQM-6900 (Proyecto de Excelencia)
Periodo/Period:	15-03-2011 / 14-03-2014
Organismo Financiador/Financial source:	Junta de Andalucía
Importe total/Total amount:	167.209,71 €
Investigador responsable/Research head:	Alberto Palmero Acebedo
Componentes/Research group:	José Cotrino Bautista, Ana Borrás Martos, Francisco Yubero Valencia, Rafael Alvarez Molina, Juan Carlos González González, Carmen López Santos

RESUMEN / ABSTRACT

En el proyecto PLASMATER abordamos el desarrollo de nuevos procesos basados en plasmas para controlar la nanoestructura, porosidad y morfología superficial de películas delgadas, con el objetivo de mejorar sus funcionalidades para aplicaciones finales. En las técnicas de deposición de películas delgadas asistida por plasma, las cantidades que definen la deposición, tales como la potencia electromagnética empleada, presión de los gases, etc., definen las propiedades del plasma, que a su vez, y a través de procesos no-lineales y fuertemente acoplados entre sí, produce el crecimiento de la película delgada en un porta-substrato. La complejidad de todos estos procesos ha dado lugar a que existan multitud de relaciones de carácter empírico entre cantidades controlables experimentales y las nanoestructuras crecidas, sin que haya una explicación clara sobre los mecanismos que controlan dicho crecimiento, y la conexión entre ambas. Este conocimiento es esencial para proponer modificaciones en las condiciones de la deposición que permitiesen un mayor control y versatilidad a la hora de sintetizar películas delgadas nanoestructuradas.

En PLASMATER nos proponemos desarrollar herramientas para controlar procesos en plasmas y obtener capas nanoestructuradas y sistemas 1D de TiO2 y ZnO soportados en substratos, para mejorar propiedades funcionales tales como foto-actividad o propiedades de mojado, entre otras. Se explorarán tres aspectos relacionados entre sí: i) diagnosis completa de la fase gaseosa (plasma y vaina) y caracterización de la nanoestructura de los materiales depositados, ii) estudio de las funcionalidades de dichos materiales, y iii) el desarrollo de códigos numéricos predictivos, a partir de los cuales se desarrollen nuevos protocolos que permitan un mayor control sobre la nanoestructura del material y, por lo tanto, sobre las funcionalidades. El uso de modelos predictivos tiene una gran relevancia debido a que, hasta nuestro conocimiento, i) será la primera vez en la literatura que se dé una visión completa del proceso de deposición y nanoestructuración de estas películas delgadas basada en fenómenos fundamentales, a partir del valor de las cantidades experimentales de control (potencia electromagnética empleada, presión de los gases, etc.), y ii) se utilizará el modelo para proponer modificaciones en el proceso de deposición que ayuden a controlar los procesos de nanoestructuración de la película y proveer de más flexibilidad y versatilidad a los materiales depositados con vista a mejorar sus funcionalidades.

Para desarrollar el proyecto PLASMATER nos proponemos seguir una estrategia mixta simulación/diagnosis experimental del proceso de deposición para desarrollar interactivamente los modelos de crecimiento en múltiples condiciones. Se considerará el estudio de las dife-

rentes escalas espaciales en el problema, desde el propio plasma (escala típica de decenas de centímetros), la vaina del plasma (por debajo de 1 milímetro), y la superficie del material (decenas de nanometros), y se utilizarán herramientas de diagnostico avanzado del plasma y de la película delgada que ayudarán al desarrollo del proyecto. Por último, la investigación también se centrará en encontrar las condiciones experimentales que permitan obtener la mejores propiedades de las capas con vista a optimizar sus aplicaciones tecnológicas e industriales.

Project PLASMATER aims at developing new plasma-based procedures to control the nanostructure, porosity and morphology of deposited thin films, and optimize the material functionalities and applications. From an experimental point of view, plasma-assisted thin film deposition techniques make use of various quantities to define the deposition conditions, such as the electromagnetic power, pressure in the reactor, etc. These quantities controls the plasma properties, which at the same time conditions the growth mechanism of the films. The complexity of the relation between experimentally controllable quantities and growth processes has produced the existence of empirical relations between experimental conditions and final film structure and composition, whose justification from a fundamental point of view is unclear.

In PLASMATER we propose to analyze three related aspects of the deposition of TiO2 and ZnO thin films assisted by plasmas: i) complete diagnosis of the plasma bulk and sheath in connection with the material microstructure, ii) functionality of the material, and iii) the development of predictive numerical codes that calculate the final film microstructure as a function of experimentally controllable quantities. This last part is of relevance because to our knowledge, i) it is the first time in the literature the deposition is fully characterized from a fundamental point of view, ii) this knowledge can be applied to suggest modifications in the deposition reactor in order to enhance different structural properties of the films.

In order to carry out the PLASMATER project, we aim at following at mixed theoretical and experimental strategy in order to interactively develop numerical codes of the thin film growth in multiple conditions. All the spatial scales involved in the description must be studied, from the plasma bulk itself (typically of few tens cm), the plasma sheath (below 1 mm), and the surface of the material (tens nm). Advanced diagnosis techniques will be employed to understand the plasma behavior and the film growth. Finally, PLASMATER will focus on the experimental conditions that lead to an optimized performance of the studied materials for advance applications in technology and industry.

Síntesis y propiedades de nanopartículas luminiscentes basadas en tierras raras para aplicaciones biomédicas Synthesis and properties of luminiscent nanoparticles base don rare earth for biological applications

Código/Code: FQM6090 (Proyecto de Excelencia)
Periodo/Period: 15-03-2011 / 14-03-2014
Organismo Financiador/Financial source: Junta de Andalucía
Importe total/Total amount: 100.000 €
Investigador responsable/Research head: Manuel Ocaña Jurado
Componentes/Research group: Angel Justo Erbez, Nuria O. Núñez Alvarez,

Fernando Cussó, Jesús Martínez de la Fuente,
Vanesa Sanz Beltrán, Sonia Rodríguez Liviano

RESUMEN / ABSTRACT

El trabajo de investigación que se propone en esta memoria está dirigido al desarrollo de nuevos métodos de síntesis, poco agresivos para el medioambiente, de materiales nanoestructurados luminiscentes constituidos por partículas uniformes con forma y tamaño de partícula controlados de fluoruros, vanadatos y fosfatos de Gd, Y o La dopados con diversos cationes lantánidos, así como al análisis de sus propiedades ópticas y magnéticas (en compuestos de Gd) y de sus posibles aplicaciones biomédicas. En concreto, se abordará el dopado con diversos cationes con luminiscencia convencional y emisión en el visible (Eu, Tb, etc.) o infrarrojo (Nd, Er, Pr) y el codopado con pares Er/Yb, Tm/Yb o Ho/Yb con luminiscencia “up-conversion”. Las principales ventajas que presentan estos materiales basados en tierras raras frente a otros materiales fluorescentes propuestos para las aplicaciones mencionadas son su menor toxicidad, su mayor estabilidad química y sobre todo, en el caso de los materiales con fluorescencia “up-conversion”, su excitación con radiación infrarroja evita que se dañen los tejidos biológicos. Las muestras preparadas se caracterizarán en términos de sus propiedades estructurales, morfológicas y composicionales y se evaluarán sus propiedades ópticas (absorción y luminiscencia) y magnéticas en relación con sus características morfológicas y estructurales. Posteriormente, se desarrollarán procedimientos de funcionalización de las nanopartículas obtenidas para obtener materiales estables en condiciones fisiológicas. Por último, se analizará la biocompatibilidad de las nanopartículas obtenidas y su eficacia para la detección de tumores.

This project is devoted to the development of new methods, environmentally friendly, for the synthesis of nanostructured luminescent materials consisting of uniform particles with controlled size and shape, based on a Gd, Y or La matrix (fluoride, vanadate or phosphate) doped with different lanthanide (Ln) cations, as well as to the analysis of theirs optical and magnetic (Gd compounds) properties and the evaluation of theirs biomedical applications. Several Ln cations with down-conversion and emissions in the visible (Eu, Tb) or near-infrared (NIR) (Nd, Er, Pr) and up-coversion (Er/Yb, Tm/Yb, Ho/Yb) luminescence have been selected. The main advantages that these Ln based nanomaterials present over other luminescent systems with potential bioapplications are their lower toxicity and higher chemical stability. In addition, in the case of up-converting nanophosphors, they are excited with NIR radiation which, in contrast with ultraviolet excitation, does not cause damage to biological tissues. Several procedures for the functionalization of the obtained nanoparticles will be essayed in order to obtain stable dispersions in physiological media. Finally, the nanophosphors biocompatibility and their efficiency for the detection of tumors will be also evaluated.

Nanoestructuras híbridas flexibles para aplicaciones con filtros de radiación ultravioleta, visible e infrarroja

Flexible hybrid nanostructures for applications as ultraviolet, visible and near infrared filters

Código/Code: FQM6090 (Proyecto de Excelencia)

Periodo/Period:	03-02-2010 / 03-02-2013
Organismo Financiador/Financial source:	Junta de Andalucía
Importe total/Total amount:	193.431,68 €
Investigador responsable/Research head:	Hernán Míguez García
Componentes/Research group:	Mauricio Calvo Roggiani, Agustín Mihi Cervelló, Silvia Colodrero Pérez, Nuria Hidalgo Serrano, Gabriel Lozano Barbero, Olalla Sánchez Sobrado

RESUMEN / ABSTRACT

El objetivo principal de esta propuesta es el desarrollo de filtros interferenciales flexibles que reflejen rangos seleccionados de radiación ultravioleta (UV), visible (Vis) o infrarroja (IR). Se persigue, además, que sean transferibles y adhesivos, de forma que puedan adaptarse a distintos tipos de superficies. Se explorarán aplicaciones inmediatas de estos nuevos espejos dieléctricos como protectores adhesivos y transparentes de la piel contra radiaciones solares de alta energía (principalmente, el rangos conocido como UVA, de 315 nm a 400 nm), por lo que se pondrá especial énfasis en la integración de polímeros que sean compatibles con la piel humana. El interés y la originalidad de la aproximación aquí propuesta radica en la ausencia en el mercado de filtros de este tipo no absorbentes, es decir, no basados en procesos de absorción de luz que implican necesariamente un calentamiento, si no que funcionen como un espejo dieléctrico que refleje el rango de frecuencias deseado sin que causen un aumento local de la temperatura. En general, estos nuevos materiales permitirían proteger de la radiación no deseada cualquier tipo de superficie, de rugosidad y composición arbitraria. Del mismo modo, y en referencia a otro ámbito de aplicación, se buscará que los filtros propuestos proporcionen color a superficies arbitrarias, a las que se adaptarán y adherirán, reflejando un rango de frecuencias cuya posición central y anchura puede determinarse con precisión en todo el espectro visible. Por último, se explorarán aplicaciones en el IR como protectores contra calentamiento o, por el contrario, como recubrimientos transparentes en el rango visible pero que eviten las perdidas de calor, según la configuración empleada.

This project aims at developing radiation filters and screens in the shape of films and capable of blocking or selecting ultraviolet (UV), visible (Vis) or near infrared (NIR) radiation within well-defined spectral ranges. Biocompatibility, flexibility and specific adhesive properties will be sought after in order to make these films usable to protect all types of ill, wounded or burnt skin. The aim is to fill a currently existing hole in the field of skin phototherapy based on the healing properties of UV-Vis-NIR light, which is the absence of biocompatible patches in which selected ranges of the electromagnetic spectrum wavelengths can be sharply blocked or allowed to pass depending on the needs of the patient. For clinical cases that so required, an integral approach to skin photo-healing will be taken, devising materials that allow therapeutic wavelengths to reach the skin while blocking harmful ones and providing the controlled topical release of substances that have a beneficial effect on the skin. This project is based on a new series of novel prototype materials that have recently been developed in the group headed by the applicant in the Institute of Materials Science of Seville.

Sistemas para la Detección de Explosivos en Infraestructuras Públicas Systems for the detection of explosives in publlic infrastructures

Periodo/Period: 1-09-2010 / 31-10-2011
Organismo Financiador/Financial source: Centro para el Desarrollo Tecnológico Industrial (Programa CENIT) Ministerio de Industria (Contrato: ARQUIMEA)
Investigador responsable/Research head: Barranco Quero, A.
Componentes/Research group: Aparicio, F., González-Elipe, A.R., Borrás Martos, A., Espinós, J.P.

RESUMEN / ABSTRACT

El objetivo de este proyecto es el desarrollo de láminas delgadas con propiedades ópticas adecuadas como elementos activos en sensores ópticos capaces de responder a la presencia de gases y/o productos volátiles procedentes de la descomposición parcial de explosivos.

The objective of the project is the development of thin films with adequate optical properties for their use as active elements in optical gas sensors capable of responding to the presence of gases and/or volatile products produced by the partial decomposition of explosives.

TRANSFERENCIA / TECHNOLOGICAL TRANSFER

CONVENIOS Y CONTRATOS / CONTRACTS AND AGREEMENTS

Síntesis y aplicación de materiales nanostructurados multifuncionales en aglomerados pétreos

Periodo/Period: 01-06-2010 / 01-09-2012
Organismo Financiador/Financial source: Cosentino, S.A.
Investigador responsable/Research head: Manuel Ocaña Jurado
Componentes/Research group: Hernán R. Míguez García, Mauricio Calvo Roggiani, Nuria O. Nuñez Alvarez

CONSOLIDER-INGENIO 2010 - CSD 2007-00007 - Proyecto: Hybrid optoelectronic and photovoltaic devices for renewable energy

Periodo/Period: 01-06-2010 / 01-09-2012
Organismo Financiador/Financial source: Universitat Jaume I de Castello
Investigador responsable/Research head: Hernán R. Míguez García
Componentes/Research group: Manuel Ocaña Jurado, Mauricio Calvo Roggia-

ni, Nuria O. Nuñez Alvarez

Síntesis y aplicación de materiales nanostructurados multifuncionales en aglomerados pétreos

Periodo/Period: 01-06-2010 / 01-09-2012
Organismo Financiador/Financial source: Cosentino, S.A.
Investigador responsable/Research head: Francisco Yubero Valencia
Componentes/Research group: Agustín R. González-Elipe, Juan Pedro Espinós, Alberto Palmero, José Cotrino Bautista, Angel Barranco Quero, Jorge Gil Rostra, Victor H. Rico

Desarrollo de láminas delgadas fluorescentes sensibles a agentes del entorno y utilizables para fabricar sensores ópticos

Periodo/Period: 01-01-2010 / 31-12-2011
Organismo Financiador/Financial source: ARQUIMEA
Investigador responsable/Research head: Angel Barranco Quero

Validación de la tecnología "Thin Film" fotovoltáica a escala piloto

Periodo/Period: 1-01-2010 / 31-12-2013
Organismo Financiador/Financial source: Abengoa Solar
Investigador responsable/Research head: Agustín R. González-Elipe

Estudio sobre el uso de combinaciones de reactores de descarga de barrera dieléctrica para la producción de hidrógeno a partir del reformado de hidrocarburos

Periodo/Period: 01-01-2011 / 31-12-2012
Organismo Financiador/Financial source: HYNERGREEN
Investigador responsable/Research head: José Cotrino Bautista

Sol y visión para la energía térmica actual SOLVENTA

Periodo/Period: 01-01-2011 / 31-12-2014
Organismo Financiador/Financial source: Proyecto INNPACTO acuerdo con la empresa ABENGOA SOLAR NEW TECHNOLOGIES
Investigador responsable/Research head: Agustín R. González-Elipe

EXPERIMENTOS CON RADIACIÓN SINCROTRÓN Y GRANDES INSTALACIONES
SYNCHROTRON RADIATION AND LARGE FACILITY EXPERIMENTS

GISAXS Analysis of metal-oxide composite films with asymetric structure and presenting optical dichroism

Agustín R. González-Elipe

HASYLAB, Hamburgo , Alemania

PUBLICACIONES / PUBLICATIONS

ARTÍCULOS PUBLICADOS EN REVISTAS SCI / PAPERS IN SCI JOURNALS

Selective Dichroic Patterning by Nanosecond Laser Treatment of Ag Nanostripes
Sanchez-Valencia, JR; Toudert, J; Borras, A; Barranco, A; Lahoz, R; de la Fuente, GF; Frutos, F; Gonzalez-Elipe, AR
Advanced Materials, **23** (2011) 848-853
DOI: 10.1002/adma.201003933

A simple route for the fabrication of dichroic optical structures based on Ag nanoparticles deposited onto SiO_2 nanocolumns is presented. The strict control of the optical response is achieved after infrared laser treatment of the supported nanoparticles with a commercial nanosecond pulsed laser. Preliminary examples of the utilization of the laser-treated AgNPs/SiO_2 nanocolumn system for optical recoding and encryption are shown.

Transparent Nanometric Organic Luminescent Films as UV-Active Components in Photonic Structures
Aparicio, FJ; Holgado, M; Borras, A; Blaszczyk-Lezak, I; Griol, A; Barrios, CA; Casquel, R; Sanza, FJ; Sohlstrom, H; Antelius, M; Gonzalez-Elipe, AR; Barranco, A
Advanced Materials, **23** (2011) 761-765
DOI: 10.1002/adma.201003088

A new kind of visible-blind organic thin-film material, consisting of a polymeric matrix with a high concentration of embedded 3-hydroxyflavone (3HF) dye molecules, that absorbs UV light and emits green light is presented. The thin films can be grown on sensitive substrates, including flexible polymers and paper. Their suitability as photonic active components in photonic devices is demonstrated.

Interplay of Resonant Cavity Modes with Localized Surface Plasmons: Optical Absorption Properties of Bragg Stacks Integrating Gold Nanoparticles
Sanchez-Sobrado, O; Lozano, G; Calvo, ME; Sanchez-Iglesias, A; Liz-Marzan, LM; Miguez, H
Advanced Materials, **23** (2011) 2108
DOI: 10.1002/adma.201004401

A procedure to prepare porous photonic crystal resonators containing gold nanoparticles is reported. The optical absorption of the ensemble, resulting from the excitation of the localized surface plasmon of the metallic beads, is finely tuned by a gradual shift of the cavity mode. This is achieved by infiltration of the void network with different guest compounds.

Aligned TiO_2 nanocolumnar layers prepared by PVD-GLAD for transparent dye sensitized solar cells
Gonzalez-Garcia, L; Gonzalez-Valls, I; Lira-Cantu, M; Barranco, A; Gonzalez-Elipe, AR
Energy & Environmental Science, **4** (2011) 3426-3435
DOI: 10.1039/c0ee00489h

Transparent thin film electrodes made of vertically aligned nanocolumns of TiO(2) with well-controlled oblique angles were grown by physical vapor deposition at glancing incidence (PVD-GLAD). For an electrode thickness of 500 nm, we report a 40% variation on solar cell efficiency (from 0.6% to 1.04%) when the deposition angle was modified between 60 degrees and 85 degrees. Transparent thicker films with higher surface area deposited at the optimal angle of 70 degrees were grown with a zigzag morphology which confers high mechanical strength to the thin films. Using this topology, the application of an electrode thickness of 3 mu m in a DSC resulted in a power conversion efficiency of 2.78% maintaining electrode transparency.

Porous one dimensional photonic crystals: novel multifunctional materials for environmental and energy applications
Calvo, ME; Colodrero, S; Hidalgo, N; Lozano, G; Lopez-Lopez, C; Sanchez-Sobrado, O; Miguez, H
Energy & Environmental Science, **4** (2011) 4800-4812
DOI: 10.1039/c1ee02081a

In recent times, several synthetic pathways have been developed to create multilayered materials of diverse composition that combine accessible porosity and optical properties of structural origin, i.e., not related to absorption. These materials possess a refractive index that varies periodically along one direction, which gives rise to optical diffraction effects characteristic of Bragg stacks or one-dimensional photonic crystals (1DPCs). The technological potential of such porous optical materials has been demonstrated in various fields related to energy and environmental sciences, such as detection and recognition of targeted biological or chemical species, photovoltaics, or radiation shielding. In all cases, improved performance is achieved as a result of the added functionality porosity brings. In this review, a unified picture of this emerging field is provided.

Porous Supramolecularly Templated Optical Resonators Built in 1D Photonic Crystals
Hidalgo, N; Calvo, ME; Bellino, MG; Soler-Illia, GJAA; Miguez, H
Advanced Functional Materials, **21** (2011) 2534-2540
DOI: 10.1002/adfm.201002486

A synthetic route to attain photonic multilayers that presents controlled porosity only at the middle-layer level is shown. The spectral resonance associated with this porous layer shows strong sensitivity to the presence of vapors adsorbed or condensed within the void network, providing a potentially relevant material for gas detection. The importance of the interplay between pore and probe-molecule diameters is studied and its implications in size-selective detection are discussed.

Enhanced gas sensing performance of TiO_2 functionalized magneto-optical SPR sensors
Manera, MG; Montagna, G; Ferreiro-Vila, E; Gonzalez-Garcia, L; Sanchez-Valencia, JR; Gonzalez-Elipe, AR; Cebollada, A; Garcia-Martin, JM; Garcia-Martin, A; Armelles, G; Rella, R
Journal Of Materials Chemistry, **21** (2011) 16049-16056
DOI: 10.1039/c1jm11937k

Porous TiO_2 thin films deposited by glancing angle deposition are used as sensing layers to monitor their sensing capabilities towards Volatile Organic Compounds both in a standard Surface Plasmon Resonance (SPR) sensor and in Magneto-Optical Surface Plasmon Resonance (MO-SPR) configuration in order to compare their sensing performances. Here our results on the enhanced sensing capability of these TiO(2) functionalized MO-SPR sensors with Au/Co/Au transducers with respect to traditional SPR gas sensors are presented.

Microwave-Assisted Synthesis and Luminescence of Mesoporous REDoped YPO4 (RE = Eu, Ce, Tb, and Ce plus Tb) Nanophosphors with Lenticular Shape
Rodriguez-Liviano, S; Aparicio, FJ; Rojas, TC; Hungria, AB; Chinchilla, LE; Ocana, M
Crystal Growth & Design, **12** (2011) -635
DOI: 10.1021/cg201358c

Mesoporous tetragonal RE:YPO4 nanophosphors (RE = Eu, Ce, Tb, and Ce + Tb) with a lenticular morphology, narrow size distribution, and high surface area have been prepared by an homogeneous precipitation procedure consisting of aging, at low temperature (80-120 degrees C) in a microwave oven, ethylene glycol solutions containing only yttrium acetylacetonate and phosphoric acid. This synthesis method involves important advantages such as its simplicity, rapidness (reaction time = 7 min), and high reaction yields. The mechanism of nanoparticle growth has been also addressed finding that the lenticular nanoparticles are formed through an ordered aggregation of smaller entities, which explains their porosity. In all cases, the doping levels were systematically varied in order to optimize the nanophosphors luminescence. All optimum nanophosphors presented a high luminescence quantum yield (QY). In particular, for the Eu and Tb doped systems, the obtained QY values (60% for Eu and 80% for Tb) were the highest so far reported for this kind of nanomaterial. The morphological, microstructural, and luminescent properties of these nanophosphors and their dispersibility in water make them suitable for biomedical applications.

Novel Guests for Porous Columnar Thin Films: The Switchable Perchlorinated Trityl Radical Derivatives
Oliveros, M; Gonzalez-Garcia, L; Mugnaini, V; Yubero, F; Roques, N; Veciana, J; Gonzalez-Elipe, AR; Rovira, C
Langmuir, **27** (2011) 5098-5106
DOI: 10.1021/la200470f

TiO_2 and SiO_2 porous thin films consisting of tilted nanocolumrts prepared by glancing angle evaporation (GLAD) have been infiltrated with guest derivatives belonging to the family of perchlorinated trityl radicals, novel guest molecules presenting an open-shell electronic configuration associated with paramagnetism, fluorescence, and electroactivity. The main driving forces for infiltration from aqueous solutions of the carboxylate-substituted radical derivatives are the electrostatic interactions between their negative charge and the net positive charges induced on the film pores. Positive charges on the internal surface of the films were induced by either adjusting the radical solution pH at values lower than the point of zero charge (PZC) of the oxide or passivating the nanocolumns oxide surface with a positively charged aminosilane. The infiltrated composite thin films are robust and easy to handle thanks to the physical protection exerted by the film columns. They also keep the multifunctionality of the used guests, as confirmed by electron paramagnetic resonance (EPR), UV-vis spectroscopy, and fluorescence spectroscopy. To prove the electroactivity of the infiltrated porous films, a porous TiO_2 host layer was supported onto conductive indium tin oxide (ITO). By application of an appropriate redox potential, the guest radical molecules have been reversibly switched from their open-shell electronic configuration to their diamagnetic state and hence changed their optical properties. On the basis of these results, it is herein proposed that the appropriate surface functionalization of the pore internal surface of GLAD thin films can be used to prepare novel radical-oxide composite thin films usable for the development of robust switchable electrically driven photonic and magnetic devices.

Aspects of Heterogeneous Enantioselective Catalysis by Metals
Kyriakou, G; Beaumont, SK; Lambert, RM
Langmuir, **27** (2011) 9687-9695
DOI: 10.1021/la200009w

Some aspects of metal-catalyzed heterogeneous enantioselective reactions are reviewed with specific reference to four different systems where the phenomena that control enantioselection appear to be very different. In the case of glucose electro-oxidation, it is clear that any intrinsic chirality present at the metal surface plays a vital role. With alpha-keto hydrogenation, achiral surfaces modified by the adsorption of chiral agents become effective enantioselective catalysts and the formation of extended arrays of chiral species appears not to be of importance: instead a 1:1 docking interaction controlled by hydrogen bonding between the adsorbed chiral modifier and the prochiral reactant determines the outcome. Hydrogen bonding also plays a central role in beta-ketoester hydrogenation, but here fundamental studies indicate that the formation of ordered arrays involving the reactant and chiral ligand is of importance. Asymmetric C=C hydrogenation, though relatively little studied, has the potential for major impact in synthetic organic chemistry both on the laboratory scale and in the manufacture of fine chemicals and pharmaceuticals. The structural attributes that determine whether a given chiral ligand is effective have been identified; the ability to form strong covalent bonds with the metal surface while also resisting hydrogenation and displacement by the strongly adsorbing reactant under reaction conditions is an essential necessary condition. Beyond this, ligand rigidity in the vicinity of the chirality center coupled with resistance to SAM formation is a critically important factor whose absence results in racemic chemistry.

Tuning from blue to magenta the up-converted emissions of YF3:Tm3+/Yb3+ nanocrystals
Quintanilla, M; Nuñez, NO; Cantelar, E; Ocaña, M; Cusso, F
Nanoscale, **3** (2011) 1046-1052
DOI: 10.1039/c0nr00676a

Monodisperse YF3:Tm3+/Yb3+ nanocrystals have been synthesized to explore the visible up-converting properties under near infrared (975 nm) excitation. It has been found that the nanoparticles exhibit intense red up-converted emissions, in addition to the characteristic UV and blue Tm3+-bands. It is demonstrated that, by carefully selecting Tm3+ and Yb3+ contents, the relative intensity of the different emissions can be changed producing an overall emission colour that can be tuned from blue to magenta.

Soft plasma processing of organic nanowires: a route for the fabrication of 1D organic heterostructures and the template synthesis of inorganic 1D nanostructures
Alcaire, M; Sanchez-Valencia, JR; Aparicio, FJ; Saghi, Z; Gonzalez-Gonzalez, JC; Barranco, A; Zian, YO; Gonzalez-Elipe, AR; Midgley, P; Espinos, JP; Groening, P; Borras, A
Nanoscale, **3** (2011) 4554-4559
DOI: 10.1039/c1nr11001b

Hierarchical (branched) and hybrid metal-NPs/organic supported NWs are fabricated through controlled plasma processing of metalloporphyrin, metallophthalocyanine and perylene nanowires. The procedure is also applied for the development of a general template route for the synthesis of supported metal and metal oxide nanowires.

Angular emission properties of a layer of rare-earth based nanophosphors embedded in one-dimensional photonic crystal coatings
Sanchez-Sobrado, O; Yacomotti, AM; Calvo, ME; Martinez, OE; Ocaña, M; Nuñez, N; Levenson, JA; Miguez, H
Applied Physics Letters, **99** (2011) -51111
DOI: 10.1063/1.3619814

The angular properties of light emitted from rare-earth based nanophosphors embedded in optical resonators built in one-dimensional photonic crystal coatings are herein investigated. Strong directional dependence of the photoluminescence spectra is found. Abrupt angular variations of the enhancement caused by the photonic structure and the extraction power are observed, in good agreement with calculated polar emission patterns. Our results confirm that the optical cavity favors the extraction of different wavelengths at different angles and that integration of nanophosphors within photonic crystals provides control over the directional emission properties that could be put into practice in phosphorescent displays.

Structural elucidation of beta-$(Y,Sc)_2Si_2O_7$: combined use of ^{89} Y MAS NMR and powder diffraction

Allix, M; Alba, MD; Florian, P; Fernandez-Carrion, AJ; Suchomel, MR; Escudero, A; Suard, E; Becerro, AI

Journal Of Applied Crystallography, **44** (2011) 846-852

DOI: 10.1107/S0021889811021303

Although the structures of pure $Sc_2Si_2O_7$ and beta-$Y_2Si_2O_7$ have been described in the literature using the C2/m space group, ^{29}Si magic angle spinning (MAS) NMR measurements of the intermediate members of the $Sc_2Si_2O_7$-beta-$Y_2Si_2O_7$ system indicate a lowering of the symmetry to the C2 space group. Indeed, these compositions exhibit a unique Si crystallographic site and an Si-O-Si angle lower than 180 degrees, incompatible with the C2/m space group. C2 is the only possible alternative. Space group Cm can be discarded with regard to its two different Si sites per unit cell. Moreover, ^{89}Y MAS NMR data have revealed the existence of two different Y sites in the structure of the intermediate members of the $Sc_2Si_2O_7$-beta-$Y_2Si_2O_7$ system, confirming the lowering of the symmetry to the C2 space group. The viability of the C2 model has therefore been tested and confirmed by refinement of synchrotron and neutron powder diffraction data for the different members of the system. The structural evolutions across the $Sc_2Si_2O_7$-beta-$Y_2Si_2O_7$ system are discussed.

Rhodamine 6G and 800 J-heteroaggregates with enhanced acceptor luminescence (HEAL) adsorbed in transparent SiO2 GLAD thin films

Sanchez-Valencia, JR; Aparicio, FJ; Espinos, JP; Gonzalez-Elipe, AR; Barranco, A

Physical Chemistry Chemical Physics, **13** (2011) 7040-7051

DOI: 10.1039/c0cp02421j

An enhanced fluorescent emission in the near infrared is observed when the Rhodamine 800 (Rh800) and 6G (Rh6G) dyes are coadsorbed in porous SiO2 optical thin films prepared by glancing angle deposition (GLAD). This unusual behavior is not observed in solution and it has been ascribed to the formation of a new type of J-heteroaggregates with enhanced acceptor luminescence (HEAL). This article describes in detail and explains the main features of this new phenomenology previously referred in a short communication [J. R. Sanchez-Valencia, J. Toudert, L. Gonzalez-Garcia, A. R. Gonzalez-Elipe and A. Barranco, Chem. Commun., 2010, 46, 4372-4374]. It is found that the efficiency and characteristics of the energy transfer process are dependent on the Rh6G/Rh800 concentration ratio which can be easily controlled by varying the pH of the solutions used for the infiltration of the molecules or by thermal treatments. A simple model has been proposed to account for the observed enhanced acceptor luminescence in which the heteroaggregates order themselves according to a "head to tail" configuration due to the geometrical constrains imposed by the SiO2 porous matrix thin film. The thermal stability of the dye molecules within the films and basic optical (absorption and fluorescence) principles of the HEAL process are also described.

Enhanced Photoactivity in Bilayer Films with Buried Rutile-Anatase Heterojunctions
Romero-Gomez, P; Borras, A; Barranco, A; Espinos, JP; Gonzalez-Elipe, AR
Chemphyschem, **12** (2011) 191-196
DOI: 10.1002/cphc.201000734

Herein, we study the photoactivity of anatase-rutile bilayer thin films consisting of an anatase overlayer of variable thickness from some tenths to some hundred nanometers deposited onto a rutile thin film. As references single anatase layers of equivalent thickness were deposited onto silicon. All the films were characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM) and Raman spectroscopy. The photoactivity of the samples was assessed by following the evolution with the UV illumination time of both the wetting angle on the thin film surface and the decoloration of a dye in a water solution. While a similar efficiency is found for the first type of experiments irrespective of the anatase thickness, in the second type a maximum in the photoactivity is found for a thickness of the anatase layer of about 130 nm. This enhanced photoactivity in bilayer systems with a buried anatase-rutile heterojunction is related to the formation of different Schottky potential barriers in the anatase layer, depending on its thickness and the substrate (i.e. rutile or SiO2) where it is deposited.

Synthesis, through pyrolysis of aerosols, of YIn(1-x)Mn(x)O(3) blue pigments and their efficiency for colouring glazes
Ocaña, M; Espinos, JP; Carda, JB
Dyes and Pigments, **91** (2011) 501-507
DOI: 10.1016/j.dyepig.2011.03.009

Mn-doped YInO(3) blue pigments have been synthesised at a much lower temperature (1100 degrees C) than that required by the traditional solid state method (1400 degrees C). The developed procedure, which is based on the pyrolysis at 600 degrees C of aerosols generated from aqueous solutions of Y, In and Mn nitrates followed by an annealing treatment at 1100 degrees C, yields spherical pigments particles with heterogeneous size in the optimum range required for ceramic applications (<10 mu m). The amount of Mn introduced in the YInO(3) matrix has been systematically varied in order to evaluate the effects of the Mn content on the colour properties of the pigments. It has been found that the optimum pigment composition (bluer colour with the lowest Mn content) is given by the formula YIn(0.90)Mn(0.10)O(3). The technological performance of these YIn(1-x)Mn(x)O(3) blue pigments has also been evaluated by testing their efficiency for colouring ceramic glazes of different composition (boracic and plumbic) and properties, aiming to find a less toxic alternative for the Co-based pigments commonly used by the ceramic industry. (C) 2011 Elsevier Ltd. All rights reserved.

A facile single-step procedure for the synthesis of luminescent Ln($^{3+}$): YVO$_4$ (Ln=Eu or Er+Yb)-silica nanocomposites
Ocaña, M; Cantelar, E; Cusso, F
Materials Chemistry And Physics, **125** (2011) 224-230
DOI: 10.1016/j.matchemphys.2010.09.011

A simple and single-step method for the production of Ln-doped YVO_4 nanocrystals and their simultaneous encapsulation in a silica network based on the pyrolysis of liquid aerosols at 800 degrees C is reported. The procedure is illustrated for Yb,Er:YVO_4-silica nanocomposites consisting of spherical particles, which present up-converted green luminescence after IR excitation whose efficiency increased on annealing up to 1000 degrees C due to the release of impurities (adsorbed water, and residual anions). XPS spectroscopy and TEM observations revealed that the surface of the composite particles was enriched in silica, which would facilitate their functionalisation required to use them in biological applications. The procedure can also be used to prepare other rare earth doped systems as illustrated for the case of Eu-doped YVO_4/silica having down-converted red luminescence.

Bacterial adherence on UHMWPE with vitamin E: an in vitro study
Gomez-Barrena, E; Esteban, J; Molina-Manso, D; Adames, H; Martinez-Morlanes, MJ; Terriza, A; Yubero, F; Puertolas, JA
Journal Of Materials Science-Materials In Medicine, **22** (2011) 1701-1706
DOI: 10.1007/s10856-011-4340-5

Orthopaedic materials may improve its capacity to resist bacterial adherence, and subsequent infection. Our aim was to test the bacterial adherence to alpha-tocopherol (frequently named vitamin E, VE) doped or blended UHMWPE with S. aureus and S. epidermidis, compared to virgin material. Collection strains and clinical strains isolated from patients with orthopaedic infections were used, with the biofilm-developing ability as a covariable. While collection strains showed significantly less adherence to VE-UHMWPE, some clinical strains failed to confirm this effect, leading to the conclusion that VE doped or blended UHMWPE affects the adherence of some S. epidermidis and S. aureus strains, independently of the concentration in use, but the results showed important intraspecies differences and cannot be generalized.

Influence of OH- concentration on the illitization of kaolinite at high pressure
Mantovani, M; Escudero, A; Becerro, AI
Applied Clay Science, **51** (2011) 220-225
DOI: 10.1016/j.clay.2010.11.021

The products of hydrothermal reactions of kaolinite at 300 degrees C and 1000 bars were studied in KOH solutions covering an OH^- concentration, $[OH^-]$, of 1 M to 3.5 M. XRD patterns indicated a notable influence of the $[OH^-]$ on the reaction. At [OH]>= 3 M. the only stable phase was muscovite/illite. The content of muscovite/illite was calculated from the analysis of the diagnostic 060 reflections of kaolinite and muscovite/illite. The results showed a linear dependence of kaolinite and muscovite/illite contents with [OH-]. Al-27 MAS NMR spectroscopy revealed the formation of small nuclei of K-F zeolite at high $[OH^-]$. Finally, modelling of the Si-29 MAS NMR spectra indicated that the Si/Al ratio of the muscovite/illite formed was very close to that of muscovite, at least in the mineral formed at low $[OH^-]$. In good agreement with the XRD data, the quantification of the reaction products by Si-29 MAS NMR indicated a linear decrease of the kaolinite content with increasing OH- concentration.

Solid solubility of $Yb_2Si_2O_7$ in beta-, gamma- and delta-$Y_2Si_2O_7$
Fernandez-Carrion, AJ; Alba, MD; Escudero, A; Becerro, AI
Journal Of Solid State Chemistry, **184** (2011) 1882-1889
DOI: 10.1016/j.jssc.2011.05.034

This paper examines the structural changes with temperature and composition in the $Yb_2Si_2O_7$-$Y_2Si_2O_7$ system: members of this system are expected to form in the intergranular region of Si_3N_4 and SiC structural ceramics when sintered with the aid of Yb_2O_3 and Y_2O_3 mixtures. A set of different compositions have been synthesised using the sol-gel method to obtain a xerogel, which has been calcined at temperatures between 1300 and 1650 degrees C during different times. Isotherms at 1300 and 1600 degrees C have been analysed in detail to evaluate the solid solubility of $Yb_2Si_2O_7$ in beta-$Y_2Si_2O_7$ and gamma-$Y_2Si_2O_7$. Although $Yb_2Si_2O_7$ shows a unique stable polymorph (beta), Yb^{3+} is able to replace Y^{3+} in gamma-$Y_2Si_2O_7$ and delta-$Y_2Si_2O_7$ at high temperatures and low Yb contents. IR results confirm the total solid solubility in the system and suggest a constant SiOSi angle of 180 degrees in the Si_2O_7 unit across the system. The temperature-composition diagram of the system, obtained from powder XRD data, is dominated by the beta-RE_2Si2O_7 polymorph, with gamma-$RE_2Si_2O_7$ and delta-$RE_2Si_2O_7$ showing reduced stability fields. The diagram is in accordance with Felsche's diagram if average ionic radii are assumed for the members of the solid solution at any temperature, as long as the beta-gamma phase boundary is slightly shifted towards higher radii.

Nitrogen plasma functionalization of low density polyethylene
Lopez-Santos, C; Yubero, F; Cotrino, J; Gonzalez-Elipe, AR
Surface & Coatings Technology, **205** (2011) 3356-3364
DOI: 10.1016/j.surfcoat.2010.11.038

Low density polyethylene (LDPE) films have been treated with different nitrogen containing plasmas with the purpose of incorporating nitrogen functional groups on its surface and analyzing the changes experienced in their surface tension. Effects of a dielectric barrier discharge (DOD) at atmospheric pressure and a microwave discharge (MW) at reduced pressure are compared with those obtained by using an atom source supplied with N-2 and mixtures Ar + NH_3 as plasma gas. X-ray photoelectron spectroscopy (XPS) analysis has provided information about the chemical surface changes whereas the surface topography of the treated samples has been examined by atomic force microscopy (AFM). Non-destructive depth profiles of oxygen and carbon have been obtained for the treated and one month aged samples by means of the non-destructive Tougaard's method of XPS background analysis. Generally, an oxygen enrichment of the deeper region of treated LDPE surfaces has been observed. Chemical derivatization of the treated samples has shown that a DBD plasma with a mixture of Ar + NH_3 was the most efficient treatment for nitrogen and amine group functionalization. It is argued that the high concentration of NW species in this plasma is the most important factor in enhancing the nitrogen functionalization of this polymer. It has been also found that the observed increase in hydrophilicity and surface tension cannot be attributed to the anchored nitrogen functional groups formed on plasma treated LDPE. Differences in the plasma activation behaviour of LDPE and that of other polymers subjected to similar treatments are stressed.

Theoretical and experimental characterization of TiO_2 thin films deposited at oblique angles
Alvarez, R; Gonzalez-Garcia, L; Romero-Gomez, P; Rico, V; Cotrino, J; Gonzalez-Elipe, AR; Palmero, A
Journal Of Physics D-Applied Physics, **44** (2011) 385302
DOI: 10.1088/0022-3727/44/38/385302

The microstructural features of amorphous TiO_2 thin films grown by the electron beam physical vapour deposition technique at oblique angles have been experimentally and theoretically studied. The microstructural features of the deposited films were characterized by considering both the column tilt angle and the increase in the column thickness with height. A Monte Carlo model of film growth has been developed that takes into account surface shadowing, short-range interaction between the deposition species and the film surface, as well as the angular broadening of the deposition flux when arriving at the substrate. The good match between simulations and experimental results indicates the importance of these factors in the growth and microstructural development of thin films deposited at oblique angles.

Supported plasma-made 1D heterostructures: perspectives and applications
Borras, A; Macias-Montero, M; Romero-Gomez, P; Gonzalez-Elipe, AR
Journal Of Physics D-Applied Physics, **44** (2011) 174016
DOI: 10.1088/0022-3727/44/17/174016

Plasma-related methods have been widely used in the fabrication of carbon nanotubes and nanofibres (NFs) and semiconducting inorganic nanowires (NWs). A natural progression of the research in the field of 1D nanostructures is the synthesis of multicomponent NWs and NFs. In this paper we review the state of the art of the fabrication by plasma methods of 1D heterostructures including applications and perspectives. Furthermore, recent developments on the use of metal seeds (Ag, Au, Pt) to obtain metal@oxide nanostructures are also extensively described. Results are shown for various metal substrates, either metal foils or supported nanoparticles/thin films of the metal where the effects of the size, surface coverage, percolation degree and thickness of the metal seeds have been systematically evaluated. The possibilities of the process are illustrated by the preparation of nanostructured films and supported NFs of different metal@oxides (Ag, Au and SiO_2, TiO_2, ZnO). Particularly, in the case of silver, the application of an oxygen plasma treatment prior to the deposition of the oxide was critical for efficiently controlling the growth of the 1D heterostructures. A phenomenological model is proposed to account for the thin-film nanostructuring and fibre formation by considering basic phenomena such as stress relaxation, inhomogeneities in the plasma sheath electrical field and the local disturbance of the oxide growth.

Analysis of artificial opals by scanning near field optical microscopy
Barrio, J; Lozano, G; Lamela, J; Lifante, G; Dorado, LA; Depine, RA; Jaque, F; Miguez, H
Journal Of Applied Physics, **109** (2011)
DOI: 10.1063/1.3573777

Herein we present a detailed analysis of the optical response of artificial opal films realized employing a near-field scanning optical microscope in collection and transmission modes. Near-field patterns measured at the rear surface when a plane wave impinges on the front face are presented with the finding that optical intensity maps present a clear correlation with the periodic arrangement of the outer surface. Calculations based on the vector Korringa-Kohn-Rostoker method reproduce the different profiles experimentally observed as well as the response to the polarization of the incident field. These observations constitute the first experimental confirmation of the collective lattice resonances that give rise to the optical response of these three dimensional periodic structures in the high-energy range.

Nitridation of nanocrystalline TiO2 thin films by treatment with ammonia
Romero-Gomez, P; Rico, V; Espinos, JP; Gonzalez-Elipe, AR; Palgrave, RG; Egdell, RG
Thin Solid Films, **519** (2011) 3587-3595
DOI: 10.1016/j.tsf.2011.01.267

Nanocrystalline anatase (TiO_2) thin films prepared by a physical vapour deposition method were nitrided by annealing in flowing NH3 at temperatures ranging between 650 degrees C and 700 degrees C. It was established that there was a narrow window of temperatures which allowed both incorporation of interstitial nitrogen into the films with retention of the anatase phase without chemical reduction and preservation of the characteristic nanocrystalline morphology. These optimally modified films responded to visible light in photowetting tests and showed the ability to degrade an organic dye under visible light irradiation.

Lateral and in-depth distribution of functional groups on diamond-like carbon after oxygen plasma treatments
Lopez-Santos, C; Yubero, F; Cotrino, J; Gonzalez-Elipe, AR
Diamond And Related Materials, **20** (2011) 49-56
DOI: 10.1016/j.diamond.2010.11.024

A diamond like carbon material has been exposed to a low pressure microwave and atmospheric pressure plasma of oxygen to enhance its hydrophilicity and surface energy. For comparison, data are also reported after activation with a beam of neutral atoms of oxygen. The surface incorporation of oxygenated functional groups and the determination of the in-depth distribution of this element have been analysed by means of the X ray photoemission spectroscopy (XPS). Atomic force microscopy (AFM) has been used to get information of the surface topography and, by recording friction maps of the surface, the lateral distribution of oxygenated functional groups formed after the different activation treatments. Differences in surface composition, topography and in-depth and lateral distribution of oxygen have been correlated with the intrinsic characteristics of the activation plasma processes.

Comments on "An Essay on Contact Angle Measurements": Determination of Surface Roughness and Modeling of the Wetting Behavior
Terriza, A; Alvarez, R; Yubero, F; Borras, A; Gonzalez-Elipe, AR
Plasma Processes And Polymers, **8** (2011) 998-1002
DOI: 10.1002/ppap.201100081

This commentary addresses the problem of determining surface roughness values and their use to assess the wetting behavior of surfaces. For very rough surfaces it is shown that depending on the observation scale by atomic force microscopy (AFM) quite different RMS roughness values can be obtained and that only the values taken at saturation can be used for properly describing the roughness of the examined materials. This effect has clear consequences when trying to apply wetting models to account for the influence of roughness on contact angles. These ideas are discussed with examples taken from rough polymer surfaces subjected to plasma etching.

Colored semi-transparent Cu-Si oxide thin films prepared by magnetron sputtering
Gil-Rosta, J; Yubero, F; Fernandez, R; Vilajoana, T; Artus, P; Dursteler, JC; Cotrino, J; Ortega, I; Gonzalez-Elipe, AR
Optical Materials Express, **1** (2011) 1100-1112

Colored semi-transparent Cu-Si oxide thin films have been prepared by reactive magnetron sputtering from a single cathode of copper-silicon composition. Thin films of different composition and optical response were obtained by changing process parameters like the relative amount of copper in the target and the O(2)/Ar mixture of the reactive plasma gas. The film characteristics were analyzed by several techniques. Their optical properties (refractive index, absorption coefficient, color) have been correlated with the process parameters used in the film preparation as well as with the film stoichiometry and chemistry.

Determination of pore size distribution at the cell-hydrogel interface
Leal-Egana, A; Dietrich-Braumann, U; Diaz-Cuenca, A; Nowicki, M; Bader, A
Journal Of Nanobiotechnology, **9** (2011) 24
DOI: 10.1186/1477-3155-9-24

Background: Analyses of the pore size distribution in 3D matrices such as the cell-hydrogel interface are very useful when studying changes and modifications produced as a result of cellular growth and proliferation within the matrix, as pore size distribution plays an important role in the signaling and microenvironment stimuli imparted to the cells. However, the majority of the methods for the assessment of the porosity in biomaterials are not suitable to give quantitative information about the textural properties of these nano-interfaces. Findings: Here, we report a methodology for determining pore size distribution at the cell-hydrogel interface, and the depth of the matrix modified by cell growth by entrapped HepG(2) cells in microcapsules made of 0.8% and 1.4% w/v alginate. The method is based on the estimation of the shortest distance between two points of the fibril-like network hydrogel structures using image analysis of TEM pictures. Values of pore size distribution determined using the presented method and those obtained by nitrogen physisorption measurements were compared, showing good agreement. A combination of these methodologies and a study of the cell-hydrogel interface at various cell culture times showed that after three days of culture, HepG(2) cells growing in hydrogels composed of 0.8% w/v alginate had more coarse of pores at depths up to 40 nm inwards (a phenomenon most notable in the first 20 nm from the interface). This coarsening phenomenon was weakly observed in the case of cells cultured in hydrogels composed of 1.4% w/v alginate. Conclusions: The method purposed in this paper allows us to obtain information about the radial deformation of the hydrogel matrix due to cell growth, and the consequent modification of the pore size distribution pattern surrounding the cells, which are extremely important for a wide spectrum of biotechnological, pharmaceutical and biomedical applications.

ARTÍCULOS PUBLICADOS EN REVISTAS NO-SCI / PAPERS IN NON-SCI JOURNALS

Hydroxyapatite Synthesis On Mesoporous Silica: A High Resolution Electron Microscopy Study
Acosta, DR; Diaz-Cuenca, A
Acta Microscopica, **20** (2011) 29-35

Effect of titanium ion substitution in the barium hexaferrite studied by Mössbauer spectroscopy and X-ray diffraction
Quiroz, P.; Halbedel, B.; Bustamante, A.; González, J.C.
Hyperfine Interact, **202** (2011) 97-106

Kinetic study of the thermal transformation of limonite to hematite by X-ray diffraction, μ-Raman and Mössbauer spectroscopy
P.R. Palacios, A. Bustamante, P. Romero-Gómez, J.C. González
Hyperfine Interact, **203** (2011) 113-118

Visual gas sensors based on dye thin films and resonant waveguide gratings
L. Davoine, M. Schnieper, A. Barranco, F.J. Aparicio
Proceedings of SPIE, **8073** (2011) 807312

CONGRESOS Y REUNIONES INTERNACIONALES / INTERNATIONAL CONGRESS AND MEETINGS

COMUNICACIONES EN CONGRESOS Y REUNIONES / COMMUNICATIONS IN CONGRESS AND MEETINGS

MRS 2011 Spring Meeting. Symposium S: Plasma-Assisted Materials Processing and Synthesis

25 – 29 abril [San Francisco, EE.UU.]

Surface functionalization of polymers and DLC materials by plasma treatments
A. Terriza, F. Yubero, A.R. González-Elipe, M.C. López Santos
Comunicación oral

From Plasma Deposited Thin Films to the preparation of supported oxide Nanofibers
A.R. González-Elipe
Conferencia invitada

E-MRS ICAM IUMRS 2011 Spring Meeting

9 – 13 mayo [Niza, Francia]

Aligned Semiconductor Oxide Nanostructures for Dye Sensitized Solar Cells
I. Gonzalez-Valls, L. González-García I. Gonzalez-Valls, L. González-García, M Lira-Cantú, A. Barranco, A.R. González-Elipe
Comunicación oral

Aligned TiO2 Nanocolumnar layers prepared by GLAD-PVD for Transparent Dye Sensitized Solar Cells
L. González-García I. Gonzalez-Valls, L. González-García, M Lira-Cantú, A. Barranco, A.R. González-Elipe
Poster

Dichroic Au-TiO2 Nanocomposite Thin Films prepared by glancing angle evaporation and infiltration of gold
L. González-García, Julian Parra, Angel Barranco, Agustín R. González-Elipe
Poster

3rd international Conference on Hybrid and Organic Photovoltaics

15 – 18 mayo [Valencia, España]

Effect of the inclusion of diffuse scattering particles on the light harvesting efficiency and optical absorption profile in dye sensitized solar cells

F.E. Gálvez, H. Míguez
Poster

Optimization of porous 1DPC as back reflectors for dye sensitized solar cells
C. López-López, S. Colodrero, A. Forneli, E. Palomares, H. Lindström, H. Míguez
Poster

TERMIS-EU Meeting
7 – 10 junio [Granada, España]

Normal human osteoblasts response to PECVD TiO2 functionalized PLGA membranes designed for guided tissue regeneration (GTR)
M. Salido, A. Terriza, J.L. Vilches, A. Díaz-Cuenca, A. Barranco, A.R. González-Elipe, J. Vilches
Poster

Nanolayers of PECVD TiO2 suitability for human osteoblasts growth for tissue engineering
M. Salido, A. Terriza, D. Torres, E. De la Orden, A. Barranco, A. Díaz-Cuenca, J. Vilches, A.R. González-Elipe
Poster

ICMAT 2011, International Conference on Materials for Advanced Technologies
26 junio – 1 julio [Suntec, Singapur]

Aligned Semiconductor Oxide Nanostructures for Dye Sensitized Solar Cells
I. Gonzalez-Valls, L. González-García, M Lira-Cantú, A. Barranco, A.R. González-Elipe
Comunicación oral

XVIII International Symposium on Metastable, Amorphous and Nanostructured Materials (ISMANAM)
26 junio – 1 julio [Gijón, España]

Interplay Between Controlled Porosity and Optical Performance in Nanostructured Photonic Materials
M.E. Calvo
Conferencia Invitada

8th International Conference on Nanosciences & Nanotechnologies (NN11)
12 – 15 julio [Thessaloniki, Grecia]

Citrate mediated synthesis and properties of uniform spheres of LnPO4 (Ln = La, Ce) monazite and Ln:LaPO4 (Ln = Eu, Ce, Ce+Tb) phosphors
N. O-Nuñez, S. Rodríguez-Liviana, M. Ocaña
Poster

ICPIG 2011 Conference

28 agosto – 2 septiembre [Belfast, Irlanda del Norte]

Growth of SiO2 Thin Films by Plasma-Assisted Reactive Magnetron Sputtering Under the Impingement of Positive and Negative Ions
M. Macias-Montero, F.J. Garcia-Garcia, R. Álvarez, J. Gil-Rostra, F. Yubero, A. R. Gonzalez-Elipe, A. Palmero, J. Cotrino
Poster

14th European Conference on Applications of Surface and Interface Analysis ECASIA'11

4 – 9 septiembre [Cardiff, UK]

Experimental evaluation of IMFP of photoelectrons in compact and mesoporous SiO_2 films with kinetic energies between 8 and 13 keV
F.J. Ferrer, L. González, J. Gil-Rostra, J. Rubio-Zuazo, G. Castro, F. Yubero
Comunicación oral

Software package to calculate the effects of core hole and surface excitations on XPS
S. Tougaard, F. Yubero
Comunicación oral

Interpretation of eRBS spectra for H quantification at surfaces
R. Álvarez, K. Tokesi, F. Yubero
Comunicación oral

Low refractive index SiOF thin films prepared by reactive magnetron sputtering
J. Gil-Rostra, F.J. Ferrer, F.J. García-García, A.R. González-Elipe, F. Yubero
Poster

EUROMAT 2011

12 – 15 septiembre [Montpellier, Francia]

Resonators built in one dimensional photonic crystals for modification of the optical properties of nanoparticles
O. Sánchez-Sobrado, M. Calvo, G. Lozano, N. Núñez, M. Ocaña, A. Sánchez-Iglesias, L. Liz-Marzán, H. Míguez
Poster

Mesostructured thin films as building blocks for multifunctional photonic crystals
N. Hidalgo Serrano, M. Calvo, H. Míguez
Poster

Flexible, self-standing and selective UV-VIS-NIR optical filters based on polymer infiltration of nanoparticle layers
M.E. Calvo, O. Sánchez Sobrado, H. Míguez
Comunicación oral

5th UHMWPE International Meeting

22 – 23 septiembre [Philadelphia, UK]

Detection of vitamin E in ultra high molecular weight polyethylene by colorimetry and water contact angle techniques
A. Terriza, M.J. Martínez-Morlanes, F. Yubero, J.A. Puértolas
Poster

Diamond like carbon coatings for UHMWPE: a way to minimize wear and bacterial adherence
G. del Prado, A. Terriza, A. Ortiz-Pérez, D. Molina-Manso, I. Mahillo, F. Yubero, J.E. Puértolas, E. Gómez-Barrena, and J. Esteban
Poster

Materials Research Society (MRS) Fall Meeting 2011, Symposium R

28 noviembre – 2 diciembre [Boston, Estados Unidos de América]

Angular response of photonic crystal based dye sensitized solar cells
C. López-López, J.M. Luque, S. Colodrero, G. Lozano, M.E. Calvo, H. Míguez
Poster

Flexible, self-standing and selective UV-VIS-NIR optical filters based on polymer infiltration of nanoparticle layers
M.E. Calvo, J.R. Castro Smirnov, H. Míguez
Comunicación oral

Effect of light scattering design on the incident photon to current conversion efficiency of dye solar cells
F.E. Gálvez, E. Kenppainen, J. Halme, H. Míguez
Comunicación oral

Optimized design of porous 1DPC for DSC: effect on conversion efficiency and optical properties
S. Colodrero, C. López-López, G. Lozano, A. Forneli, E. Palomares, D. Colonna, A. Di Carlo, H. Míguez
Comunicación oral

CONGRESOS Y REUNIONES NACIONALES / NATIONAL CONGRESS AND MEETINGS

COMUNICACIONES EN CONGRESOS Y REUNIONES / COMMUNICATIONS IN CONGRESS AND MEETINGS

IMAGINENANO 2011, Nano&Med Conference
11 – 14 abril [Bilbao, España]

The potential of combining silica-based mesoporous materials with osteoprogenitor cells for bone repair
L. Santos-Ruiz, D. Amat, A. Díaz-Cuenca, P.J. Maireles, J. Becerra
Poster

Magneto-Plasmonic Nanostructured Materials for Gas Sensors Applications
L. González-García M.G. Manera, G. Montagna, E. Ferreiro-Vila, , J.R. Sánchez-Valencia, A.R. González-Elipe, A. Cebollada, J.M. García-Martín, A. García-Martín, G. Armelles, R. Rella
Comunicación oral

VII Reunión Española de Optoelectrónica
29 junio – 1 julio [Santander, España]

Del Azul al Magenta: Sintonizabilidad del color de la emisión de “up-conversion” en nano-cristales de YF_3:Tm,Yb
M. Quintanilla, N.O. Nuñez, E. Cantelar, M. Ocaña, F. Cussó
Poster

V Jornadas Anuales CIBER-BBN
12 – 13 septiembre [Zaragoza, España]

Osteoprogenitor cells interaction with mesoporous ceramic materials. In vitro and in vivo assays
D. Amat, A. Díaz-Cuenca, P.J. Maireles, J. Becerra, L. Santos-Ruiz
Poster

Novel materials for endoprosthesis and bone substitutes in orthopaedic surgery
L. Santos-Ruiz, R. Rico, D. Amat, E. Guerado, D. Monopoli, A. Díaz-Cuenca, P.J. Maireles, F. Orgaz, J. Becerra
Poster

Reunión Bienal de Física
19 – 23 septiembre [Santander, España]

Plasmas de baja temperatura y aplicaciones en nanotecnología de superficies
A. R. Gonzalez-Elipe
Conferencia invitada

VI Congreso de la Sociedad Española de Terapia Génica y Celular
21 – 23 septiembre [Zaragoza, España]

Adhesión celular in vitro e in vivo sobre materiales Cerámicos mesoporosos nanoestructurados: SBA-15, HA-SBA-15 y MCM-41
D. Amat, A. Díaz-Cuenca, J. Becerra, L. Santos-Ruiz
Poster

XIV Congreso de la Sociedad Española de Biología Celular
12 – 15 diciembre [Málaga, España]

Exploring novel materials and surface treatments to improve endoprosthesis
L. Santos-Ruiz, R. Rico, D. Amat, E. Guerado, D. Monopoli, A. Díaz Cuenca, P.J. Maireles, F. Orgaz, J. Becerra
Poster

FORMACION / TRAINING

TESIS DOCTORALES/ DOCTOR DEGREE THESIS

Título:	**Desarrollo de láminas luminiscentes por tecnología de plasma para su integración en sensores fotónicos**
Autor:	Francisco Javier Aparicio Rebollo
Director:	Angel Barranco Quero
Centro:	Universidad de Sevilla
Título:	**Propiedades fotofuncionales de nanoestructuras superficiales de óxidos preparadas mediante plasma y haces de iones**
Autor:	Pablo Romero Gómez
Director:	Agustín R. González-Elipe
Centro:	Universidad de Sevilla
Título:	**Optical Absorption and Emission of Nanomaterials Integrated in One-Dimensional Photonic Crystals**
Autor:	Olalla Sánchez Sobrado
Directores:	Hernán Míguez García

Centro: Universidad de Sevilla

Título: **Transformación hidrotermal de silicatos laminares en presencia de fluidos alcalinos. Escenarios naturales y artificiales**
Autor: Marco Mantovani
Directores: Ana Isabel Becerro Nieto
Calificación: Sobresaliente “Cum Laude”
Centro: Universidad de Sevilla

Formación de Graduados / Master Degree Thesis

Título: **Estudio de las propiedades Opticas de nanoestructuras columnares de Plata**
Autor: Alejandro Nicolás Fillipin
Directores: Ana Borrás Martos y Agustín R. González-Elipe
Grado: Trabajo Fin de Master
Centro: Universidad de Sevilla
Año Académico: 2010-2011

Título: **Crecimiento de nanoestructuras orgánicas soportadas en sustratos heteroestructurados de microestructura controlada**
Autor: Miguel Angel Betanzo Flor
Directora: Ana Borrás Martos
Grado: Trabajo Fin de Master
Centro: UNED
Año Académico: 2010-2011

Equipamiento Científico Available Equipment

- Sistema de Magnetron Sputttering para la preparación de láminas delgadas
- Potenciostato y sistema electroquímico
- Sistema de medida de ángulos de contacto (advancing and receding)
- Equipo de crecimiento en vacío de nanofibras y otros materiales nanoestructurados
- Microscopio de efecto túnel (STM)
- Sistema de desorción térmica programada
- Espectrómetro de Fotoemisión (XPS)
- Analizador de potencial Z, tamaño de partícula y pesos moleculares (Malvern, ZS90)
- Bomba híbrida de vacío resistente a químicos VACUUBRAND RC-6
- Software y sondas para monitorización para equipo de liofilización CHRIST EPSILON 2-4 LSC

- Liofilizador de altas prestaciones Epsilon 2-4 (CHRIST)
- Estufa de desecación de 90 litros (RAYPA)
- Cámara Incubadora Opaq + Orbital Maxi (OVAN)
- pH & Ion-metro GLP 22+ (CRISON A)
- Malvern, Modelo Zetasizer Nano: para determinar mediante "Dynamic light scattering" la distribución de tamaños de partícula de sistemas coloidales en suspensión (disolvente acuoso u orgánico) en los rangos 1-3000 nanómetros. Este equipo también es adecuado para la evaluación del potencial "Z" de sistemas coloidales en suspensión (disolvente acuoso u orgánico) mediante medidas de Movilidad Electroforética.
- Colorímetro Dr. Lange: para la medida de parámetros de color (x, y, Y/L*a*b*, etc.) de superficies y polvos
- Ellipsómetro spectroscopico Woolan VB-400 con rango de frecuencias entre 300 y 1700 nm. Medida de índices de refracción y coeficiente de extención de capas delgadas y superficies.
- Espectrómetro visible-UV CARY-100. Medidas de coeficiente de absorción con luz normal y polarizada.
- Fluorímetro espectroscópico (HORYBA Jobin Yvon Fluorolog) con accesorio para la determinación de tiempos de vida. Microscopio de fluorescencia (HORYBA Jobin Yvon sigle photon controller: FluoroHub).
- Medidor de ángulos de contacto líquidos. Medidas ángulos de avance y retroceso, así como de energías de adhesión de líquidos sobre superficies (Dataphysics Contact Angle System SCA 20).
- Medida de cuatro puntos de conductividad eléctrica en superficies y láminas delgadas (Fuente de corriente Keithley 617 y voltímetro Keithley 2400).
- Medidas eléctricas en capas delgadas en función de la temperatura y la atmósfera
- Microscopio de Fuerzas atómicas (AFM) para la caracterización de superficies (Cervantes de Nanotec).
- Microscopio de efecto túnel (STM) con posibilidad de trabajar desde nitrógeno líquido hasta 600 ºC (VT-STM de Omicrom).
- Técnicas de caracterización de plasmas: sonda de Langmuir (Plasma Consult single and double sound), espectroscopía de emisión óptica (Avantes 200-900 nm resolución 1 nm) y espectrometría de masas (Hyden=
- Espectrómetro FT-IR con celda DRIFT (Pelkin elmer Spectrum One)
- Sistema de medida de porosidades en capas delgadas.
- Sistema de desorción térmica programada dotado con espectroscopía Auger (VG-8047).
- Espectrómetro de XPS (espectrómetro VSW) con sistema REELS de alta resolución (Kimball Physics EGPS-1022B) y fuente de átomos incorporada (Oxford Scientific Osprey plasma Source).

DISEÑO DE NANOMATERIALES Y MICROESTRUCTURAS

TAILORED NANOMATERIALS AND MICROSTRUCTURE

PROYECTOS DE INVESTIGACIÓN / RESEARCH PROJECTS

Laboratorio avanzado para el análisis de nanomateriales funcionales Advanced laboratory for the nano-analysis of novel functional materials (AL-NANOFUNC)

Código/Code:	REGPOT-CT-2011-285895
Periodo/Period:	01-10-2011 / 30-03-2015
Organismo Financiador/Financial source:	Unión Europea
Importe total/Total amount:	2.687.409 €
Investigador responsable ICMS Research head ICMS:	Asunción Fernández Camacho
Componentes/Research group:	T. Cristina Rojas, M.Carmen Jiménez, Gisela Arzac, Olga Montes, Inmaculada Rosa, Rafael Alvarez, Vanda Godinho, Juan Carlos Sánchez-López, Hernán Míguez, Agustín R. González-Elipe, Manuel Ocaña, M. Jesús Sayagués, Lionel Cervera, Roland Schierholz, Salah Rouillon, Lucia Castillo, Rocío García, Carlos García-Negrete, Jaime Caballero

RESUMEN / ABSTRACT

El proyecto AL-NANOFUNC ha sido diseñado para poner en marcha en el Instituto de Ciencia de los Materiales de Sevilla (ICMS, CSIC-Univ.Sevilla, España) un laboratorio avanzado para el Nano-análisis de nuevos materiales funcionales. Las técnicas de Nanoscopía avanzada, basadas en equipos de microscopía electrónica de última generación, se dedicarán a la investigación de vanguardia en temas específicos de gran interés: i) Nanomateriales para aplicaciones energéticas sostenibles; ii) películas delgadas multifuncionales y recubrimientos nanoestructurados; iii) materiales nano-estructurados para fotónica y sensores.

Para situar a los laboratorios del ICMS en una posición de liderazgo que sea competitiva en un escenario mundial, el proyecto AL-NANOFUNC contempla la puesta al día del potencial investigador actual en varias direcciones: i) Mejorar las capacidades de equipamiento en relación a la microscopía electrónica analítica de alta resolución; ii) mejorar el impacto de la investigación básica a través de la contratación de investigadores especializados y el intercambio transnacional con los centros de referencia en Europa, iii) desarrollar y mejorar el potencial de innovación de la investigación del ICMS abriendo las nuevas instalaciones a empresas y centros relacionados; iv) organizar talleres, conferencias y actividades de difusión para mejorar la visibilidad de la investigación.

En el proyecto se propone también una estrecha colaboración con centros de referencia y empresas de Lieja (Bélgica), Graz (Austria), Jülich (Alemania), Oxford (Inglaterra), Cambridge (Inglaterra), Dübendorf (Suiza) y Rabat (Marruecos), así como con laboratorios de Universidades Andaluzas.

Cinco empresas en Andalucía colaborarán también en estrecha sinergia para promover las líneas estratégicas de interés a largo plazo de la región en los productos de piedra natural y artificial y los sectores de energía solar y energías renovables.

The AL-NANOFUNC project has been designed to install and fully develop at the Materials Science Institute of Seville (ICMS, CSIC-Univ.Seville, Spain) an advanced laboratory for the Nano-analysis of novel functional materials. Advanced Nanoscopy facilities, based on latest generation electron microscopy equipments, will be devoted to breakthrough research in specific topics of high interest: i) Nanomaterials for sustainable energy applications; ii) protective and multifunctional thin film and nanostructured coatings; iii) nanostructured photonic materials and sensors.

To take the ICMS laboratories to a leading position that is competitive in a world-wide scenario, the AL-NANOFUNC project is contemplated to up-grade the actual research potential in several directions: i) improve equipment capabilities regarding the Analytical High Resolution Electron Microscopy facilities; ii) improve the impact and excellence of basic research through hiring of experienced researchers and transnational exchange with the reference centers in Europe; iii) develop and improve the innovation potential of the ICMS's research by opening the new facilities to companies and stakeholders; iv) organize workshops and conferences, dissemination and take-up activities to improve research visibility.

Close collaborations with reference centers and companies in Liège (Belgium), Graz (Austria), Jülich (Germany), Oxford (England), Cambridge (England), Dübendorf (Switzerland) and Rabat (Morocco), as well as with laboratories at Andalucian Universities, are foreseen in this project.

Five companies in Andalusia will also collaborate in close synergies to promote the long-term strategic lines of interest for the region in the natural and artificial stone products and solar and renewable energy sectors.

Desarrollo y diseminación de nuevas técnicas de caracterización nanomecánica y standards

Creating and disseminating novel nano-mechanical characterization techniques and standars (NANOINDENT)

Código/Code:	NMP3-CA-2008-218659
Periodo/Period:	01-09-2008 / 31-08-2011
Organismo Financiador/Financial source:	Unión Europea
Importe total/Total amount:	14.500 €
Investigador responsable ICMS /Research head ICMS:	Fernández, A.
Componentes/Research group:	Godinho, V., Philippon, D.

RESUMEN / ABSTRACT

El proyecto se dedica al desarrollo, mejora, y standarización de las técnicas de caracterización, los métodos y los equipos en los ensayos nano-mecánicos. Las actividades a nivel Europeo, coordinadas por un centro virtual, mejorarán la metrología de nanoindentación actual y permitirán un conocimiento más profundo de la relación estructura-propiedades en la nano-escala. Estos métodos son una herramienta única para caracterizar el comportamiento mecánico en la nanoescala de nanocomposites, nanocapas e interfases. Este trabajo también producirá una base sólida para definer y preparer nuevos standards que soporten la metodología de caracterización de los nanomateriales. Las etapas incluyen el desarrollo de los métodos clásicos de nanoindentación dinámica y su aplicación a campos nuevos como el rayado y las medidas de desgaste y la aplicación de nano-indentadores modificados. También se trabajará en la determinación uniforme de los parámetros instrumentals y en la definición de standards par alas nuevas aplicaciones. El centro virtual diseminará la información sobre la base de una nueva "Base de datos para la caracterización Nano-mecánica". Esto se conseguirá a través de los trabajos de "round robin" entre los socios é incluirá igualmente datos de otras fuentes de investigación y la búsqueda bibliográfica.

Our project aims to gather, improve, catalogue and present characterisation techniques, methods and equipment for nanomechanical testing. European-wide activities coordinated by a new virtual centre will improve existing nanoindentation metrology to reveal structure-properties relationship at the nano-scale. These methods are the only tools to characterise nanocomposite, nanolayer and interface mechanical behaviours in the nanometre range. This work will also lay down a solid base for subsequent efforts for defining and preparing new standards to support measurement technology in the field of nanomaterials characterisation. Steps include development of the classical and the dynamic nanoindentation method and its application to new fields, application of modified nano-indenters to new fields as scratching and wear measurement, firm and uniform determination of instrumental parameters and defining new standard samples for the new applications. The virtual centre will disseminate information based on a new "Nanocharacterisation database" built on two definite levels: on a broader level partners will inventory and process all novel nanocharacterisation techniques and, in narrower terms, they will concentrate on nanomechanical characterisation. This will be achieved through the synchronisation of efforts set around a core of round robins but the database will include data of other channels as parallel research work and literature recherché.

Estructura, empaquetamiento y propiedades tribológicas de monocapas autoensambladas de alquilaminas lineales de cadena larga

Structure, packing and tribology of Fatty Self-assembled monolayers of Alkylamines

Código/Code:	CTQ2008-00188
Periodo/Period:	01-01-2009 / 31-12-2011
Organismo Financiador/Financial source:	Ministerio de Ciencia e Innovación
Importe total/Total amount:	77.440 €
Investigador responsable/Research head:	Benítez Jiménez, José Jesús
Componentes/Research group:	Salmeron, M., Garzón Garzón, E., Sánchez Soto, P.J., Heredia Guerrero, J.A.

RESUMEN / ABSTRACT

El presente proyecto se encuadra en la línea de investigación que analiza las propiedades tribológicas de monocapas autoensamblas. Más concretamente en la contribución de eventos a escala molecular en la propiedades fricciónales de sistemas modelos a base de monocapas autoensambladas de moléculas alquílicas. La información de que se dispone para sistemas modelo a base de tioles sobre oro y alquisilanos sobre mica empleando técnicas de sonda de proximidad, fundamentalmente AFM (atomic force microscopy), es muy amplia. La aportación que proporciona este proyecto es más novedosa y parte del empleo de otro sistema modelo, alquilaminas de cadena larga sobre mica. La interacción del grupo funcional amino con el soporte mica es considerablemente menor que la propia del tiol-oro y el silano-mica lo que se traduce en una menor calidad del empaquetamiento molecular. El control de la calidad del empaquetamiento mediante el ajuste de las condiciones de preparación permitiría disponer de un sistema con gran contenido de defectos sobre el que establecer la influencia de éstos en las propiedades friccionales. La consistencia mecánica de las capas de alquilaminas sobre mica impide su resolución estructural a nivel molecular empleando el microscopio AFM en modo de contacto, por lo que se propone una metodología que englobe y complemente el característico análisis friccional y la microscopia SPFM (scanning polarization force microscopy). La técnica SPFM se basa en la medida de la fuerza electrostática que se establece entre una sonda polarizada y las cargas, dipolos permanentes o inducidos a nivel superficial. Dadas las marcadas diferencias entre las magnitudes dieléctricas de la mica y la monocapa alquílica, la metodología propuesta parte del análisis del efecto de pantalla de la capa autoensamblada sobre la señal en polarización del soporte y su relación con el grado de compactación de ésta. La técnica SPFM es especialmente sensible a la presencia de agua dado su elevada constante dieléctrica por lo que resulta muy adecuada para la detección de vacantes o intersticios susceptibles de adsorber agua en el seno de la capa autoensamblada. En último extremo, el proyecto tiene por objeto la correlación de las propiedades friccionales con la evaluación SPFM del grado de empaquetamiento de las capas preparadas.

The aim of this research project is to study the contribution of molecular scale events to the tribological properties of self-assembled monolayers of alkyl molecules. The amount of topographic and frictional AFM data available on typical self-assembled systems such as thiols on gold and silanes on mica is very extensive. Here, we propose alkylamines on mica as a new self-assembled system. The reason is that the weaker interaction between the amino end group and mica, if compared with S-gold and silane-mica, leads to a less effective molecular packing. The ability to control the quality of molecular packing by tunning the preparation conditions is a good model to test the contribution of defects to friction. Molecular resolution using contact AFM is not possible on alkylamine self-assembled monolayers, so there is a lack of structural information on this system. The new methodology described in this project proposes the use of Scanning Polarization Force Microscopy (SPFM) to address this issue based on the high polarization signal contrast between mica and self-assembled layers. Furthermore, the high sensitivity of SPFM to the presence of water molecules filling vacancies, can be used to evaluate the quality of the molecular packing by monitoring the screening effect exerted by the self-assembled layer. Consequently, the study of both, the frictional and the SPFM properties of self-assembled monolayers of alquilamines, are complementary to describe the contribution of defects to friction.

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Recubrimientos nanoestructurados multifuncionales para aplicaciones mecánicas y tribológicas (NANOMETRIB)

Multifunctional nanostructured coatings for mechanical and tribological applications (NANOMETRIB)

Código/Code: MAT2007-66881-C02-01 (Plan Nacional)
Periodo/Period: 01-10-2007 / 30-09-2011
Organismo Financiador/Financial source: Ministerio de Ciencia e Innovación
Importe total/Total amount: 232.320 €
Investigador responsable/Research head: Juan Carlos Sánchez López
Componentes/Research group: Asunción Fernández Camacho, Cristina Fernández, Miguel Angel Muñoz-Márquez, Said El Mrabet, Vanda Godinho, M. David Abad

RESUMEN / ABSTRACT

En el campo de las aplicaciones mecánicas y tribológicas, las investigaciones se dirigen al desarrollo de nuevos sistemas que consigan aumentar la eficiencia de operaciones industriales, equipos o herramientas mediante el incremento de la dureza, la reducción de la fricción y la velocidad del desgaste de los materiales en contacto o la resistencia a la oxidación. Estas mejoras suponen un ingente ahorro económico y energético al alargar la vida media de los materiales sin necesidad de su reparación o cambio, como también, una reducción del empleo de emulsiones lubricantes con aceites o grasas. Este proyecto se propone el desarrollo de nuevos recubrimientos nanoestructurados multifuncionales por la técnica de PVD-Magnetron Sputtering para aplicaciones mecánicas y tribológicas en los que se alcance un equilibrado compromiso entre todas las propiedades mencionadas de fricción, dureza, estabilidad térmica. La combinación de múltiples funciones en un mismo material dota de un extraordinario valor añadido al sistema. Para lograr este objetivo general se van a preparar recubrimientos caracterizados donde el tamaño y distribución de las fases componentes, la composición química y su microestructura estén confinados en el rango nanométrico. Los sistemas elegidos comprenden cristales de materiales duros (nitruros, carburos o boruros de metales de transición: Cr, Ti, W) que pueden estar rodeados de una segunda fase que actúe como lubricante a base de C o dicalcogenuros de W) y dopados con ciertos metales para incrementar su resistencia térmica (V ó Nb). En todos los casos, el proyecto comprende su síntesis, caracterización estructural y química, así como su validación práctica en ensayos mecánicos y tribológicos. El estudio de la relación existente entre la microestructura y las propiedades medidas será un objetivo esencial puesto que permitirá una mayor comprensión de los mecanismos de actuación, y por ende, la optimización de tales sistemas nanoestructurados para su mejor aprovechamiento tecnológico.

In this In the field of mechanical and tribological applications, the investigations are oriented towards the development of new systems capable to increase the performance of industrial operations, machines or tools by increasing the hardness and diminution of the friction and wear rate of materials under contact or increasing the oxidation resistance. These improvements suppose an energy-saving and cost reduction due to increase of tool life-time

without needs of reparation as well as a reduction in the employment of lubricant emulsions with oils and greases. This project goal is to develop bew multifunctional nanostructured systems by the Magnetron Sputtering PVD technique for mechanical and tribological applications where an adequate balance among the above-mentioned properties as friction, hardness and thermal stability are searched. The combination of multiple functions into a materials increase noticeably the material added value. To achieve this general objective, different coatings will be prepared by confinement of size and distribution of phases, chemical composition and microstructure in the nanometric regime. The chosen systems are constituted by crystals of hard materials (nitrides, carbides and borides of transition metals: Cr, Ti, W) that can be surrounded by a second phase that acts as lubricant based on C or dichalcogenides of W and doped with certain metals to increase their thermal resistance (V or Nb). In all cases, the project comprises their synthesis, chemical and structural characterization, and their practical validation in tribological tests of friction and wear. The establishment of the relationships between microstructure and measured properties will be an essential objective, since it enables the better understanding of the action mechanisms, and thus, the optimisation of such nanostructured multifunctional systems for an improved technological benefit.

Recubrimientos nanoestructurados para operar en vacío

Nanostructured films for operating under vacuum

Código/Code: MAT2010-21597-C02-01 (Plan Nacional)
Periodo/Period: 01-10-2011 / 31-12-2011
Organismo Financiador/Financial source: Ministerio de Ciencia e Innovación
Importe total/Total amount: 14.520 €
Investigador responsable/Research head: Juan Carlos Sánchez López
Componentes/Research group: T. Cristina Rojas Ruiz, Santiago Domínguez Meister

RESUMEN / ABSTRACT

En este proyecto se desarrollarán recubrimientos nanoestructurados por la técnica de magnetron sputtering para lubricación de componentes mecánicos en aplicaciones aeroespaciales. Estos materiales deben proporcionar protección frente al desgaste y baja fricción cuando se usen en condiciones atmosféricas o vacío. Los sistemas elegidos para lograr este compromiso están formados por nanocristales de WC dispersados en una fase amorfa de dicalcogenuro (WS2 or WSe2). Estos lubricantes se esperan que pueden mejorar la resistencia al desgaste, mecánica y a la oxidación en comparación con los recubrimientos convencionales (MoS2 or DLC) usados para estos fines.

In this project, nanostructured coatings will be prepared using a magnetron sputtering process for lubrication of mechanical components used in aerospace applications. These materials must provide wear protection and low friction when operating in ambient air or vacuum environment. The chosen systems to obtain this compromise are constituted by WC nanocrystals dispersed in an amorphous dichalchogenide phase (WS2 or WSe2). These solid lubricant coatings are proposed to enhance the wear resistance, mechanical strength and oxidation resistance in comparison to their conventional MoS2 or DLC coatings for this kind of applications.

Papel de los aditivos en los sistemas composites de hidruros metálicos reactivos para almacenamiento de hidrógeno
Role of additives in the reactive hydride composite systems for hydrogen storage

Código/Code: CTQ2009-13440
Periodo/Period: 01/01/2010 AL 31/12/2012
Organismo Financiador/Financial source: Ministerio de Educación y Ciencia
Importe total/Total amount: 174.240 €
Investigador responsable/Research head: Fernández Camacho, A.
Componentes/Research group: Fernandez Camacho, A., López Cartés, C., Rojas Ruíz, T.C., Arzac, G.; Hufschmidt, D., Cecchini, R., Deprez, E

RESUMEN / ABSTRACT

Dada la problemática actual por el agotamiento a corto-medio plazo de los combustibles fósiles y los cambios climáticos causados por el efecto invernadero, se hace necesaria la reconsideración de una política energética global. El hidrógeno como vector de transporte y almacenamiento de energía es un candidato muy atractivo por tratarse de una alternativa viable y limpia.

En el presente proyecto se propone el estudio de los llamados sistemas composites de hidruros reactivos (RHC) para almacenamiento de hidrógeno. Estos sistemas se basan en acoplar un hidruro metálico sencillo (i.e. MgH_2) con un hidruro complejo (típicamente un compuesto borohidruro, i.e $LiBH_4$) para dar una reacción reversible que produce o consume hidrógeno. El sistema puede así usarse como material para almacenamiento de hidrógeno de acuerdo a la siguiente reacción: $MgH_2+2LiBH_4 \leftrightarrow MgB_2+LiH+4H_2$ (11.4 wt% capacidad de almacenamiento de hidrógeno). La reacción mejora el balance de calor, en comparación con el MgH2 puro, al reducir la liberación de calor durante el proceso de carga. Para mejorar los aspectos cinéticos (reducción de las temperaturas y tiempos de operación) se ha propuesto el uso de catalizadores y/o aditivos. El principal objetivo del proyecto es comprender el papel de estos aditivos para mejorar las cinéticas de sorción de hidrógeno. En particular se han seleccionado como aditivos para este estudio los productos comerciales Ti-Isopropoxide ($TiO_4C_{12}H_{28}$), TiO_2 y VCl_3 . También se prepararan en nuestro laboratorio otros catalizadores como Co_3B, Ni_3B o RuCo que igualmente se ensayarán.

Los sistemas se prepararán y activarán por molienda de alta energía de los dos materiales hidruros molidos juntos con ó sin aditivos (5-10 mol%). Los estudios cinéticos se llevarán a cabo a través de medidas de sorción gravimétrica y volumétrica de hidrógeno (desorción o absorción vs. tiempo a T constante) y de la calorimetría de barrido diferencial (DSC). Se llevará también a cabo un estudio exhaustivo de caracterización microestructural y química de los sistemas en las diferentes etapas (tras la molienda, desorbidos y re-absorbidos) con las si-

guientes técnicas: Difracción de rayos X (XRD), microscopía electrónica de transmisión (TEM) acoplada al análisis EDX (energía dispersiva de rayos X) y EELS (espectroscopía de pérdida de energía de electrones), espectroscopía de fotoemisión (XPS) y espectroscopía de absorción de rayos X (XAS). El estudio comparativo de las muestras con y sin aditivos y la correlación entre los estudios cinéticos y el análisis microestructural y químico, deben clarificar el mecanismo de la mejora cinética producida por los aditivos. Estos mecanismos están a día de hoy lejos de ser comprendidos. Sobre la base del conocimiento adquirido se espera mejorar de manera significativa estos sistemas en relación a sus aplicaciones para almacenamiento de hidrógeno.

Due to the expected short-medium term exhaustion of fossil fuels and due to clime changes produced by the green house effect, it is necessary to reconsider a new global energy policy. Hydrogen, as a vector for energy storage and transport, is an attractive candidate for a clean handling of energy.

In the present project it is proposed the study of the so called reactive hydride composite systems (RHC) for hydrogen storage. These systems are based in the coupling of a single metal hydride (i.e. MgH_2) with a complex hydride (typically a borohydride compound, i.e $LiBH_4$) to give a reversible reaction that is producing or consuming hydrogen. The system can so be used as a hydrogen storage material according to following reaction: $MgH_2+2LiBH_4 \leftrightarrow MgB_2+LiH+4H_2$ (11.4 wt% hydrogen storage capacity). The reaction is improving the heat transfer handling, as compared to pure MgH_2, by reducing heat release during the charging process. To improve the kinetic aspects (reduction of operation temperatures and times) it has been proposed the use of catalysts a/o additives. The main objective of the project is to understand the role of these additives to improve the hydrogen sorption kinetics. In particular commercial Ti-Isopropoxide ($TiO_4C_{12}H_{28}$) , TiO_2 and VCl_3 have been selected as additives for this study. Also other catalysts like Co_3B, Ni_3B or RuCo will be prepared in our laboratory and also tested.

The systems will be prepared and activated by high energy ball milling of the two hydride materials milled together with or without the additives (5-10 mol%). Kinetic studies will be carried out by gravimetric and volumetric hydrogen sorption measurements (hydrogen desorption or adsorption vs. time at constant T) and differential scanning calorymetry (DSC) analysis. An exhaustive microstructural and chemical analysis of the systems at the different step (as prepared, desorbed and re-absorbed) will be undertaken by following techniques: X-Ray Diffraction (XRD), Transmission Electron Microscopy (TEM) coupled to EDX (energy dispersive X-Ray) and EELS (Electron Energy Loss Spectroscopy) analysis, X-Ray Photoelectrton Spectroscopy (XPS) and X-Ray absorption Spectroscopy (XAS). The comparative study of the samples, with and without additives, and the correlation between the kinetic studies and the microstructural and chemical analysis, should clarify the mechanisms of the kinetic improvements produced by the additives. These mechanisms are today far from being understood. On basis of the acquired knowledge we expect to significantly improve the systems with respect to hydrogen storage applications.

Estudio de la viabilidad de procesos de carbonatación de CO2 mediante compuestos tipo Wollastonita para su aplicación en procesos industriales de captura y reutilización de CO2

Study of the viability of carbonation process through wollastonite-like composites for CO2 capture and re-use industrial processes

Código/Code:	CIT-44000-209-1
Periodo/Period:	01/01/2009 – 31/12/2011
Organismo Financiador/Financial source:	Ministerio de Educación y Ciencia
Importe total/Total amount:	105.825 €
Investigador responsable/Research head:	Esquivias Fedriani, L.
Componentes/Research group:	Esquivias Fedriani, L., Santos Sánchez, Alberto, Morales Flórez, Víctor, Cárdenas Escudero, Cristian, Pereda Briones, Laura

RESUMEN / ABSTRACT

El proyecto Wollastonita aborda el reto actual de reducir las emisiones de dióxido de carbono asociadas a los procesos energéticos e industriales. Es por ello que su principal consiste en el desarrollo de un sistema capaz de capturar grandes cantidades de CO2 y otros gases de efecto invernadero (GEI) de misión localizada, típicamente plantas térmicas de generación de energía eléctrica u cementeras, escalable a nivel industrial. Con la realización de este Proyecto se tratará por una parte de analizar la viabilidad técnica y económica de los procesos de secuestro de CO2 mediante compuestos de sílice y calcio, como es el caso de la wollastonita, y por otra parte, se tratarán de identificar las especificaciones requeridas para el diseño de un sistema integrado de captura y secuestro de CO2 aplicado a una instalación industrial generadora de grandes cantidades de este gas.

Dado que el subproducto de la carbonatación puede ser un mineral valioso, medioambientalmente seguro y termodinámicamente estable, este puede ser reutilizado como materia prima en determinados procesos industriales, dependiendo de su morfología, pureza y tamaño de partícula. Por ello, se estudiarán las posibles aplicaciones de este producto, tratando de establecer en cada caso la relación coste/beneficio. Estas posibilidades supondrían el hecho de conseguir un ciclo completo para el proyecto, desarrollando un proceso viable para la reducción de los GEI y su eliminación o reutilización completa ulterior.

The Wollastonite Project deals the current challenge of reducing the industrial carbon dioxide emissions. Its main goal consists in developing a system able to capture huge amounts of CO2 and other green-house gasses (GHG) from localized sources, typically, thermal plants and cement factories, so the designed technology could be scaled-up at an industrial level. On

the one hand, the economic and technological viability of the carbon dioxide capturing processes based on composites of calcium and silica, typically wollastonite, will be assessed, and on the other hand, the required technical features of an scaled-up industrial process able to capture CO2 from industrial plants will be researched.

Given that the by-product of carbon mineral capture processes based on calcium silicates can be a valuable mineral, namely calcium carbonate, a valuable environmental safe compound and thermodynamically stable, it can be re-used as raw material from some industrial processes, depending on its morphology, purity or grain size. Therefore, the possible applications of the carbon mineral capture by-product will be researched, assessing on each process the energetic and economical ratio costs/profits. This applications will allow the design of an integral industrial process, able to reduce GHG emissions and subsequently able to re-use the by-product in an industrial process.

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Acoplamiento dinámica de fronteras de grano - segregación de impurezas en policristales nanoestructurados: aplicación a la circonia tetragonal dopada con itrio policristalina (YTZP)

The coupling of grain boundary dynamics and impurity segregation in nanostructured polycrystals: application to yttria tetragonal zirconia polycrystal (YTZP).

Código/Code: MAT2009-14351-C02-01
Periodo/Period: 01/01/2010 – 31/12/2012
Organismo Financiador/Financial source: Ministerio de Educación y Ciencia
Importe total/Total amount: 87.120 €
Investigador responsable/Research head: Gómez García, D.
Componentes/Research group: Francisco Luis Cumbrera Hernández, Arturo Domínguez Rodríguez, Robert Luis González Romero

RESUMEN / ABSTRACT

El proyecto que se presenta estudiará, mediante simulación por ordenador a distintas escalas, la evolución microestructural de un policristal a temperatura constante y bajo la aplicación de un campo de tensiones mecánicas; en particular, se prestará especial atención a los sistemas nanométricos. Para abordar con rigor este problema es indispensable conocer la ley de movilidad de las fronteras de grano en función de la temperatura y de las tensiones locales. En presencia de impurezas, esta ley depende crucialmente de la concentración de especies atómicas segregadas en dichas fronteras y su evolución durante el régimen dinámico (i. e. durante la deformación). A su vez, la segregación se ve alterada por el propio movimiento de la frontera de grano, de modo que ambos fenómenos están acoplados entre sí. El estudio de la segregación se realizará mediante simulación por Dinámica Molecular (DM); asimismo, se utilizará la DM para caracterizar la movilidad de una única frontera de grano conteniendo impure-

zas. Estos datos serán empleados en un modelo mesoscópico que se usará para estudiar la dinámica de un conjunto de granos de tamaño nanométrico y, por ende, la plasticidad de este sistema policristalino modelo.

El objetivo último de este proyecto es el de determinar la ley de evolución de los centros de masas de los granos para obtener, previo tratamiento estadístico, la ley constitutiva para la plasticidad en un policristal nanométrico. Esta ley macroscópica se contrastará finalmente con resultados experimentales en el sistema itria-zirconia policristalino (YTZP) nanométrico, en el que el equipo ha adquirido amplia experiencia en los últimos años.

This project aims to study, by computer simulation at different length scales, the microstructural evolution of a polycrystal at elevated temperature and under an applied mechanical stress field, with an emphasis on nanometric systems. For this study it is essential to know the law of mobility of the grain boundaries as a function of the temperature and the local stresses. When impurities are present, this law depends critically upon the concentration of segregated chemical species at these boundaries and upon their evolution during the dynamic regime (i.e., during deformation). As segregation itself is altered by the movement of the grain boundary, the two phenomena are coupled. The study of segregation will be carried out by Molecular Dynamics (MD) simulations; MD will also be used to characterize the mobility of a single grain boundary containing impurities. These data will be used as input in a mesoscopic model, which will allow the study of the dynamics of an ensemble of nanometric grains and, consequently, plasticity in this model polycrystalline system.

The final objective of this project is to determine the law of evolution of the centers of mass of the grains in order to get, via a statistical treatment, the constitutive law for plasticity in a nanometric polycrystal. This macroscopic law will then be compared with experimental results in nanometric YTZPa system in which the research team has wide experience in recent years.

Desarrollo de recubrimientos composite de carbono para aplicaciones biomédicas

Development of carbón-based composites for biomedical applications

Código/Code:	P10-TEP 06782 (Proyecto de Excelencia)
Periodo/Period:	15-03-2011 / 15-03-2014
Organismo Financiador/Financial source:	Junta de Andalucía
Importe total/Total amount:	96.000 €
Investigador responsable/Research head:	Juan Carlos Sánchez López
Componentes/Research group:	T. Cristina Rojas, Carlos López Cartes, David Abad, Vanda Godinho, Santiago Domínguez, Inmaculada Rosa

RESUMEN / ABSTRACT

El proyecto comprende el desarrollo de recubrimientos basados en carbono desde su síntesis a medida, caracterización, evaluación en tests de desgaste y estudios de biocompatibilidad para su uso en implantes artificiales. El control del tipo de enlace químico del carbono (sp2/sp3) y la composición química, incluyendo metales como (Ag, Ti) u otros elementos (B, N, O), permitirá modular las propiedades mecánicas y tribológicas (dureza, fricción y resistencia al desgaste) con objeto de incrementar su comportamiento final. Para ello se propone el empleo de la técnica de pulverización catódica (del inglés magnetron sputtering) para depositar estos recubrimientos avanzados sobre los materiales usados en los implantes (acero, aleaciones de Ti o polímeros) bajo diferentes condiciones de síntesis. Seguidamente, éstos composites de carbono serán evaluados de forma comparativa en ensayos de fricción y desgaste que simulen las condiciones que estos materiales se encontrarán en la aplicación final. De esta manera será posible establecer una correlación entre el comportamiento observado y las características químicas y estructurales de las capas preparadas bajo diferentes condiciones de síntesis. Finalmente, la biocompatibilidad será estudiada en ensayos de adhesión celular, citotoxicidad y actividad antibacteriana. Este completo conjunto de análisis aportará una excelente perspectiva de las posibilidades de transferencia tecnológica de estos materiales avanzados a la biomedicina.

This project pursues the development of carbon-based coatings including the tailored synthesis, characterization, evaluation in wear tests and biocompatibility study for the application in artificial implants. The control of the carbon chemical bonding (sp2/sp3) and the chemical composition, including metals as (Ag, Ti) or other elements (B, N, O) will enable to tune the mechanical and tribological properties (hardness, friction and wear resistance) with the aim of improving the final performance. To achieve this goal, the use of magnetron sputtering technique is envisaged to deposit advanced coatings under different synthesis conditions. Next, these carbon composites will be evaluated comparatively in friction and wear tests that simulate the conditions that these materials will face in the final application. In this way, it will be possible to establish the correlation between the observed behavior and chemical and structural characteristics of the prepared layers in cell adhesion tests, cytotoxicity and antibacterial activity. This complete characterization will provide an excellent overview of the possibilities of technological transfer of these advanced materials to the biomedicine.

Nanopartículas funcionalizadas para aplicaciones de hipertermia y evaluación de su ecotoxicidad Functionalized for hypethermia applications and evaluation of ecotoxicity

Código/Code:	P09-FQM-4554 (Proyecto de Excelencia)
Periodo/Period:	03-02-2010 / 02-02-2013
Organismo Financiador/Financial source:	Junta de Andalucía (Proyecto Internacional)
Importe total/Total amount:	172.598,68 €
Investigador responsable/Research head:	Asunción Fernández Camacho
Componentes/Research group:	J. Blasco, M. Hampel, Carlos López, L.M. Lubián, I. Moreno, Miguel Angel Muñoz, David Philippon, T. Cristina Rojas, Inmaculada Rosa, Carlos García-Negrete

RESUMEN / ABSTRACT

En este Proyecto de Excelencia se parte de la experiencia previa del grupo TEP-217 en el desarrollo y caracterización de nanopartículas funcionalizadas potencialmente biocompatibles y se pretende avanzar en cuatro direcciones. a) Continuar con el desarrollo de nanopartículas basadas principalmente en Au, Ag y óxidos magnéticos con distintas funcionalizaciones y microestructura. b) Profundizar en la fisico-química de su interacción con campos electromagnéticos (en un amplio rango de frecuencias desde kHz a GHz) para producir calentamientos localizados. Actualmente se han propuesto distintos mecanismos (corrientes inducidas, histéresis, relajación de momentos magnéticos y movimiento browniano) sin que existan todavía suficientes datos para comprender e interpretar los resultados experimentales. c) Establecer una colaboración multidisciplinar con el grupo RNM-306, especialista en ensayos de ecotoxicidad, que permita mejorar el conocimiento del impacto ambiental de las nanopartículas (principalmente de oro y plata) en los ecosistemas marinos, que son el sumidero final de una buena parte de los nanomateriales producidos en la actualidad. d) Realizar estudios preliminares de la toxicidad de las nanopartículas en función del campo electromagnético aplicado. En cualquier proyecto dedicado a la nanotecnología resulta extremadamente valioso introducir estudios que nos permitan determinar el impacto toxicológico y ambiental de los nuevos materiales que se están desarrollando en la actualidad.

Un objetivo fundamental de este proyecto es la formación de personal investigador a través de la realización de una Tesis Doctoral en el Instituto de Ciencia de Materiales de Sevilla.

This Excellence project is taking profit of the previous experience of the group TEP-217 in the development and characterization of functionalized biocompatible nanoparticles and potentially trying to advance in four directions. a) Continue with the development of nanoparticle based mainly on Au, Ag and magnetic oxides with different functionalizations and microstructure. b) To deepen the physical-chemical interaction with electromagnetic fields (in a wide range of frequencies from kHz to GHz) to produce local heating. Currently, various mechanisms have been proposed (Eddy current, hysteresis, relaxation of magnetic moments and Brownian motion) without enough data yet existing to understand and interpret the experimental results. c) Establish a multidisciplinary collaboration with the group RNM-306, a specialist in ecotoxicity testing, to improve the knowledge of the environmental impact of nanoparticles (mainly gold and silver) in marine ecosystems, which are the ultimate sink for a good part of nanomaterials currently produced. d) Conduct preliminary studies of the toxicity of nanoparticles as a function of applied magnetic field. In any project dedicated to nanotechnology is extremely valuable to introduce studies to determine the toxicological and environmental impact of new materials being developed at present.

A key objective of this project is the training of research personnel through the implementation of one doctoral thesis at the Institute of Materials Science of Seville.

OTROS PROYECTOS / OTHER PROJECTS

Caracterización mediante técnicas de Microscopia Electrónica de Transmisión a escala nanométrica de películas delgadas nanoestructuradas con aplicaciones multifuncionales

Código/Code: 201060I041

Oganismo Financiador/Financial source: CSIC (Intramural)
Importe total/Total amount: 25.000 €
Investigador responsable/Research head: T. Cristina Rojas Ruiz

Transferencia / Technological Transfer

Convenios y Contratos / Contracts and Agreements

Caracterización microestructural y química de materiales para avisadores sonoros

Periodo/Period: 19-01-2010 / 19-01-2012
Organismo Financiador/Financial source: Clarton Horn
Investigador responsable/Research head: Asunción Fernández Camacho
Componentes/Research group: Vanda C. Fortio Godinho, Inmaculada Rosa Cejudo

Estudio de la viabilidad de recubrimientos y encapsulación de micro- y nanopartículas de carbonato de calcio y aplicaciones derivadas

Periodo/Period: 01-04-2011 / 31-07-2012
Organismo Financiador/Financial source: REVERTE MINERALS
Investigador responsable/Research head: T. Cristina Rojas Ruiz
Componentes/Research group: Asunción Fernández Camacho, M. Carmen Jiménez de Haro, T. Cristina Rojas Ruiz

Diseño, construcción y puesta en marcha de un sistema para la producción de hidrógeno por hidrólisis de borohidruro en condiciones de alimentar una pila de combustible tipo PEM

Periodo/Period: 01-07-2010 / 30-06-2012
Organismo Financiador/Financial source: Abengoa Hidrógeno, S.A.
Investigador responsable/Research head: Asunción Fernández Camacho
Componentes/Research group: Gisela Arzac, Dirk Hufschmidt

Cooperación Internacional y Otros International Cooperation and Others

Phase field modeling and grain growth

Periodo/Period: 1-05-2011 / 31-08-2011

Entidad Financiadora/Financial source:	Programa Salvador de Madariaga. Ministerio de Educación y Ciencia (Cooperación con la Florida State University, EE.UU.)
Importe total/Total amount:	12.000 €
Investigador responsable/Research head:	Diego Gómez García

Patentes / Patents

Method for the synthesis of polyaleurate polyester

Inventores: José Jesús Benítez Jiménez, Antonio Heredia Bayona, José Alejandro Heredia Guerrero
Ámbito Geográfico: Internacional
PATENTE SOLICITADA. N. de solicitud: 2011/144792
Fecha Solicitud/Licencia: 20/mayo/2011
Entidades Titulares: CSIC y Universidad de Málaga

Proceso de producción de hidrógeno mediante hidrólisis catalizada de un hidruro complejo, e instalación con reactor semicontinuo para llevar a cabo el procedimiento

Inventores: M. Angeles Jiménez Domínguez, M. Mar Jiménez Vega, Belén Sarmiento Marrón, Asunción Fernández Camacho, Gisela M. Arzac, Enrique Jiménez Roca
Ámbito Geográfico: Nacional
PATENTE SOLICITADA. N. de solicitud: P201031899
Pais de Prioridad: España
Fecha Solicitud/Licencia: 22/diciembre/2010
Entidad Titular: Abengoa Hidrógeno, S.A.
Solicitud USA n. 13/268095 (7/octubre/2011)
Solicitud Patente Europea n. 11193661.3

Eliminación del dióxido de carbono y otros gases atmosféricos mediante residuos industriales ricos en calcio

Inventores: Luis Esquivias Fedriani, Victor M. Morales Florez
Ámbito Geográfico: Internacional
PATENTE SOLICITADA. N. de solicitud: PCTES2011000010
Fecha Solicitud/Licencia: 19/enero/2011
Entidad Titular: CSIC, Universidad de Cádiz y Universidad de Sevilla

Procedimiento de captura de CO_2 y SO_2

Inventores: Luis Esquivias Fedriani, Victor M. Morales Florez
Ámbito Geográfico: Nacional
PATENTE SOLICITADA. N. de solicitud: P201100536
Fecha Solicitud/Licencia: 10/mayo/2011

Entidad Titular: CSIC, Universidad de Cádiz y Universidad de Sevilla

PUBLICACIONES / PUBLICATIONS

ARTÍCULOS PUBLICADOS EN REVISTAS SCI / PAPERS IN SCI JOURNALS

The biophysical design of plant cuticles: an overview
Dominguez, E; Heredia-Guerrero, JA; Heredia, A
New Phytologist, **189** (2011) 938–949
DOI: 10.1111/j.1469-8137.2010.03553.x

The outer surfaces of epidermal cell walls are impregnated with an extracellular matrix called the cuticle. This composite matrix provides several functions at the interface level that enable plants to thrive in different habitats and withstand adverse environmental conditions. The lipid polymer cutin, which is the main constituent of the plant cuticle, has some unique biophysical properties resulting from its composition and structure. This review summarizes the progress made towards understanding the biophysical significance of this biopolymer with special focus on its structural, thermal, biomechanical, and hydric properties and relationships. The physiological relevance of such biophysical properties is discussed in light of existing knowledge on the plant cuticle.

New Insights into the Properties of Pubescent Surfaces: Peach Fruit as a Model
Fernandez, Victoria; Khayet, Mohamed; Montero-Prado, Pablo; Alejandro Heredia-Guerrero, Jose; Liakopoulos, Georgios; Karabourniotis, George; del Rio, Victor; Dominguez, Eva; Tacchini, Ignacio; Nerin, Cristina; Val, Jesus; Heredia, Antonio
Plant Physiology, **156** (2011) 2098–2108
DOI: 10.1104/pp.111.176305

The surface of peach (Prunus persica 'Calrico') is covered by a dense indumentum, which may serve various protective purposes. With the aim of relating structure to function, the chemical composition, morphology, and hydrophobicity of the peach skin was assessed as a model for a pubescent plant surface. Distinct physicochemical features were observed for trichomes versus isolated cuticles. Peach cuticles were composed of 53% cutan, 27% waxes, 23% cutin, and 1% hydroxycinnamic acid derivatives (mainly ferulic and p-coumaric acids). Trichomes were covered by a thin cuticular layer containing 15% waxes and 19% cutin and were filled by polysaccharide material (63%) containing hydroxycinnamic acid derivatives and flavonoids. The surface free energy, polarity, and work of adhesion of intact and shaved peach surfaces were calculated from contact angle measurements of water, glycerol, and diiodomethane. The removal of the trichomes from the surface increased polarity from 3.8% (intact surface) to 23.6% and decreased the total surface free energy chiefly due to a decrease on its nonpolar component. The extraction of waxes and the removal of trichomes led to higher fruit dehydration rates. However, trichomes were found to have a higher water sorption capacity as compared with isolated cuticles. The results show that the peach surface is composed of two different materials that establish a polarity gradient: the trichome network, which has a higher surface free energy and a higher dispersive component, and the cuticle underneath, which has a lower surface free energy and higher surface polarity. The significance of the data concerning water-plant surface interactions is discussed within a physiological context.

Surface-functionalized fluorescent silica nanoparticles for the detection of ATP
Moro, AJ; Schmidt, J; Doussineau, T; Lapresta-Fernandez, A; Wegener, J; Mohr, GJ
Chemical Communications, **47** (2011) 6066–6068
DOI: 10.1039/c1cc10419e

The design of two-dyed fluorescent silica nanoparticles for ATP detection is presented. The indicator dye possesses a dipicolylamine (DPA) unit complexed with Zn(II) as a receptor function for ATP while a rhodamine derivative is used as the reference dye. The nanoparticles were fully characterized regarding analytical performance, morphology and cytocompatibility.

Boron Compounds as Stabilizers of a Complex Microstructure in a Co-B-based Catalyst for NaBH(4) Hydrolysis
Arzac, GM; Rojas, TC; Fernandez, A
Chemcatchem, **3** (2011) 1305–1313
DOI: 10.1002/cctc.201100101

Co-B-based materials are widely used as catalysts for hydrogen generation through sodium borohydride self-decomposition. In the mid 1990s, the aqueous and organic chemistry involved in Co-B synthesis and handling was studied. Nevertheless, the exact microstructure of these catalysts has remained unsolved. Herein we present an exhaustive study which shows a new and complete microstructural view of a Co-B-based material together with the chemistry of the cobalt and boron involved. By using nanoscale-resolution microscopy and spectroscopy techniques, we have elucidated the role of boron compounds as stabilizers in a complex microstructure, which also explains its high catalytic performance and long-term stability. The catalyst is proposed to be made up of 1-3 nm hcp Co(0) nanoparticles embedded in amorphous Co(x)B (x = 1, 2, 3), Co(x)O(y), Co(BO(2))(2), and B(2)O(3) phases alternatively or all together. All of these amorphous phases protect the nanocrystalline metallic core from growth and oxidation.

Optimized hydrogen generation in a semicontinuous sodium borohydride hydrolysis reactor for a 60W-scale fuel cell stack
Arzac, GM; Fernandez, A; Justo, A; Sarmiento, B; Jimenez, MA; Jimenez, MM
Journal of Power Sources, **196** (2011) 4388–4395
DOI: 10.1016/j.jpowsour.2010.10.073

Catalyzed hydrolysis of sodium borohydride (SBH) is a promising method for the hydrogen supply of fuel cells. In this study a system for controlled production of hydrogen from aqueous sodium borohydride (SBH) solutions has been designed and built. This simple and low cost system operates under controlled addition of stabilized SBH solutions (fuel solutions) to a supported CoB catalyst. The system works at constant temperature delivering hydrogen at 1 L min(-1) constant rate to match a 60-W polymer electrolyte membrane fuel cell (PEMFC). For optimization of the system, several experimental conditions were changed and their effect was investigated. A simple model based only on thermodynamic considerations was proposed to optimize system parameters at constant temperature and hydrogen evolution rate. It was found that, for a given SBH concentration, the use of the adequate fuel addition rate can maximize the total conversion and therefore the gravimetric storage capacity. The hydrogen storage capacity was as high as 3.5 wt% for 19 wt% SBH solution at 90% fuel conversion and an operation temperature of 60 degrees C. It has been demonstrated that these optimized values can also be achieved for a wide range of hydrogen generation rates. Studies on the durability of the catalyst showed that a regeneration step is needed to restore the catalytic activity before reusing.

Structure and Chemical State of Octadecylamine Self-Assembled Monolayers on Mica

Benitez, JJ; San-Miguel, MA; Dominguez-Meister, S; Heredia-Guerrero, JA; Salmeron, M
Journal of Physical Chemistry C, **115** (2011) 19716–19723
DOI: 10.1021/jp203871g

Structural and chemical data on n-octadecylamine self-assembled monolayers on mica (ODA/mica SAMs) have been obtained from ATR-FTIR and XPS spectroscopies. The analysis of the methylene modes concludes that alkylamine molecules are arranged in a rigid and well-ordered packing. Besides, the magnitude of the splitting of the methylene scissoring deflection is consistent with a molecular tilted configuration within the self-assembled layer, as already reported from topographic AFM data. Molecular dynamics simulations have supported this conclusion. XPS has revealed the presence of an important fraction of protonated amino groups (-NH(3)(+)) even in freshly prepared ODA/mica SAMs in air at RT. Two sources of protonation are proposed: (i) the acid-base reaction of (-NH(2)) end groups with the water adlayer on the surface of hydrophilic mica and (ii) the formation of an allcylamonium alkylcarbamate by a fast reaction with the atmospheric CO(2) dissolved in such water adlayer. Though the water induced amino protonation is hypothetical, the presence of carbamate is univocally confirmed by ATR-FTIR Upon extended contact with air (ripening) the conformational ordering in ODA/mica SAMs is slightly improved. Besides, further amino group protonation takes place with no additional carbamate formation. The process is described by a tentative mechanism in which protons are transferred from water molecules at the edges of SAMs islands to the inside. On the other side, carbamation is hindered by the steric effect of CO(2) molecules trying to penetrate the close packed structure of octadec-ylamine molecules.

Magnetic core-shell fluorescent pH ratiometric nanosensor using a Stober coating method

Lapresta-Fernandez, A; Doussineau, T; Moro, AJ; Dutz, S; Steiniger, F; Mohr, GJ
Analytica Chimica Acta, **707** (2011) 164–170
DOI: 10.1016/j.aca.2011.09.008

We describe the use of a modified Stober method for coating maghemite (gamma-Fe(2)O(3)) nanocrystals with silica shells in order to built magnetic fluorescent sensor nanoparticles in the 50-70 nm diameter range. In detail, the magnetic cores were coated by two successive silica shells embedding two fluorophores (two different silylated dye derivatives), which allows for ratiometric pH-measurements in the pH range 5-8. Silica coated magnetic nanoparticles were prepared using maghemite nanocrystals as cores (5-10 nm in diameter) coated by tetraethoxyorthosilicate via hydrolysis/condensation in ethanol, catalyzed by ammonia. In the inner shell was covalently attached a sulforhodamine B, which was used as a reference dye; while a pH-sensitive fluorescein was incorporated into the outer shell. Once synthesized, the particles were characterized in terms of morphology, size, composition and magnetization, using dynamic light scattering (DLS), transmission electron microscopy (TEM), X-ray diffraction (XRD) and vibrating sample magnetometry (VSM). TEM analysis showed the nanoparticles to be very uniform in size. Wide-angle X-ray diffractograms showed, for uncoated as well as coated nanoparticles, typical peaks for the spinel structure of maghemite at the same diffraction angle, with no structural changes after coating. When using VSM, we obtained the magnetization curves of the resulting nanoparticles and the typical magnetization parameters as saturation magnetization (M(s)), coercivity (H(c)). and remanent magnetization (M(r)). The dual-dye doped magnetic-silica nanoparticles showed a satisfactory magnetization that could be suitable for nanoparticle separation and localized concentration of them. Changes in fluorescence intensity of the pH indicator in the different pH buffered solutions were observed within few seconds indicating an easy accessibility of the embedded dye by protons through the pores of the silica shell. The relationship between the ratio in fluorescence (sensor/reference dyes) and pH was adjusted to a sigmoidal fit using a Boltzmann type equation. Finally, the proposed method was statistically validated against a reference.

Structure and support induced structure disruption of soft nanoparticles obtained from hydroxylated fatty acids

Heredia-Guerrero, JA; San-Miguel, MA; Luna, M; Dominguez, E; Heredia, A; Benitez, JJ
Soft Matter, **7** (2011) 4357–4363
DOI: 10.1039/c0sm01545h

Soft and spherical nanoparticles, named as cutinsomes, have been prepared from concentrated 9(10), 16-dihydroxypalmitic acid (diHPA) in aqueous solution. After isolation, cutinsomes have been chemically and structurally characterized by ATR-FTIR, TEM and dynamic atomic force microscopy (dynamic AFM). The nanoparticle can be described as a lipidic, liquid-like and mostly esterified core surrounded by a polar shell of carboxylate/carboxylic acid molecules. Molecular dynamic (MD) simulations have been used to support this model. The structural stability of soft cutinsomes has been tested by deposition on both non-polar (HOPG) and polar (mica) flat substrates. It has been found that the magnitude of the interaction between the polar shell of cutinsomes and the support determines their structure conservation or its spreading or rupture and spill out of the liquid-like content. The structural consistence of these nanoparticles as a function of the polarity of substrate is of interest in elucidating the formation mechanism of cutin, the most abundant biopolyester in nature and a very interesting biomaterial to be mimetized.

Procedure to use phosphogypsum industrial waste for mineral CO(2) sequestration

Cardenas-Escudero, C; Morales-Florez, V; Perez-Lopez, R; Santos, A; Esquivias, L
Journal of Hazardous Materials, **196** (2011) 431–435

DOI: 10.1016/j.jhazmat.2011.09.039

Industrial wet phosphoric acid production in Huelva (SW Spain) has led to the controversial stockpiling of waste phosphogypsum by-products, resulting in the release of significant quantities of toxic impurities in salt marshes in the Tinto river estuary. In the framework of the fight against global climate change and the effort to reduce carbon dioxide emissions, a simple and efficient procedure for CO(2) mineral sequestration is presented in this work, using phosphogypsum waste as a calcium source. Our results demonstrate the high efficiency of portlandite precipitation by phosphogypsum dissolution using an alkaline soda solution. Carbonation experiments performed at ambient pressure and temperature resulted in total conversion of the portlandite into carbonate. The fate of trace elements present in the phosphogypsum waste was also investigated, and trace impurities were found to be completely transferred to the final calcite. We believe that the procedure proposed here should be considered not only as a solution for reducing old stockpiles of phosphogypsum wastes, but also for future phosphoric acid and other gypsum-producing industrial processes, resulting in more sustainable production.

A comparative study of the role of additive in the MgH(2) vs. the LiBH(4)-MgH(2) hydrogen storage system

Fernandez, A; Deprez, E; Friedrichs, O

International Journal of Hydrogen Energy, **36** (2011) 3932–3940

DOI: 10.1016/j.ijhydene.2010.12.112

The objective of the present work is the comparative study of the behaviour of the Nb- and Ti-based additives in the MgH(2) single hydride and the MgH(2) + 2LiBH(4) reactive hydride composite. The selected additives have been previously demonstrated to significantly improve the sorption reaction kinetics in the corresponding materials. x-Ray Diffraction (XRD), X-Ray Absorption Spectroscopy (XAS), X-Ray Photoelectron Spectroscopy (XPS) and Electron Microscopy (TEM) analysis were carried out for the milled and cycled samples in absence or presence of the additives. It has been shown that although the evolution of the oxidation state for both Nb- and Ti-species are similar in both systems, the Nb additive is performing its activity at the surface while the Ti active species migrate to the bulk. The Nb-based additive is forming pathways that facilitate the diffusion of hydrogen through the diffusion barriers both in desorption and absorption. For the Ti-based additive in the reactive hydride composite, the active species are working in the bulk, enhancing the heterogeneous nucleation of MgB(2) phases during desorption and producing a distinct grain refinement that favours both sorption kinetics. The results are discussed in regards to possible kinetic models for both systems.

Magnetic and fluorescent core-shell nanoparticles for ratiometric pH sensing

Lapresta-Fernandez, A; Doussineau, T; Dutz, S; Steiniger, F; Moro, AJ; Mohr, GJ

Nanotechnology, **22** (2011) 415501

DOI: 10.1088/0957-4484/22/41/415501

This paper describes the preparation of nanoparticles composed of a magnetic core surrounded by two successive silica shells embedding two fluorophores, showing uniform nanoparticle size (50-60 nm in diameter) and shape, which allow ratiometric pH measurements in the pH range 5-8. Uncoated iron oxide magnetic nanoparticles (similar to 10 nm in diameter) were formed by the coprecipitation reaction of ferrous and ferric salts. Then, they were added to a water-in-oil microemulsion where the hydrophilic silica shells were obtained through hydrolysis and condensation of tetraethoxyorthosilicate together with the corresponding silylated dye derivatives-a sulforhodamine was embedded in the inner silica shell and used as the reference dye while a pH-sensitive fluorescein was incorporated in the outer shell as the pH indicator. The magnetic nanoparticles were characterized using vibrating sample magnetometry, dynamic light scattering, transmission electron microscopy, x-ray diffraction and Fourier transform infrared spectroscopy. The relationship between the analytical parameter, that is, the ratio of fluorescence between the sensing and reference dyes versus the pH was adjusted to a sigmoidal fit using a Boltzmann type equation giving an apparent pK(a) value of 6.8. The fluorescence intensity of the reference dye did not change significantly (similar to 3.0%) on modifying the pH of the nanoparticle dispersion. Finally, the proposed method was statistically validated against a reference procedure using samples of water and physiological buffer with 2% of horse serum, indicating that there are no significant statistical differences at a 95% confidence level.

Corrigendum to "Segregation-induced grain boundary electrical potential in ionic oxide materials: A first principles model (vol 58, pg 6404, 2010)"
Gomez-Garcia, D; Melendez, JJ; Gonzalez-Romero, RL; Dominguez-Rodriguez, A
Acta Materialia, **59** (2011) 1848
DOI: 10.1016/j.actamat.2010.11.009

Artificial weathering pools of calcium-rich industrial waste for CO2 sequestration
Morales-Florez, V; Santos, A; Lemus, A; Esquivias, L
Chemical Engineering Journal, **166** (2011) 132–137
DOI: 10.1016/j.cej.2010.10.039

Processes of carbonation of calcium-rich aqueous industrial wastes from acetylene production were performed mimicking rock weathering, using the atmospheric carbon dioxide as reactant. This residue was carbonated exposing it to the air in artificial pools with controlled solid-to-liquid and surface-to-volume ratios, and the efficiency of this simple mineral carbonation process was maximized. Considering realistic values of just one acetylene production plant, the intelligent handling of the calcium-rich waste would make it possible to counteract the emission of around 800t of carbon dioxide per year, so the CO2 emissions of the acetylene production could be completely compensated and its carbon footprint significantly reduced. X-ray diffraction patterns and thermogravimetric analyses reported the conversion, up to 88%, of the calcium hydroxide into calcium carbonate under atmospheric conditions. So, considering a realistic industrial scale-up, 476 kg of CO2 could be captured with it of dry waste. The morphology of the grains is resolved by electron microscopy, and can be described as needles 15 nm wide and 200 nm long arranged in grains smaller than 1 micron. We exploit these nanometric textural parameters (nanometric pores and particles having a specific surface area similar to 50m(2)/g) to design an efficient carbon fixation procedure. The aim of this work is to propose this simple carbonation technology, based on aqueous alkaline industrial waste, as a contribution to reducing global CO2 emissions.

Cation diffusion in yttria-zirconia by molecular dynamics
Gonzalez-Romero, RL; Melendez, JJ; Gomez-Garcia, D; Cumbrera, FL; Dominguez-Rodriguez, A; Wakai, F
Solid State Ionics, **204** (2011) 1–6
DOI: 10.1016/j.ssi.2011.10.006

This paper presents a novel methodology to calculate cation diffusion coefficients and activation energies in cubic Y(2)O(3)-ZrO(2) by Molecular Dynamics. The calculation is based upon modulating the interaction potential to promote cation mobility within the lattice. The technique was calibrated by measuring static properties and oxygen self-diffusion characteristics, and then applied to cation diffusion. The respective activation energies and diffusion coefficients agree well with experimental findings. Preliminary results about grain boundary cation diffusion are presented for the first time as a proof of the potentiality of the procedure.

Identification of Ternary Phases in TiBC/a-C Nanocomposite Thin Films: Influence on the Electrical and Optical Properties
Abad, MD; Sanjines, R; Endrino, JL; Gago, R; Andersson, J; Sanchez-Lopez, JC
Plasma Processes and Polymers, **8** (2011) 579–588
DOI: 10.1002/ppap.201000182

The local structure of TiBC and amorphous carbon (a-C) nanocomposite films (TiBC/a-C) was correlated with their optical and electrical properties. TiBC/a-C films with increasing C content were deposited by magnetron co-sputtering from TiC:TiB(2) (60: 40) and graphite targets. Chemical composition is determined by electron energy-loss spectroscopy. Grazing incidence X-ray diffraction reveals that the microstructure of the films is amorphous with small nanocrystallites emerging by increasing the C content that could be attributed to the formation of ternary (TiB(x)C(y)) or mixed binary (TiB(2) and TiC) phases. Further information was then obtained by studying the chemical bonding by measuring the near-edge fine structure (NES) by electron energy-loss (B K-, C K-, and Ti L-edges) and X-ray absorption (B K- and Ti L-edges) spectroscopies. The NES analysis indicates the formation of a nanocrystalline ternary TiB(x)C(y) compound concomitant with the segregation of an a-C phase as the carbon content is increased. The optical properties were studied by spectroscopic ellipsometry and the electrical resistivity was measured by the Van der Pauw method between 20 and 300 K. The films continuously lose their metallic character in terms of optical constants and resistivity with increasing carbon content. Theoretical fitting of the electrical properties using the grain-boundary scattering model supported the formation of a nanocomposite structure based on a ternary TiB(x)C(y) phase embedded in a matrix of a-C. The electron transport properties are mainly limited by the high density of point defects, grain size, and transmission probability.

Structural, chemical surface and transport modifications of regenerated cellulose dense membranes due to low-dose gamma-radiation
Vazquez, MI; Heredia-Guerrero, JA; Galan, P; Benitez, JJ; Benavente, J
Materials Chemistry and Physics, **126** (2011) 734–740
DOI: 10.1016/j.matchemphys.2010.12.051

Modifications caused in commercial dense regenerated cellulose (RC) flat membranes by low-dose gamma-irradiation (average photons energy of 1.23 MeV) are studied. Slight structural, chemical and morphological surface changes due to irradiation in three films with different RC content were determined by ATR-FTIR, XRD, XPS and AFM. Also, the alteration of their mechanical elasticity has been studied. Modification of membrane performance was determined from solute diffusion coefficient and effective membrane fixed charge concentration obtained from NaCl diffusion measurements. Induced structural changes defining new and effective fracture propagation directions are considered to be responsible for the increase of fragility of irradiated RC membranes. The same structural changes are proposed to explain the reduction of the membrane ion permeability through a mechanism involving either ion pathways elongation and/or blocking.

Combined x-ray photoelectron spectroscopy and scanning electron microscopy studies of the LiBH4-MgH2 reactive hydride composite with and without a Ti-based additive
Deprez, E; Munoz-Marquez, MA; de Haro, MCJ; Palomares, FJ; Soria, F; Dornheim, M; Bormann, R; Fernandez, A
Journal of Applied Physics, **109** (2011) 14913
DOI: 10.1063/1.3525803

A detailed electronic and microstructural characterization is reported for the LiBH4-MgH2 reactive hydride composite system with and without titanium isopropoxide as additive. Surface characterization by x-ray photoelectron spectroscopy combined to a morphological study by scanning electron microscopy as well as elemental map composition analysis by energy dispersive x-ray emission are presented in this paper for the first time for all sorption steps. Although sorption reactions are not complete at the surface due to the unavoidable superficial oxidation, it has been shown that the presence of the additive is favoring the heterogeneous nucleation of the MgB2 phase. Ti-based phases appear in all the samples for the three sorption steps well dispersed and uniformly distributed in the material. Li-based phases are highly dispersed at the surface while the Mg-based ones appear, either partially covered by the Li-based phases, or forming bigger grains. Ball milling is promoting mixing of phases and a good dispersion of the additive what favors grain refinement and heterogeneous reactions at the interfaces.

Mechanical, microstructural and oxidation properties of reactively sputtered thin Cr-N coatings on steel
Cecchini, R; Fabrizi, A; Cabibbo, M; Paternoster, C; Mavrin, BN; Denisov, VN; Novikova, NN; Haidopoulo, M
Thin Solid Films, **519** (2011) 6515-6521

DOI: 10.1016/j.tsf.2011.04.115

Thin (40 nm and 160 nm) Cr-N coatings were deposited on steel by reactive magnetron sputtering deposition, varying the N(2) flow. The coatings were characterized in the as-deposited condition and after annealing in air at 500 degrees C for 1 h, by X-Ray Diffraction, Transmission Electron Microscopy, Raman and Fourier Transform Infrared spectroscopies. Hardness was measured by nanoindentation. Coatings have a nanocrystalline microstructure with the phase shifting from Cr(2)N to CrN, increasing grain size, thermal stability and resistance to oxidation with increasing N(2). Also intrinsic coating hardness is influenced by both N(2) flow during deposition and film thickness, as a result of changes in phase composition and microstructural properties.

Endurance of TiAlSiN coatings: Effect of Si and bias on wear and adhesion

Philippon, D; Godinho, V; Nagy, PM; Delplancke-Ogletree, MP; Fernandez, A
Wear, **270** (2011) 541-549
DOI: 10.1016/j.wear.2011.01.009

In this work, the endurance of TiAlSiN nanocomposite thin films subjected to tribological solicitation is studied. These coating were deposited on M2 steel substrate by magnetron sputtering. Dry sliding experiments were conducted at ambient temperature against WC-Co ball. Coefficients of friction, wear rates and endurances were correlated with the composition, microstructure, mechanical properties, residual stress and adhesion of the coatings. The hardness and elastic modulus were found dependent not only on the composition but also on the residual stress induced by the deposition process. Friction coefficient was found to be independent on Si content while the wear rate is strongly reduced for higher Si contents. The formation of a nanocomposite microstructure, the amount of amorphous Si-based phase and both, wear resistance and adhesion are shown as the critical factors to determine the endurance of the coating.

Microstructure and chemical bonding of DLC films deposited on ACM rubber by PACVD

Martinez-Martinez, D; Schenkel, M; Pei, YT; Sanchez-Lopez, JC; De Hosson, JTM
Surface & Coatings Technology, **205** (2011) S75-S78
DOI: 10.1016/j.surfcoat.2011.01.025

The microstructure and chemical bonding of DLC films prepared by plasma assisted chemical vapor deposition on acrylic rubber (ACM) are studied in this paper. The temperature variation produced by the ion impingement during plasma cleaning and subsequent film deposition was used to modify the film microstructure by controlling the different degrees of strain applied to the substrate. The film microstructure is studied by top view and cross sectional SEM. The observed patch sizes are correlated with the variation of temperature that occurred during deposition. Finally, the chemical bonding of the samples is studied by Raman spectroscopy. All the samples show similar spectra regardless the bias voltage used.

Comparative investigation of Al- and Cr-doped TiSiCN coatings

Shtansky, DV; Kuptsov, KA; Kiryukhantsev-Korneev, PV; Sheveiko, AN; Fernandez Camacho, A; Petrzhik, MI
Surface & Coatings Technology, **205** (2011) 4640-4648
DOI: 10.1016/j.surfcoat.2011.04.012

The aim of this work was a comparative investigation of the structure and properties of Al- and Cr-doped TiSiCN coatings deposited by magnetron sputtering of composite TiAlSiCN and TiCrSiCN targets produced by self-propagating high-temperature synthesis method. Based on X-ray diffraction, scanning and transmission electron microscopy. X-ray photoelectron spectroscopy, and Raman spectroscopy data, the Al- and Cr-doped TiSiCN coatings possessed nanocomposite structures (Ti,Al)(C,N)/a-(Si,C) and (Ti,Cr)(C,N)/a-SiCxNy/a-C with cubic crystallites embedded in an amorphous matrix. To evaluate the thermal stability and oxidation resistance, the coatings were annealed either in vacuum at 1000, 1100, 1200, and 1300 degrees C or in air at 1000 degrees C for 1 h. The results obtained show that the hardness of the Al-doped TiSiCN coatings increased from 41 to 46 GPa, reaching maximum at 1000 degrees C, and then slightly decreased to 38 GPa at 1300 degrees C. The Cr-doped TiSiCN coatings demonstrated high thermal stability up to 1100 degrees C with hardness above 34 GPa. Although both Al-and Cr-doped TiSiCN coatings possessed improved oxidation resistance up to 1000 degrees C, the TiAlSiCN coatings were more oxidation resistant than their TiCrSiCN counterparts. The TiCrSiCN coatings showed better tribological characteristics both at 25 and 700 degrees C and superior cutting performance compared with the TiAlSiCN coatings.

Electrical properties and applications of carbon based nanocomposite materials: An overview

Sanjines, R; Abad, MD; Vaju, C; Smajda, R; Mionic, M; Magrez, A
Surface & Coatings Technology, **206** (2011) 727-733
DOI: 10.1016/j.surfcoat.2011.01.025

The allotropic forms of carbon (amorphous and polycrystalline graphite, carbon black, fullerenes, nanotubes, graphene) exhibit a large variety of charge transport properties which have been stimulating fundamental and applied research for the development of new devices based on micro and nano-sized electronic systems. Carbon based nanocomposites offer the possibility to improve the device performances and to develop novel multifunctional material systems by combining the properties of each individual phase. In this paper we review the electrical properties of carbon materials and some of the most exciting carbon based nanocomposites, as well as their potential technological applications. First, the electrical properties of amorphous and polycrystalline graphitic materials and those of their related nanocomposites materials are discussed. Second, an overview of the state-of-art on research and applications of carbon nanotube-based composites is presented. Third, we discuss briefly the emerging area of research related to graphene materials. Finally, the electrical properties and applications of conducting carbon black aggregates and carbon black/polymer composites are overviewed.

Identification of the wear mechanism on WC/C nanostructured coatings

El Mrabet, S; Abad, MD; Sanchez-Lopez, JC

Surface & Coatings Technology, **206** (2011) 1913-1920
DOI: 10.1016/j.surfcoat.2011.07.059

A series of WC/C nanostructured films with carbon contents ranging from 30 to 70 at.% was deposited on M2 steel substrates by magnetron sputtering of WC and graphite targets in argon. Depending on the amorphous carbon (a-C) incorporated in the coatings, nanocrystalline coating (formed mainly by WC(1-x) and W(2)C phases) or nanocomposite (WC(1-x)/a-C) were obtained with tunable mechanical and tribological properties. Ultrahardness values of 36-40 GPa were measured for the nanocrystalline samples whilst values between 16 and 23 GPa were obtained in the nanocomposite ones depending on the a-C content. The tribological properties were studied using a pin-on-disk tester versus steel (100Cr6) balls and 5 N of applied load in dry sliding conditions and the failure modes by scratch adhesion tests. Three different zones were identified according to the observed tribological behavior: I (mu > 0.8; adhesive wear), II (mu: 0.3-0.6; abrasive wear) and III(mu similar to 0.2; self-lubricated). The wear tracks and the ball scars were observed by scanning electron microscopy (SEM) and Raman spectroscopy in order to elucidate the tribochemical reactions appearing at the contact and to determine the wear mechanism present in each type. A correlation among structure, crystalline phases, a-C content and tribomechanical properties could be established for the series of WC/C coatings and extended to understand the trends observed in the literature for similar coatings.

Recent insights into xerogel and aerogel mineral composites for CO(2) mineral sequestration
Morales-Florez, V; Santos, A; Esquivias, L
Journal of Sol-Gel Science and Tecnology, **59** (2011) 417-423
DOI: 10.1007/s10971-010-2276-8

Supercritically dried composites have already been analysed and proposed as carbon dioxide sequesters. However, the economical and energetic costs of the supercritical drying process had to be re-evaluated, and were eventually found not to enhance the feasibility of the proposed route for CO(2) mineral sequestration. Different composites series were synthesised with the only difference being the drying method. The structures of the porous matrix were characterised as well as their ability to capture CO(2). The first results showed that the xerogel matrix is as good a host as the aerogel one, and also avoids expensive procedures such as supercritical drying for sample preparation without losing CO(2) capture capacity and enhancing the efficiency of the whole carbon sequestration process. In this case, the sample preparation was simplified as much as possible, with the aim of reducing energetic and economic costs. Although good carbonation efficiencies were obtained with these cheap samples, the first results showed that previous high carbonation efficiencies could not be repeated.

Surface-modified Pd and Au nanoparticles for anti-wear applications
Sanchez-Lopez, JC; Abad, MD; Kolodziejczyk, L; Guerrero, E; Fernandez, A
Tribology International, **44** (2011) 720-726
DOI: 10.1016/j.triboint.2009.12.013

This work reports the employment of metallic nanoparticles (palladium and gold) with a mean particle size of 2.2 nm surface-protected with tetraalkylammonium and alkanethiolate chains, respectively, as lubricant additives. Dispersions of both types of nanoparticles (5 wt%) are prepared using tetrabutylammonium acetate (TBA) and paraffin as base oils, respectively. The tribological properties are then evaluated by a ball-on-disc tribometer at two different loads (7 and 15 N) with excellent results: friction (< 0.1), wear rate (similar to 10(-10) mm(3)/Nm) The excellent anti-wear response is explained by the formation of a metal-containing transfer film and their action as counterface spacers avoiding direct contact.

ARTÍCULOS PUBLICADOS EN REVISTAS NO-SCI / PAPERS IN NON-SCI JOURNALS

Propiedades tribológicas de capas de carbono amorfo dopadas con plata para aplicaciones biomédicas
J.C. Sánchez-López, J.L. Endrino, R. Escobar Galindo
Libro de Actas del VI Congreso Ibérico de Tribología (2011) 211-222
(Nº ISBN: 978-84-694-5705-4)

Mejora de las propiedades conductoras en grasas antigripante mediante el empleo de nanopartículas de Pd
J.C. Sánchez-López, M.A. Roldán, M.L. Merino, C. Esteban
Libro de Actas del VI Congreso Ibérico de Tribología (2011) 335-344
(Nº ISBN: 978-84-694-5705-4)

Structure of Diamond-Like Carbon films deposited by femtosecond and nanosecond pulsed laser ablation
A. Sikora, F. Garrelie, C. Donnet, A.S. Loir, J. Fontaine, J.C. Sanchez-Lopez, T.C. Rojas
Virtual Journal of Ultrafast Science, Vol 10, issue 1 (2011).

LIBROS Y OTRAS PUBLICACIONES / BOOKS AND OTHER PUBLICATIONS

Self-Assembly and Polymerization of Natural Occurring Fatty Acids
José Alejandro Heredia Guerrero, Eva Domínguez, Miguel Angel San-Miguel, José Jesús Benítez and Antonio Heredia
En: Advances in Materials Science Research
Editorial Nova Science Publishers (Eds. Maryann C. Wythers)
ISBN: 978-1-61209-116-7

CONGRESOS Y REUNIONES INTERNACIONALES / INTERNATIONAL CONGRESS AND MEETINGS

PARTICIPACIÓN EN LA ORGANIZACIÓN DE CONGRESOS Y REUNIONES / PARTICIPATION IN ORGANISING CONGRESSES AND MEETINGS

International Conference on Metallurgical Coatings and Thin Films, ICMCTF'2011

2 – 6 mayo [San Diego, Estados Unidos de América]
Juan Carlos Sánchez López [Miembro del Comité Organizador]

E-MRS 2011 Spring Meeting, Symposium K "Protective Coatings and Thin Films11

9 – 13 mayo [Niza, Francia]
Juan Carlos Sánchez López [Miembro del Comité Organizador]

VI Congreso Ibérico de Tribología

16 – 17 junio [Madrid, España]
Juan Carlos Sánchez López [Miembro del Comité Científico]

18th International Symposium on Metastable, Amorphous and Nanostructured Materials

26 junio – 1 julio [Gijón, España]
Asunción Fernández Camacho [Miembro del National Advisory Committee]

ITFPC-MIATEC 2011, Innovation in Thin Film Processing and Characterization & Magnetron, Ion processing and Arc Technologies European Conference

14 – 17 noviembre [Nancy, Francia]
Juan Carlos Sánchez López [Miembro del Comité Científico]

COMUNICACIONES EN CONGRESOS Y REUNIONES / COMMUNICATIONS IN CONGRESS AND MEETINGS

Faraday Discussion 151: Hydrogen Storage Materials

18 – 20 abril [Didcot, Oxon, Reino Unido]

Synergistic effect in Ru-Co-B catalysts for hydrogen production through sodium borohydride self-hydrolisis: A microstructural and chemical view
G.M.Arzac, T.C.Rojas, C.López-Cartés, A.Fernández
Poster

Stable hydrogen generation in a semicontinuous sodium borohydride hydrolysis reactor for a 60W-scale fuel cell stack
G.M.Arzac, M.A.Jimenez, B.Sarmiento, M.M.Jimenez, D. Hufschmidt, A.Fernández
Poster

International Conference on Metallurgical Coatings and Thin Films, ICMCTF'2011
2 – 6 mayo [San Diego, Estados Unidos de América]

Identification of the wear mechanism on WC/C nanostructured coatings.
S. El Mrabet, M.D. Abad, J.C. Sánchez-López
Comunicación oral

E-MRS 2011 Spring Meeting, Symposium K "Protective Coatings and Thin Films11
9 – 13 mayo [Niza, Francia]

Chemical and microstructural characterization of (Y or Zr)-doped CrAlN coatings
T.C. Rojas, S. El Mrabet, M. Brizuela, A. García-Luis, J.C. Sánchez-López
Poster

Comparative tribological study on carbon-based PVD coatings deposited on WC-Co balls
E. Almandoz, G.G. Fuentes, R. Martínez, J. Rodrigo, R.J. Rodríguez, M.D. Abad, A. Mariscal, J.C. Sanchez-Lopez
Poster

Corrosion behaviour of protective TiBC/a-C and WC/a-C coatings
A. Conde, I. Garcia, M.A. Arenas, M.D. Abad, A. Mariscal, J.C. Sánchez-López
Poster

Thermal stability of CrSiN nanocomposite coatings and its consequences regarding the high temperature oxidation behaviour
T. Schmitt, P. Steyer, N. Mary, J. Fontaine, F. Sanchette, J.C. Sanchez-Lopez, F. Mompiou, M. O'Sullivan
Comunicación oral

PRIMO 16, Pollutant Responses in Marine Organisms
15 – 18 mayo [Long Beach, California, Estados Unidos de América]

Effect of the exposure of the clam Ruditapes Philippinarum to gold nanoparticles, evaluation of enzymatic and molecular endpoints
M.Volland, M.Hampel, C.García-Negrete, A.Lapresta-Fernández, T.C.Rojas, M.C.Jiménez de Haro, A.Fernández, J.Blasco
Comunicación oral

Jornada de Ingeniería de Cerámicos para Ambientes Extremos

10 junio [Sevilla, España]

Sistemas Autoensamblados como Modelo para el Estudio de las Interacciones Intermoleculares
J.A. Heredia-Guerrero; M.A. San Miguel; A. Heredia; J.J. Benítez
Comunicación oral

Obtención de Bioplásticos a Partir de Hidroxiácidos de Cadena Larga
J.A. Heredia-Guerrero; A. Heredia; J.J. Benítez
Comunicación oral

VI Congreso Ibérico de Tribología

16 – 17 junio [Madrid, España]

Mejora de las propiedades conductoras en grasas antigripante mediante el empleo de nanopartículas de Pd
J.C. Sánchez-López, M.A. Roldán, M.L. Merino, C. Esteban
Comunicación oral

Propiedades tribológicas de capas de carbono amorfo dopadas con plata para aplicaciones biomédicas
J.C. Sánchez-López, J.L. Endrino, R. Escobar Galindo
Comunicación oral

Estudio de la resistencia al rayado de composites de alúmina con nanotubos de carbono
F. Gutiérrez-Mora, R. Poyato, J.C. Sánchez-López y A. Domínguez-Rodríguez
Comunicación oral

18th International Symposium on Metastable, Amorphous and Nanostructured Materials

26 junio – 1 julio [Gijón, España]

Characterization by TEM techniques with nano-scale resolution of nanostructured-multifunctional thin films prepared by magnetron sputtering
T.C.Rojas, V. Godinho, D. Philippon, J.C. Sánchez-López, M. Brizuela, A. García-Luis, A. Fernández
Conferencia Invitada

Amorphous SiOxNy thin films with controlled closed porosity and its effects on refractive index and mechanical properties
V. Godinho, T.C. Rojas, A. Fernández
Comunicación oral

8th International Conference on Nanosciences & Nanotechnologies – NN11
12 – 15 julio [Thessaloniki, Grecia]

Scratch Characterization of a-C:H and TiN coatings: from Micro to Macro Range
R.Cecchini, V.Godinho, A.Fernández, T.Chudoba, P.Ricci, M.Cabibbo
Comunicación oral

Advanced Complex Inorganic Materials-ACIN2011
11 – 14 septiembre [Namur, Bélgica]

Synthesis of silicon carbide nano powders by microwave-assisted carbothermal reduction
B.M. Moshtaghioun, R. Poyato, A. Monshi, D. Gómez-García y A. Domínguez-Rodríguez
Poster

6th Int. Conf. on the Environmental Effects of Nanoparticles and Nanomaterials
19 – 21 septiembre [The Royal Society, Londres, Reino Unido]

Enzymatic and molecular responses on the Manila clam Ruditapes Philippinarum to gold nanoparticles and dissolved gold
J.Blasco, M.Volland, M.Hampel, C.García-Negrete, A.Lapresta-Fernández, T.C.Rojas, M.C.Jiménes de Haro, A.Fernández
Comunicación oral

8th European Congress of Chemical Engineering
25 – 29 septiembre [Berlin, Alemania]

Hydrogen Storage using Sodium Borohydride
M.A. Jiménez, M. Maynar, M. Tejada, G.M. Arzac, A.Fernández
Poster

Specialist Meeting on Carbon 2011
26 – 28 septiembre [Puerto Vallarta, México]

Tribological behaviour of amorphous carbon-based coatings
J.C. Sánchez-López
Conferencia Invitada

IV International Conference on Surfaces, Materials and Vacuum
26 – 30 septiembre [Puerto Vallarta, México]

Protection of surfaces exposed to wear by nanoengineered coatings
J.C. Sánchez-López
Conferencia Invitada

2nd Joint Congress of the Portuguse and Spanish Microscopy Societies:Microscopy at the frontiers of science
18 – 21 octubre [Aveiro, Portugal]

Multifuntional thin film prepared by Magnetron Sputtering containing embedded voids: A nano-scale characterization by electron microscopy techniques
T.C.Rojas, V. Godinho, M.C. Jiménez de Haro, A. Fernández
Comunicación oral

Boron Compounds as stabilizers of a complex microstructure in a Co-B based catalyst for NaBH4 hydrolysis
G.M. Arzac; T.C. Rojas; A. Fernández
Comunicación oral

ITFPC-MIATEC 2011, Innovation in Thin Film Processing and Characterization & Magnetron, Ion processing and Arc Technologies European Conference
14 – 17 noviembre [Nancy, Francia]

Thermal stability and oxidation resistance of hard nanocomposite Ti-(Al,Cr,Y)-Si-CN coatings produced by ion implantation assisted magnetron sputtering
P.V. Kiryukhantsev-Korneev, K.A. Kuptsov, A.N. Sheveyko, C.Rojas, A.Fernández, D. Shtansky
Comunicación oral

CONGRESOS Y REUNIONES NACIONALES / NATIONAL CONGRESSES AND MEETINGS

COMUNICACIONES EN CONGRESOS Y REUNIONES / COMMUNICATIONS IN CONGRESS AND MEETINGS

I Jornada Ingeniería de Cerámicos para Ambientes Extremos
10 junio [Sevilla, España]

Autoensamblado molecular sobre soportes de baja interacción como estrategia para el estudio de las interacciones intermoleculares
José Jesús Benítez Jiménez
Comunicación oral

FORMACION / TRAINING

TESIS DOCTORALES/ DOCTOR DEGREE THESIS

Título: **Autoensamblaje Molecular y Síntesis de Materiales Biomiméticos a partir de Hidroxiácidos derivados de Cutinas Vegetales**
Autor: José Alejandro Heredia Guerrero
Directores: José Jesús Benítez Jiménez, Antonio Heredia Bayona
Calificación: Apto "Cum Laude"
Centro: Universidad de Málaga

Título: **Study and characterization of magnetrón sputtered thin films of the Ti-Al-Si-N(O) system**
Autor: Vanda Godinho
Directores: M.P. Delplancke-Ogletree y Asunción Fernández Camacho
Calificación: Sobresaliente "Cum Laude"
Centro: Université Libre de Brussels y la Universidad de Sevilla

Título: **Study of the Reactive Hydride Composite 2LiBH4+MgH2 and its additives for hydrogen storage applications**
Autor: Emilie Deprez
Directores: Asunción Fernández Camacho
Calificación: Sobresaliente "Cum Laude"
Centro: Université Libre de Brussels y la Universidad de Sevilla

FORMACIÓN DE GRADUADOS / MASTER DEGREE THESIS

Título: **Comportamiento tribológico a alta temperatura de recubrimientos duros de CrAlN dopados con Y ó Zr**
Autor: Antonio José Contreras Sánchez
Directore: Juan Carlos Sánchez López
Grado: Ingenería de Materiales
Centro: Universidad de Sevilla
Año Académico: 2010-2011

Título: **Caracterización química y estructural de un catalizador Co-B para la hidrólisis del borohidruro sódico: Una nanoestructura singular estabilizada por compuestos basados en Boro**
Autor: Gisela Mariana Arzac de Calvo
Directore: Asunción Fernández Camacho y T. Cristina Rojas Ruiz
Grado: Trabajo Fin de Master

Centro:	Universidad de Sevilla
Año Académico:	2010-2011

Título:	**Exposición del molusco Ruditapes Philippinarum a nanopartículas de oro: Estudio de localización mediante microscopía electrónica**
Autor:	Carlos Andrés García Negrete
Directore:	Asunción Fernández Camacho y T. Cristina Rojas Ruiz
Grado:	Trabajo Fin de Master
Centro:	Universidad de Sevilla
Año Académico:	2010-2011

EQUIPAMIENTO CIENTÍFICO AVAILABLE EQUIPMENT

Spin coater
UV/Ozonone cleaner
Horno a vacío de baja temperatura
Cromatógrafo
Pila de combustible (100W)
Medidor y sonda de temperatura por fluorescencia
Cabeza magnetrón de 2”
Bomba FLODOS
Electrónica y controladores de flujo másico para gases

Propiedades mecánicas de superficies y recubrimientos
Tribómetro CSM (movimiento lineal y rotativo) para evaluación de coeficientes de fricción y desgaste.
Tribómetro de alta temperatura (hasta 800ºC) –Microtest
Calotest para medida de espesores y evaluación del desgaste.
Equipo de rayado (Scratch-test) hasta 200N (Tribotechnic).
Perfilómetro-rugosímetro (Mahr) de tipo táctil y resolución vertical nanométrica.

Cámaras de deposición
Tres cámaras de deposición de recubrimientos y películas delgadas por la técnica de pulverización catódica (magnetrón sputtering). Con una dotación de 7 cabezas magnetrón, 2 fuentes DC, 2 fuentes RF y 1 fuente pulsada, portamuestras girables y calentables.

Equipamiento de irradiación con campos electromagnéticos
Analizador de redes AGILENT con amplificadores y celda GTEM

Laboratorio de síntesis de NPs y catalizadores por vía química
Reactores y material de vidrio convencional
Rotavapor, sistemas de filtrado
Cámara seca MBRAUN
Reactores de producción de hidrógeno

Laboratorio de síntesis de NPs y catalizadores por vía química
Reactores y material de vidrio convencional
Rotavapor, sistemas de filtrado
Cámara seca MBRAUN
Reactores de producción de hidrógeno

Laboratorio AFM/STM
Microscopio AFM aire/liquido modelo Explorer marca Topometrix.
Microscopio AFM aire/atmósfera controlada modelo Cervantes con unidad de control Dulcinea marca Nanotec.
Microscopio STM aire/atmósfera controlada con unidad de control Dulcinea marca Nanotec.
Microscopio STM aire/líquido modelo Discoverer con controlador TMX2000 marca Topometrix.
Balanza Langmuir-Blodgett modelo Minitrough termostatizada con dipper controlado por software marca KSV.

UNIDAD EXTERNA DE INVESTIGACIÓN: FÍSICA DE MATERIALES

EXTERNAL UNIT: PHYSICS OF MATERIALS

PROYECTOS DE INVESTIGACIÓN / RESEARCH PROJECTS

Compuestos cerámico/cnts: procesado, caracterización y propiedades mecánicas Ceramic/SWNT composites: processing, characterization and mechanical properties

Código/Code:	MAT2009-11078
Periodo/Period:	01-10-2009 / 30-09-2012
Organismo Financiador/Financial source:	Ministerio de Ciencia e Innovación
Importe total/Total amount:	211.750,01 €
Investigador responsable/Research head:	Antonio Muñoz Bernabé
Componentes/Research group:	Arturo Domínguez Rodríguez, Ángela Gallardo López, Felipe Gutiérrez Mora, Ana Morales Rodríguez, Nitin P. Padture, Rosalía Poyato Galán

RESUMEN / ABSTRACT

Con este proyecto se pretende, en primer lugar, la fabricación de materiales compuestos nanoestructurados con matrices cerámicas de Al_2O_3 y ZrO_2 estabilizada con Ytria (8Y-SZP), reforzadas con diferentes concentraciones de nanotubos de carbono (CNTs). En ambos tipos de materiales se partirá de polvos cerámicos de alta pureza (> 99 %) y diferentes tamaños de grano, entre 30 y 40 nm para el Al_2O_3 y entre 20 y 300 nm para el 8Y-SZP. Se utilizarán diferentes técnicas tendentes a lograr la dispersión uniforme de los CNTs en la matriz cerámica, uno de los principales problemas que persisten en la actualidad para la fabricación de este tipo de materiales con características reproducibles y propiedades mecánicas mejoradas respecto de la matriz. En segundo lugar, se pretende estudiar la influencia de la microestructura (segregación en los bordes de grano, distribución de nanotubos, tamaño de grano,...) en las propiedades mecánicas de los materiales obtenidos, a baja temperatura (resistencia a la fractura y al desgaste) y también a alta temperatura (resistencia a la fluencia).

La sinterización se realizará usando técnicas de nueva generación como el horno de microondas (MW) y el spark plasma sintering (SPS), equipos de los que dispone nuestro grupo de investigación y que actualmente se encuentran plenamente operativos. Estas técnicas permiten el sinterizado de las matrices cerámicas en un tiempo corto y, en el caso del SPS, a temperaturas relativamente bajas en comparación con los métodos tradicionales lo que permite la densificación del material conservando el tamaño nanométrico de los polvos cerámicos de partida y sin producir daños importantes en los CNTs.

Los policristales obtenidos serán caracterizados microestructuralmente mediante técnicas de microscopia electrónica de transmisión tales como TEM, HRTEM, EDX y PEELS, microscopia electrónica de barrido de alta resolución (HRSEM), difracción de rayos X y espectroscopia Raman. La caracterización mecánica incluye ensayos de resistencia a la fractura y al desgaste a temperatura ambiente y temperaturas moderadas y ensayos de deformación a alta temperatura, controlando tensión, temperatura y atmósfera de trabajo.

Los parámetros macroscópicos y microscópicos obtenidos se analizarán en términos de los modelos existentes y en caso de no encontrar en ellos la justificación adecuada se intentará avanzar en la modelización de los mecanismos que contribuyen a la deformación de estos materiales compuestos nanoestructurados y con segundas fases de CNTs.

The aim of this Project is two fold: firstly the fabrication of nanostructured composites of alumina and yttria stabilized zirconia polycrystals (8Y-SZP) reinforced with different concentrations of carbon nanotubes (CNTs). In both materials, the powder used will have a high purity (> 99%) and different grain sizes; between 30 and 40 nm in the case of alumina and between 20 and 300 nm in the case of 8Y-SZP, and secondly to study the influence of the microstructure (grain boundary segregation and nanotubes distribution) on the mechanical properties at low temperature (fracture and wear resistance) as well as at high temperature (creep resistance).

To obtain the polycrystals nanostructured, two techniques of new generation (both equipments belong to our research group) will be used, such as the microwave furnace (MW) and the spark plasma sintering (SPS); this techniques allow to sinter the powder in a short time and at low temperature in the case of SPS which is a fundamental requirement to keep the nanostructure of the as-received powder without destroying the CNTs.

The obtained polycrystals will be microstructurally characterized using techniques such as SEM, TEM, HRTEM, EDX, PEELS, X-Ray diffraction and Raman spectroscopy. The mechanical characterization includes fracture and wear resistance tests at moderate temperature and creep test at high temperature as a function of stress, temperature and controlled atmosphere.

The macroscopic and microscopic parameters will be analyzed using the existent models and, if needed, by formulating new models in order to establish the master chart of the mechanical behaviour of these ceramics composites.

Unión Europea
Fondo Europeo de Desarrollo Regional
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MINISTERIO DE CIENCIA E INNOVACIÓN

Propiedades termomagnéticas de materiales y optimización de su eficiencia energética Thermomagnetic properties of materials and optimization of energy efficiency

Código/Code: MAT2010-20537
Periodo/Period: 01-01-2011 / 31-12-2013
Organismo Financiador/Financial source: Ministerio de Ciencia e Innovación
Importe total/Total amount: 121.000 €
Investigador responsable/Research head: Alejandro Conde Amiano
Componentes/Research group: Clara F. Conde Amiano, Josefa María Borrego Moro, Victorino Franco García, Javier S. Blázquez Gámez, Rafael Caballero Flores

RESUMEN / ABSTRACT

Se propone un estudio de propiedades termomagnéticas de materiales magnéticos blandos, preparados por técnicas de solidificación rápida y aleado mecánico. Se trata de profundizar en la relación composición-microestructura-propiedades como vía para la optimización de materiales en dos direcciones: magnéticos blandos para aplicaciones a alta temperatura y materiales para refrigeración magnética en el entorno de la temperatura ambiente. En el

primer caso se trata de aumentar el límite térmico de comportamiento blando del material y de disminuir el coeficiente de temperatura de sus propiedades. En el segundo caso se trata de acercar la temperatura de transición magnética del material a la temperatura ambiente y de maximizar su respuesta magnetocalórica. Se abordará también la modelización de diferentes procesos implicados en la formación de aleaciones (aleado mecánico, cinética de nanocristalización), de las interacciones entre partículas y sus efectos en el comportamiento termomagnético del material, de la dependencia de la respuesta magnetocalórica con el campo magnético aplicado, etc.

A study of the thermomagnetic properties of soft magnetic materials obtained by rapid quenching and mechanical alloying techniques is proposed. The aim of the project is to improve the knowledge of the composition-microstructure-properties relationship as a way to optimize the material properties in two lines: soft magnetic materials for high temperature applications and materials for magnetic refrigeration near room temperature. In the first case, the aim is to enhance the thermal limit for the soft magnetic behavior of the materials and to decrease the temperature coefficient of their properties. In the second case, the aim is to bring the magnetic transition temperature of the material close to room temperature and to maximize the magnetocaloric response. It will be also contemplated modeling of different processes involved in the alloy formation (mechanical alloying, nanocrystallization kinetics), of the interactions between particles and their effects on the thermomagnetic behavior of the material, of the dependency of the magnetocaloric response with the applied magnetic field, etc.

Materiales magnéticos blandos; su optimización para un uso eficiente de la energía

Código/Code:	P10-FQM-6462 (Proyecto de Excelencia)
Periodo/Period:	15-03-2011 / 15-03-2014
Organismo Financiador/Financial source:	Junta de Andalucía
Importe total/Total amount:	153.190,75 €
Investigador responsable/Research head:	Alejandro Conde Amiano
Componentes/Research group:	Clara F. Conde Amiano, Josefa María Borrego Moro, Victorino Franco García, Javier S. Blázquez Gámez, Rafael Caballero Flores

OTROS PROYECTOS / OTHER PROJECTS

Magnetocaloric effect in amorphous and multiphase materials: experiments and models

Código/Code:	N00014-11-1-0311
Periodo/Period:	1-05-2011 / 31-01-2012
Oganismo Financiador/Financial source:	OTROS PROGRAMAS, ORGANISMOS PÚBLICOS (EXTERNOS) OFFICE OF NAVAL RESEARCH

(USA)
Importe total/Total amount: 99.430 $ USA
Investigador responsable/Research head: Victorino Franco García
Componentes/Research group: Clara F. Conde Amiano, Alejandro Conde Amiano, Javier S. Blázquez Gámez, B. Ingale

COOPERACIÓN INTERNACIONAL Y OTROS INTERNATIONAL COOPERATION AND OTHERS

Estudio y optimización de nanocomposites para refrigeración magnética

Periodo/Period: 1-01-2010 / 31-12-2011
Entidad Financiadora/Financial source: Ministerio de Ciencia e Innovación (Proyecto FR2009-0101) Acciones Integradas
Importe total/Total amount: 12000 €
Investigador responsable/Research head: Victorino Franco García

PUBLICACIONES / PUBLICATIONS

ARTÍCULOS PUBLICADOS EN REVISTAS SCI / PAPERS IN SCI JOURNALS

Cellular automata simulations on nanocristallization processes: from instantaneous growth approximation to limited growth
J.S. Blázquez, C.F. Conde, A. Conde
Journal of Non-Crystalline Solids, **357** (2011) 2833–2839
DOI: 10.1016/j.jnoncrysol.2011.03.018

Cellular automata simulations have been performed to simulate the crystallization process under a limited growth approximation. This approximation resembles several characteristics exhibited by nanocrystalline microstructures and nanocrystallization kinetics. Avrami exponent decreases from a value n = 4 indicating interface controlled growth and constant nucleation rate to a value n ~ 1 indicating absence of growth. A continuous change of the growth contribution to the Avrami exponent from zero to 3 is observed as the composition of the amorphous phase becomes richer in the element present in the crystalline phase.

Magnetic and structural characterization of Mo-Hitperm alloys with different Fe/Co ratio
Conde, C.F., Borrego, J.M., Blázquez, J.S., Conde, A., Svec, P., Janickovic, D.
Journal of Alloys and Compounds, **509** (2011) 1994–2000
DOI: 10.1016/j.jallcom.2010.10.113

The influence of the Co content on the microstructure and magnetic behaviour of a series of amorphous and nanocrystalline (FeCo) $_{79}$Mo $_{8}$Cu $_{1}$B $_{12}$ alloys is reported. Changes in the magnetic properties provoked by the microstructural evolution upon different thermal treatments of as-cast samples are analyzed as well. Kinetics of nanocrystallization process can be described by an isokinetic approach. As the Co content in the alloy increases, the Curie temperature of the amorphous as-cast samples increases while the crystallization onset temperature decreases. The crystalline volume fraction as well as the mean grain size of the nanocrystals at the end of the nanocrystallization process are slightly higher for the lowest Co content alloy but smaller than in similar Hitperm Mo-free alloys. The average magnetic field and the average isomer shift of the as-cast samples show a linear increase with two slopes with the Co content of the alloy. The same tendency is found for the saturation magnetization. Combined TEM, XRD, and MS data indicate the presence of Mo atoms in the nanocrystals. At the end of the nanocrystallization process the softest magnetic behaviour corresponds to the lowest Co content alloy. The second crystallization process provokes a magnetic hardening of these alloys.

Influence of la and Ce additions on the magnetocaloric effect of Fe-B-Cr-based amorphous alloys
Law, J.Y., Franco, V., Ramanujan, R.V.
Applied Physics Letters, **98** (2011) Article Number 192503
DOI: 10.1063/1.3589353

The magnetic entropy change (Δ S M), temperature of peak Δ S M (T pk) and refrigerant capacity (RC) in Fe (RE) 80 B 12 Cr 8 (RE=La, Ce, or Gd) alloys were studied. Increasing La, Ce, and Gd content led to relatively constant, decrease, and increase in T pk, respectively. Both the phenomenologically constructed universal curve for Δ S M and field dependence power laws demonstrated that these alloys exhibited similar critical exponents at Curie temperature. With 5% Ce added to Fe 80 B 12 Cr 8, Tpk could be tuned near room temperature with relatively constant peak Δ S M. Fe 79 B 12 Cr 8 La 1 exhibited enhanced RC compared to Gd 5 Si 2 Ge 1.9 Fe 0.1. The tunable T pk and enhanced RC are needed in active magnetic regenerators.

Magnetocaloric effect and critical exponents of Fe 77Co 5.5Ni 5.5Zr 7B 4Cu 1: A detailed study
Franco, V., Caballero-Flores, R., Conde, A., Knipling, K.E., Willard, M.A.
Journal of Applied Physics, **109** (2011) Article Number 07A905
DOI: 10.1063/1.3535191

The critical exponents of the alloy have been determined with the Kouvel-Fisher method to predict the field dependence of the magnetic entropy change δS M. The nonlinear fit of δS M (H) to a power law provides a field exponent in perfect agreement with the predictions of the relevant scaling laws using the obtained critical exponent values. It is shown that possible discrepancies between these two methods for determining the field dependence of δS M might arise due to a poor resolution in the temperature of the experiments.

Analysis of the magnetoresistance contributions in a nanocrystallized Cr-doped FINEMET alloy

Kiss, L.F., Franco, V., Csontos, M., Péter, L., Conde, C.F., Conde, A., Kemény, T., Tóth, J., Varga, L.K., Bakonyi, I.
Journal of Magnetism and Magnetic Materials, **323** (2011) 699-707
DOI: 10.1016/j.jmmm.2010.10.026

The magnetoresistance (MR) was measured at 200, 250 and 300 K in magnetic fields up to B=12 T for a nanocrystallized Fe 63.5Cr 10Nb 3Cu 1Si 13.5B 9 alloy. Both the longitudinal (LMR) and transverse (TMR) component of the magnetoresistance decreased from B=0 to about 0.1 T. This could be ascribed to a giant MR (GMR) effect due to spin-dependent scattering of conduction electrons along their path between two FeSi nanograins via the non-magnetic matrix. Such a scattering may occur if the nanograin moments are not or only weakly coupled in the absence of a strong exchange coupling (due to the high Cr content in the matrix) and/or only weak dipoledipole coupling is present (due to sufficiently large separations between the nanograins). For larger fields, the GMR saturated and a slightly nonlinear increase in MR with B was observed due to a contribution by the residual amorphous matrix. The anisotropic MR effect (AMR≡LMR-TMR) was negative for all fields and temperatures investigated. By measuring the MR of melt-quenched Fe 100-xSi x solid solutions with x=15, 18, 20, 25 and 28, the observed AMR could be identified as originating from the FeSi nanograins having a D0 3 structure.

Direct magnetocaloric measurements of Fe-B-Cr-X (X = La, Ce) amorphous ribbons

Law, J.Y., Franco, V., Ramanujan, R.V.
Journal of Applied Physics, **110** (2011) Article Number 023907
DOI: 10.1063/1.3613666

A procedure has been developed to directly measure the adiabatic temperature change of amorphous melt-spun Fe-based ribbons displaying attractive room temperature magnetocaloric properties. Polycrystalline Gd ribbons are used as a reference material to compensate for the contribution of the sample holder to the experimental values. Fe 78B 12Cr 8Ce 2 and Fe 75B 12Cr 8Ce 5 melt-spun ribbons exhibited a peak adiabatic temperature change (ΔT ad pk) ~ 58% larger than Co 82.9Si 5.9Fe 4.5Cr 4B 2.7 amorphous ribbons. The ΔT ad pk in Fe 78B 12Cr 8Ce 2, Fe 75B 12Cr 8Ce 5, and Fe 79B 12Cr 8La 1 ribbons displayed ~ 18-33% enhanced ΔT ad pk compared to a GdAl 2 alloy.

Magnetocaloric effect in melt-spun FePd ribbon alloy with second order phase transition

Prida, V.M., Franco, V., Vega, V., Sánchez-Llamazares, Suñol, J.J., Conde, A., Hernando, B.
Journal of Alloys and Compounds, **509** (2011) 190-194
DOI: 10.1016/j.jallcom.2010.09.060

Magnetic entropy change and refrigerant capacity for an applied magnetic field variation of 1.5 T have been determined in the temperature range of 293-700 K for the as-quenched polycrystalline Fe 73.2Pd 26.8 melt-spun ribbons alloy. Samples show a major magnetic phase with the fct crystal structure and a Curie temperature of 553 K, at which a second order magnetic phase transition occurs. A maximum magnetic entropy change of 1.04 J kg -1 K -1 was achieved at 550 K, while the maximum refrigerant capacity of 108 J/kg is attained at the applied field of 1.5 T. The field dependence of the magnetic entropy change for this material follows the phenomenological universal curve and at the temperature of the peak corresponds to a large field independent exponent of n = 0.84. Extrapolated value of field depending RC Area at 5 T reach above 300 J/kg, which is comparable to that of some of the best-known Fe-doped GdSiGe coolant compounds.

Optimization of the refrigerant capacity in multiphase magnetocaloric materials

Caballero-Flores, R., Franco, V., Conde, A., Knipling, K.E., Willard, M.A.
Applied Physics Letters, **98** (2011) Article Number 102505
DOI: 10.1063/1.3560445

The refrigerant capacity (RC) of magnetocaloric materials can be enhanced using multiphase materials or composites, which expand the temperature range over which a significant magnetic entropy change can be obtained. Numerical simulations show that by controlling the parameters of the composite (the fraction of the different phases and their Curie temperatures) improvements of RC of ∼83% are possible. The maximum applied field plays a crucial, nonmonotonic, role in the optimization. As a proof of concept, it is shown that the combination of two Fe88-2 x Co x Ni x Zr 7 B 4 Cu 1 alloys produces an enhancement in R C of ∼37%, making it ∼92% larger than that of Gd5 Si 2 Ge 1.9 Fe 0.1.

The magnetocaloric properties of GdScSi and GdScGe

Couillaud, S., Gaudin, E., Franco, V., Conde, A., Pottgen, R., Heying, B., Rodewald, U.Ch., Chevalier, B.
Intermetallics, **19** (2011) 1573-1578
DOI: 10.1016/j.intermet.2011.06.001

The magnetocaloric properties of the ferromagnetic compounds GdScSi (T C = 354(2) K) and GdScGe (T C = 349(2) K) (tetragonal CeScSi-type structure refined from single crystal diffractometer data, space group I4/mmm) have been determined. The field dependence of the magnetic entropy ΔS m change and of the refrigerant capacity RC have been obtained from magnetization measurements. At the T C Curie temperature, ΔS m for GdScSi and GdScGe is respectively equal to 2.5 and 3.3 J/kg Gd K for a magnetic field change of 2 T; the values are comparable to those determined previously for Gd 7Pd 3 and Gd 4Bi 3 which exhibit also a T C-temperature higher than room temperature. Both microstructural and the analysis of the magnetocaloric response are used to assess the single phase nature of the samples.

Origin of the magnetic anomaly and tunneling effect of europium on the ferromagnetic ordering in Eu 8-xSr xGa 16Ge 30(x=0,4) type-I clathrates

Phan, M.-H., Franco, V., Chaturvedi, A., Stefanoski, S., Nolas, G.S., Srikanth, H.
Physical Review B – Condensed Matter and Materials Physics, **84** (2011) 054436
DOI: 10.1103/PhysRevB.84.054436

Systematic dc magnetization studies using the Banerjee criterion, Kouvel-Fisher, and magnetocaloric effect methods provide physical insights into the origin of the magnetic anomaly and the tunneling effect of europium on the ferromagnetic ordering in Eu 8Ga 16Ge 30 type-I clathrates. We show that Eu 8Ga 16Ge 30 undergoes a second-order magnetic transition (SOMT) at T C ∼ 35 K, resulting from the magnetic interaction between the Eu2 + ions at the Eu2 sites, followed by a secondary magnetic transition at T L ∼ 10 K (indicated as a magnetic anomaly in previous studies), as a result of the magnetic interaction between the Eu2 + ions at the Eu1 and Eu2 sites. The critical exponent β=0.388 is close to that predicted from the three-dimensional Heisenberg model (β=0.365), while the critical exponent γ=0.956 is close to that predicted from the mean-field model (γ=1). The substitution of Sr2 + for Eu2 + retains the SOMT but largely reduces the transition temperatures (T C ∼ 15 K and T L ∼ 5 K), with the critical exponents β=0.521 and γ=0.917 close to those predicted from the mean-field model (β=0.5 and γ=1). These results point to the important fact that the tunneling of Eu2 + between the four equivalent sites in the tetrakaidecahedral cage tends to prevent the occurrence of a long-range ferromagnetic ordering in the type-I clathrate materials.

Tunable magnetocaloric effect in Gd-based glassy ribbons
Mayer, C., Gorsse, S., Ballon, G., Caballero-Flores, R., Franco, V., Chevalier, B.
Journal of Applied Physics, **110** (2011) Article Number 053920
DOI: 10.1063/1.3632983

The series of glassy ribbons Gd 60M 30In 10 (M = Mn, Co, Ni, Cu) was synthesized by melt-spinning. The change of transition element M in these Gd-based metallic glasses was proven to induce huge variations of the Curie temperature T C, magnetic entropy change peak values ΔS m peak, and widths at half maximum values of the magnetic entropy change δT. When M is non magnetic (M = Co, Ni, Cu), the samples behave similarly: they display high values of ΔS m peak (between -6.6 and -8.2 J/kg K in a magnetic field variation of 4.6 T), average δT values (between 77 and 120 K) and no magnetic hysteresis. On the contrary, when M carries a magnetic moment (M = Mn), some irreversibility appears at low temperature, ΔS m peak is lower (only 3.1 J/kg K for µ 0H = 4.6 T) and the magnetic transition is very large (δT = 199 K for µ 0H = 4.6 T). These features are explained by some antiparallel coupling between Mn atoms randomly located in the metallic glass. This leads to the occurrence of a cluster-glass behavior at low temperature (35 K), following the ferromagnetic transition observed at 180 K when the temperature is decreased. Also, power law fittings of ΔS m peak and δT versus µ 0H were performed and show that δT is less field dependent than ΔS m peak. We could then identify an interesting way of improving the refrigeration capacity of the material at low magnetic field.

Two milling time regimes in the evolution of magnetic anisotropy of mechanically alloyed soft magnetic powders
Ipus, J.J., Blázquez, J.S., Franco, V., Conde, C.F., Conde, A.
Journal of Alloys and Compounds, **509** (2011) 1407-1410
DOI: 10.1016/j.jallcom.2010.10.207

The milling time evolution of magnetic anisotropy of ball milled powders can be described considering two regimes. First, for short milling times, the main factor affecting the magnetic behavior of the alloy is the accumulation of internal stresses. Second, for long milling times, magnetic anisotropy can be explained using three contributions: long-range magnetoelastic, averaged short-range magnetoelastic and averaged magnetocrystalline anisotropies.

Magnetic properties and magneto-caloric effect in pseudo-binary intermetallic (Ce,R) 2Fe 17 compounds (R = Y, Pr and Dy)
Alvarez, P., Gorria, P., Sánchez Llamazares, J.L., Pérez, M.J., Franco, V., Reiffers, M., Curlik, I., Gazo, E., Kovac, J., Blanco, J.A.
Intermetallics, **19** (2011) 982-987
DOI: 10.1016/j.intermet.2011.02.020

We have synthesized three pseudo-binary (Ce,R) 2Fe 17 intermetallic alloys, where cerium has been partially substituted by R = Y, Pr and Dy, with the aim of tuning the Curie temperature (between 253 and 273 K) for obtaining the maximum magneto-caloric response of the alloys just below room temperature. The analysis of the x-ray powder diffraction patterns show that the three samples crystallize in the rhombohedral Th 2Zn 17-type crystal structure (space group R3m). We report the temperature dependence of the isothermal magnetic entropy change, ΔS M(T), the magnetic field dependence of its maximum value, ΔS M max(H), and the relative cooling power around the second-order magnetic transition for magnetic field changes μ 0ΔH max = 5 T. The collapse of the normalized ΔS M(θ)/ΔS M max vs. temperature (where θ is a rescaled temperature) into a single master curve allows the extrapolation of ΔS M(T) curves for higher magnetic field changes, and/or the estimation of the temperature dependence of the magnetic entropy for other 2:17 pseudo-binary compounds. The lower values of ΔS M max compared with those of the R 2Fe 17 compounds with R = Pr or Nd are explained in terms of the decrease of the saturation magnetization. The magnetic field dependence of the ΔS M max indicates that only Pr 1.5Ce 0.5Fe 17 alloy roughly follows a mean-field behaviour.

Congresos y Reuniones / Congress and Meetings

Congresos y Reuniones Internacionales / International Congress and Meetings

Participación en la Organización de Congresos y Reuniones / Participation in Organising Congresses and Meetings

Symposium "Magnetic Materials for Energy Application"
27 Febrero – 3 Marzo [San Diego, Estados Unidos de América]
Victorino Franco [Miembro del Comité Organizador]

Workshop "Recent Trends on Nanomagnetism, Spintronics and their Applications"
1 – 4 Junio [Ordicia, España]
Victorino Franco [Publication Editor]

56th MMM Conference
30 Octubre – 3 Noviembre [Scottsdale, Estados Unidos de América]
Victorino Franco [Publication Editor]

COMUNICACIONES EN CONGRESOS Y REUNIONES / COMMUNICATIONS IN CONGRESS AND MEETINGS

International Symposium on Metastable, Amorphous and Nanostructured Materials, ISMANAM 2011
26 Junio – 1 Julio [Gijón, España]

"Analysis of nanocrystallization kinetics and crystal size distribution under limited growth approach", Blazquez-Gamez, Javier S.; Conde-Amiano, Clara F.; Conde-Amiano, Alejandro
Comunicación oral

"Comparison of equivalent ball milling processes on Fe70Zr30 and Fe70Nb30", Blazquez-Gamez, Javier S.; Ipus-Bados, Jhon Jairo; Conde-Amiano, Clara F.; Conde-Amiano, Alejandro
Poster

European Congress and Exhibition on Advanced Materials and Processes, EUROMAT 2011
12 – 15 Septiembre [Montpellier, Francia]

"The magnetocaloric effect in amorphous and multiphase materials: phenomenological models to describe its field dependence", Franco-Garcia, Victorino; Conde-Amiano, Alejandro
Comunicación oral

20th Soft Magnetic Materials Conference 2011, SMM 20
18 – 22 Septiembre [Isla de Kos, Grecia]

"The magnetocaloric effect in soft magnetic amorphous alloys and composites", Franco-Garcia, Victorino; Conde-Amiano, Alejandro
Conferencia Invitada

56th Annual Conference on Magnetism and Magnetic Materials
30 Octubre – 3 Noviembre [Scottsdale, Estados Unidos de América]

"Enhancement of the magnetocaloric effect in composites: Experimental validation", Paticopoulus, S.; Caballero-Flores, Rafael; Franco-Garcia, Victorino; Blazquez-Gamez, Javier S.; Conde-Amiano, Alejandro; Knipling, K. E.; Willard., M. A.
Comunicación oral

FORMACION / TRAINING

TESIS DOCTORALES/ DOCTOR DEGREE THESIS

Título:	**Efecto magnetocalórico en materiales con transiciones de fase de segundo orden: Optimización de la capacidad de refrigeración.**
Autor:	Rafael Caballero Flores
Directores:	Alejandro Conde Amiano, Victorino Franco García
Calificación:	Sobresaliente "Cum Laude"
Centro:	Universidad de Sevilla

EQUIPAMIENTO CIENTÍFICO AVAILABLE EQUIPMENT

- Calorímetro de barrido diferencial (Perkin-Elmer DSC7)
- Balanza termogravimétrica (Perkin-Elmer TGA-7)
- Espectrómetro Mössbauer (Wissel MB-500) con horno.
- Coercímetro (desarrollado en el laboratorio)
- Magnetómetro de muestra vibrante (LakeShore 7000) con horno y criostato.
- Equipo de medida directa de temperatura adiabática (Advanced Magnetic Technologies).
- Molino Planetario (Fritzsch Pulverisette Vario 4)
- Equipo de solidificación por enfriamiento ultrarrápido (melt spinning, Bühler)
- Equipo de fusión por arco (MAM1, Bühler

SERVICIOS GENERALES
GENERAL SERVICES

SERVICIO DE ESPECTROSCOPÍAS / SPECTROSCOPY SERVICE

El Servicio de Espectroscopía incluye las Unidades de Espectroscopia de Resonancia Magnética Nuclear, Espectroscopía Raman, Espectroscopía Infrarroja y Espectroscopía Ultravioleta-Visible. Este servicio está dedicado a la determinación de la estructura molecular de los compuestos químicos y la caracterización de materiales.

This Service consists of four different spectroscopies: Nuclear Magnetic Resonance Spectroscopy, Raman Spectroscopy, Infrared Spectroscopy and Ultraviolet-Visible Spectroscopy. It is devoted to the determination of molecular structure of chemical compounds and materials.

RESONANCIA MAGNÉTICA NUCLEAR EN SU CONFIGURACIÓN DE ESTADO SÓLIDO / NUCLEAR MAGNETIC RESONANCE IN ITS SOLID-STATE CONFIGURATION

La Resonancia Magnética Nuclear en estado sólido es utilizada para el estudio de la estructura atómica de materiales amorfos o poco cristalinos. Se basa en el comportamiento de los momentos magnéticos de ciertos núcleos atómicos bajo la influencia de un campo magnético externo y de los campos locales creados por los núcleos vecinos y por la distribución de carga electrónica en torno al núcleo. Los espectros más comunes son representaciones de la intensidad de absorción frente a la frecuencia de resonancia y presentan señales cuya posición, forma y tamaño están íntimamente relacionados con el entorno químico del núcleo estudiado. Permite el estudio del orden a corto alcance de materiales estructuralmente desordenados y diferencia átomos con números atómicos similares.

Solid State Nuclear Magnetic Resonance is a widely use technique to study the structural properties of materials, including amorphous and not very crystalline solids. This technique is based on the behavior of the magnetic moments of the nuclei under an external magnetic fields and the local magnetic field due to the environment. Thus, the position, shape and intensity of the signals inform of the chemical environment of the nuclei.

INSTRUMENTAL DISPONIBLE / AVAILABLE EQUIPMENT

- Espectrómetro de RMN multinuclear Bruker, mod. DRX-400
  Multinuclear RMN Spectrometer (Bruker, mod. DRX-400)
- Sonda CP/MAS de 4 mm dotada de doble canal, 1H y BB (en el rango de frecuencia desde 15N a 31P)
  CP/MAS sound of 4 mm with double channel, 1H and BB (at a frequency range from 15N to 31P)
- Unidad neumática, que permite alcanzar velocidades de giro bajo ángulo mágico de hasta 15000 Hz
  Neumatic unit, that allows to reach turn velocities under a magic angle up to 15000 Hz

- Accesorio de temperatura variable dotado de una línea propia de N_2, así como de un sistema de control de temperatura que permite trabajar en un rango entre 223 K y a 373 K.
  Accessory of variable temperature with a line of its own of N_2, and with a temperature control system that allows to work at a range of 223 K - 373 K.

Responsable Científico/Scientific Responsible: Dra. María Dolores Alba Carranza
Personal Técnico/Technical Assistant: Dr. Miguel Angel Avilés Escaño

ESPECTROSCOPÍA MICRO-RAMAN / MICRO-RAMAN SPECTROSCOPY

La espectroscopia Raman se basa en un proceso fotónico en el que la radiación incidente es dispersada por la muestra, produciéndose transiciones de tipo vibracional y rotacional. En general, el espectro Raman se interpreta como un espectro vibracional que ofrece información muy similar al espectro de infrarrojo, aunque las vibraciones que se ven reflejadas en el espectro Raman no son siempre las mismas que en aquel. Para que un modo vibracional sea activo en espectroscopia Raman es necesario que se produzcan cambios en la polarizabilidad de los enlaces químicos o la molécula considerada, lo que conlleva la producción de momentos dipolares inducidos. Su campo de aplicación es muy extenso: semiconductores, compuestos del carbono (grafito, diamante, nanotubos, fibras…), catalizadores, pigmentos, etc.

Raman spectroscopy is based on a photonic process in which the incident radiation is dispersed by the sample. This latter is perturbed leading to vibrational and rotational transitions. In general, the Raman spectrum is interpreted like a vibrational one, providing information very similar to the infrared spectroscopy, although the Raman active vibrations are not always the same than excited in infrared. A Raman vibration mode is active if there is a change of polarizability of the chemical bonds or the considered molecule, which in turn results in the generation of induced dipolar momentam. Its application fields are very broad: semiconductors, carbon compounds (graphite, diamond, nanotubes, fibers…), catalysts, pigments, etc.

INSTRUMENTAL DISPONIBLE / AVAILABLE EQUIPMENT

- LabRAM Horiba Jobin Yvon dotado de un microscopia confocal y 3 longitudes de excitación (785 cm^{-1} rojo, 532 cm^{-1} verde, y 325 cm^{-1} UV)
  LabRAM Horiba Jobin Yvon equipped with a confocal microscope and 3 excitation lasers (785 cm^{-1} red, 532 cm^{-1} green, and 325 cm^{-1} UV)

Responsables Científicos/ Scientific Responsibles:: Dr. Juan Carlos Sánchez López, Dr. Hernán Míguez García y Dr. Miguel Angel Centeno Gallego
Personal Técnico/ Technical Assistant: Dr. Miguel Angel Avilés Escaño

ESPECTROSCOPÍA INFRARROJA / INFRARED SPECTROSCOPIES

La espectroscopía de Infrarrojos (FT-IR) se basa en la absorción de radiación infrarroja por parte de los materiales. Esta absorción supone un cambio en la energía vibracional de los enlaces, siempre que se produzca un cambio en la polarización de dicho enlace. El resultado obtenido es un espectro en el que se representa la radiación absorbida o transmitida en función del número de onda de la radiación, lo cual permite identificar el enlace correspondiente.
El equipo en el ICMS cubre un rango de número de ondas que va desde 5000 a 250 cm-1 (óptica de CsI) y se puede trabajar con purga o en vacío. Se halla equipado con accesorios para trabajar en los modos de Reflectancia Difusa (DRIFT), Reflectancia Total Atenuada (ATR) y Reflexión Especular. Dispone de un microscopio de Infrarrojos que tiene una resolución lateral de 10 µm.

Infrared spectroscopy (FT-IR) is based on the selective absorption of the infrared radiation by the materials. This absorption means a change in the vibrational energy of the chemical bounds, whenever it occur a change in the polarization. The result is a spectrum showing the absorbed or transmitted radiation as a function of the wavenumber of the radiation, which can be assigned to the corresponding chemical bound.
The equipment of the ICMS works in a wavenumber range from 5000 to 250 cm^{-1} (CsI optic), and can operate with a gas purge or in vacuum. It is equipped with several accessories to do Diffuse Reflectance (DRIFT), Attenuated Total Reflectance (ATR) or Specular Reflectance. It has got an Infrared Microscope with a lateral resolution of 10 µm.

INSTRUMENTAL DISPONIBLE / AVAILABLE EQUIPMENT

- JASCO FT/IR-6200 IRT-5000
  JASCO FT/IR-6200 IRT-5000

Responsables Científicos/ Scientific Responsibles: Dr. Manuel Ocaña Jurado y Dr. Ángel Barranco Quero
Personal Técnico/ Technical Assistant: Dr. Miguel Angel Avilés Escaño

ESPECTROSCOPÍA ULTRAVIOLETA / ULTRAVIOLET-VISIBLE SPECTROSCOPIES

La espectroscopía Ultravioleta-Visible (UV-Vis) informa sobre las diferencias de energía existentes entre los niveles electrónicos ocupados más externos y los desocupados más próximos.
Se dispone en el ICMS de dos equipos que cubren el rango de longitudes de onda que va desde 190 nm hasta 900 nm. Se puede trabajar tanto en el modo de Transmisión como en el de Reflectancia Difusa.

The Ultraviolet-Visible Spectroscopy (UV-Vis) report on the existing energy differences between the more external occupied electronic levels and the nearer unoccupied ones.

There are two equipments in the laboratory, which work in the wavelength range of 190 nm to 900 nm. It can operate in the Transmission mode or in Diffuse Reflectance Modes.

INSTRUMENTAL DISPONIBLE / AVAILABLE EQUIPMENT

- SHIMADZU UV-2101 PC
  SHIMADZU UV-2101 PC
- Perkin Elmer Lambda 12
  Perkin Elmer Lambda 12

Personal Técnico/ Technical Assistant: Dr. Miguel Angel Avilés Escaño

SERVICIO DE ANÁLISIS TEXTURAL Y TÉRMICO / TEXTURAL AND THERMAL ANALYSIS SERVICE

Este servicio incluye las siguientes Unidades: Análisis Térmico, Fisi-quimisorción, Análisis de Tamaño de Partícula y Potencial Z. Está dedicado a la determinación de la textura, estructura y comportamiento térmico de los materiales.

This Service includes the following units: Thermal Analysis, Physisorption and Chemisorption, Particle Size and Z-potential determination. It is devoted to the characterization of texture, microstructure and thermal behavior of advanced materials.

FISI-QUIMISORCIÓN / PHYSISORPTION-CHEMISORPTION

Este servicio constituye una herramienta básica para la caracterización microestructural de sólidos pulverulentos de distinta naturaleza, en cuanto a porosidad, superficie específica y superficie químicamente activa.

En el servicio se dispone de un analizador de adsorción de gases (Micromeritics, ASAP 2020) que proporciona isotermas de adsorción y desorción, a partir de los cuales se obtienen de ellas la superficie específica y distribución del tamaño de poro y de microporo de estos materiales, incorporando también los accesorios necesarios para medidas de quimisorción.

This service constitutes a basic tool for the microstructural characterization of powdered solids of different natures, regarding to their porosity, specific surface area and chemically active surface.

This service is composed by a phyisisorption analyser (Micromeritics, ASAP 2020) which provides the complete adsorption/desorption isotherms, from which the specific surface area, pore and micropore size distribution and concentration of reactive sites are obtained. The instrument is also equipped for carrying out chemisorption of different reactive molecules, as O_2, H_2, CO, etc.

INSTRUMENTAL DISPONIBLE / AVAILABLE EQUIPMENT

- Analizador científico de fisisorción ASAP2010 (Micromeritics)
  Physisorption analyser ASAP 2010 (Micromeritics)
- Analizador de quimisorción ASAP2010 (Micromeritics)
  Chemisorption analyser ASAP 2010 (Micromeritics)
- Analizador de fisisorción multimuestra TRISTAR II (Micromeritics)
  Multisample physisorption analyser TRISTAR II (Micromeritics)
- Analizador de fisisorción multimuestra TRISTAR II-Kr (Micromeritics)
  Multisample physisorption analyser TRISTAR II-Kr (Micromeritics)

Responsables Científicos/ Scientific Responsibles: Dr. Gerado Colón Ibáñez y Dr. Miguel Angel Centeno Gallego
Personal Técnico/ Technical Assistant: Dª Cristina Gallardo López

ANÁLISIS TÉRMICO / THERMAL ANALYSIS

Las técnicas de análisis térmico permiten estudiar aquellos cambios físicos o químicos que ocurren en los sólidos en función de la temperatura y que conlleven modificaciones en su masa o intercambios de calor con su entorno.
En el servicio se pueden realizar experimentos desde temperatura ambiente hasta 1500ºC, tanto en atmósfera inerte (N_2) como reactiva (aire, O_2,…).
Se dispone de tres técnicas: Análisis Termogravimétrico (TG), Análisis Térmico Diferencial (ATD) y Calorimetría Diferencial de Barrido (CDB).

Thermal analysis techniques allows to studying physical or chemical changes occurring in solid in samples as a function of the temperature. Those changes should involve either a mass change or a heat flow.
The experiments can be performed in the range from room temperature to 1500ºC, both under inert (N_2), or reactive (air, O_2,…) atmospheres.
Three different techniques are available: Thermogravimetry (TG), Differential Thermal Analysis (DTA) and Differential Scanning Calorimetry (DSC).

INSTRUMENTAL DISPONIBLE / AVAILABLE EQUIPMENT

- Equipo de análisis térmico simultáneo TG/ATD/CDB TA Instruments Q600
  TA Instruments Q600 Simultaneous TG/DTA/DSC instrument
- Equipo termogravimétrico TG, TA Instruments Q5000
  Thermogravimetric instrument TG, TA Instruments Q5000
- Equipo de calorimetría diferencial de barrido CDB, TA Instruments Q20
  Differential scanning calorimeter DSC, TA Instruments Q20

Responsable Científico/ Scientific Responsible: Dr. Luis A. Pérez Maqueda
Personal Técnico/ Technical Assistant: Dª Cristina Gallardo López

TAMAÑO DE PARTÍCULAS Y POTENCIAL Z / PARTICLE SIZE AND Z POTENTIAL ANALYSIS

Se dispone de las técnicas de Dispersión Dinámica de Luz y de Difracción Láser (LD), que permiten determinar la distribución de tamaños de partícula de sistemas coloidales en suspensión (disolvente acuoso u orgánico) en los rangos que van de 3 a 3000 nanómetros (DLS) o de 0.05 a 900 micras (LD).

Así mismo, se dispone de la técnica de Análisis de Movilidad Electroforética para la evaluación del potencial “Z” de sistemas coloidales en suspensión (disolvente acuoso u orgánico).

Dynamic light scattering (DLS) and Laser diffraction (LD) are available for the determination of particle size distributions of colloidal systems (dispersed in aqueous or organic dispersions solutions) in the range 3-3000 nanometers (DLS) and 0.05-900 microns (LD).

Electrophoretic mobility measurements can be also performed for the evaluation of Z potential in colloidal systems (aqueous or organic dispersions).

INSTRUMENTAL DISPONIBLE / AVAILABLE EQUIPMENT

- Malvern modelo Zetamaster (DLS) y MalvernSizer (LD)
  Malvern model Zetamaster (DLS) and MalvernSizer (LD)

Responsable Científico/ Scientific Responsible: Dr. Manuel Ocaña Jurado
Personal Técnico/ Technical Assistant: Dª Cristina Gallardo López

SERVICIO DE MICROSCOPÍA DE ELECTRONES / ELECTRON MICROSCOPY SERVICE

El servicio está dedicado a la caracterización química y estructural de muestras sólidas mediante técnicas de microscopía electrónica. Las técnicas de caracterización disponibles en el servicio son la Microscopía Electrónica de Transmisión (TEM) y la Microscopía Electrónica de Barrido (SEM), acopladas una y otra con las Espectroscopías de Energía Dispersiva de Rayos X (EDS) y de Pérdida de Energía de Electrones (EELS).
Las tareas ofrecidas por el personal técnico comprenden la preparación de muestras, su estudio por la batería de técnicas disponibles (TEM, SEM, HRTEM, SAED, EDS, EELS), la adquisición de imágenes y espectros, y en algunos casos, la interpretación de los datos experimentales.

This Service is devoted to the chemical and structural characterization of solid samples by means of electron microscopies. The characterization techniques available at ICMS are Transmission Electron Microscopy and Scanning Electron Microscopy, which are equipped with a Electron Energy Loss Spectrometre and a Energy Dispersive X-ray Analyser, respectively.
The technicians working on this service carryied out different tasks, as sample preparation, image and spectral adquisition, and in some particular cases, interpretation of experimental results.

MICROSCOPÍA ELECTRÓNICA DE BARRIDO / SCANNING ELECTRON MICROSCOPY

La microscopía electrónica de barrido proporciona información microestructural, morfológica y de composición química en escala microscópica (hasta una resolución lateral de ~ 5 nm). Se puede aplicar a todo tipo de materiales y problemáticas de estudio en ciencia de materiales: cerámicas, plásticos, metales, minerales, catalizadores, muestras de patrimonio histórico, capas finas, recubrimientos, interfases, nanopartículas, etc.

The scanning electron microscopy provides information about the microstructure, morphology and chemical composition at the microscopic scale of solid samples (upto a lateral resolution of ~ 5 nm). It can be applied to all type of materials including ceramics, polymers, metals, minerals, catalysts, samples from cultural heritage, thin films, coatings, interfaces, nanoparticles, etc.

INSTRUMENTAL DISPONIBLE / AVAILABLE EQUIPMENT

- Microscopio SEM, modelo JEOL JSM-5400, dotado de analizador EDX Oxford Isis, con resolución de 138 eV. Cañón termoiónico de filamento de W
  JEOL JSM-5400 microscope equipped with an Oxford Isis EDX analyzer with a resolution of 138 eV. Thermoionic W electron gun

- Microscopio SEM, modelo Hitachi S4800 SEM-FEG de alta resolución (1-3 nm). Dotado de analizador EDX Bruker X Flash Detector 4010 con una resolución de 133 eV. Cañón de emisión de campo y detector STEM
  Hitachi S4800 SEM-FEG microscope of high resolution (1-3 nm). Equipped with a Bruker X flash 4010 EDX detector with a resolution of 133 eV, field emission gun and STEM detector.
- Equipamiento anexo para la preparación de muestras: metalizadores, cortadoras, etc.
  Sample preparation equipment: metallization devices, cutting tools, etc.

Responsable Científico/ Scientific Responsible: Dra. Asunción Fernández Camacho
Personal Técnico/ Technical Assistant: Dra. M. Carmen Jiménez de Haro

MICROSCOPÍA ELECTRÓNICA DE TRANSMISIÓN / TRANSMISSION ELECTRON MICROSCOPY

La microscopía electrónica de transmisión es una técnica ampliamente utilizada para la caracterización estructural y química de materiales a escala microscópica y nanoscópica, pudiéndose obtener información sobre morfología, tamaño de grano, composición química, grado de cristalinidad e identificación de fases cristalinas en todo tipo de materiales. La espectroscopia de pérdida de energía de electrones (EELS) acoplada al microscopio TEM constituye una herramienta adicional para determinar la estructura electrónica, el tipo de enlace y la formación de fases.

The transmission electron microscopy is a widely used technique for the microstructural and chemical characterization at micro and nanoscales, giving information about morphology, grain size, chemical composition, crystallinity and identification of crystalline phases in all type of materials. The energy loss spectroscopy (EELS), coupled to the TEM microscope, constitutes an additional tool for the determination of electronic structure, type of bond and phase formation.

INSTRUMENTAL DISPONIBLE / AVAILABLE EQUIPMENT

- Microscopio JEM-2000EX con una resolución estructural de 2.1 Å
  JEM-2000EX microscope with a structural resolution of 2.1 Å.
- Microscopio Philips CM200 con una resolución estructural entre puntos de 2.3 Å, portamuestras de uno y dos giros, calentamiento y enfriamiento. Acoplado al equipo se dispone de un sistema de análisis por Energías Dispersivas de Rayos X (EDX) y Espectrómetro de Pérdidas de Energía Electrónica (PEELS), de GATAN modelo 766-2 keV
  Philips CM200 microscope with a structural resolution of 2.3 Å. Sample holder with one and two angles, heating and cooling. It is equipped with a X-ray Energy Dispersive Analyser (EDX) and a Electron Energy Loss Spectrometre (PEELS) (Gatan, model 766-2 keV.

- Laboratorio de preparación de muestras para microscopía, que comprende: Evaporador de carbón, pulidora, cortadoras de disco y ultrasónica, adelgazador cóncavo-convexo, adelgazadores iónicos: Balttec (modelo RES 100) y Fischione (modelo 1010)
  Sample preparation laboratory, equipped with carbón evaporator, cutting and polishing tools, dimple, ion milling guns Balttec (model RES100) and Fischione (model 1010)

Responsable Científico/ Scientific Responsible: Dra. Asunción Fernández Camacho
Personal Técnico/ Technical Assistant: Lda. Olga Montes Amorín (CicCartuja) y María Inmaculada Roja Cejudo

SERVICIO DE DIFRACCIÓN DE RAYOS X
X-RAY DIFFRACTION LABORATORY SERVICE

La difracción de rayos-X permite la identificación cualitativa y cuantitativa de sustancias cristalinas y su caracterización microestructural y textural.
El servicio dispone en la actualidad de cuatro difractómetros independientes, configurados específicamente para abordar el análisis de muestras policristalinas de muy distinta naturaleza, en lo referente a su composición, estabilidad química, cristalinidad, etc.
Asimismo, con alguno de ellos se pueden llevar a cabo, además de los análisis rutinarios (θ-2θ), otros varios mas avanzados, como pueden ser:

- Seguir las transformaciones de fase “in situ” provocadas por calentamientos en atmósfera inerte (vacio, Ar) o reactiva (H2, O2,..).
- Caracterizar materiales en la nanoescala (1-100 nm) mediante el estudio de la dispersión de rayos-X a ángulos bajos (SAXS).
- Determinar el grosor, densidad y rugosidad de películas delgadas, mediante Reflectometría de rayos-X.
- Obtener la estructura cristalina de materiales inestables a la atmósfera o muy transparentes a los rayos-X, mediante el empleo de capilares.

X-ray diffraction allows the qualitative and quantitative identification of crystalline substances and their microstructural and textural characterization.
At present, four independent diffractometers are available in this service, specifically configured to analyze the composition, chemical stability, crystallinity and many other properties in polycrystalline samples of a varied nature. Besides ordinary analyses (θ-2θ), part of the equipment can perform some advanced studies as:

- Direct monitoring of transformations undergone in materials under heating, such as phase changes, under inert o reactive atmosphere.
- To characterize materials at the nanoscale (1-100 nm) through X-ray scattering at low angles, using the SAXS technique.
- To measure some physical parameters of layers such as density, thickness and surface roughness with the reflectometry setup.

- To obtain the diffraction patterns of samples either sensitive to the atmosphere or highly transparent to X-rays (organic compounds) employing the capillary configuration.

INSTRUMENTAL DISPONIBLE / AVAILABLE EQUIPMENT

- Difractómetro Panalytical X'PERT PRO con cargador automático de muestras
  Diffractometer PANALYTICAL X'PERT PRO with automatic sample charger
- Difractómetro PHILIPS X'PERT PRO con cámara de alta temperatura (1200 ºC) ANTON PAAR HTK 1200
  Diffractometer PHILIPS X'PERT PRO with high temperature chamber (1200ºC) ANTON PAAR HTK 1200
- Difractómetro Panalytical X'PERT PRO (reflectometría, SAXS, ángulo rasante y capilares)
  Diffractometer PANALYTICAL X'PERT PRO (reflectometry, SAXS, low angle scattering and capillary)
- Difractómetro de polvo SIEMENS D5000 DUAL (reflexión y transmisión)
  Diffractometer SIEMENS D5000 DUAL (reflection and transmission)

Responsable Científico/ Scientific Responsible: Dra. Concepción Real Pérez
Personal Técnico/Technical Assistant: Ldo. José María Martínez Blanes

SERVICIO DE ANÁLISIS DE SUPERFICIE/ SURFACE ANALYSIS SERVICE

El Servicio de Análisis de superficie incluye las Unidades de Espectroscopía de Fotoelectrones de Rayos X (XPS) y de Espectroscopia de Descarga Luminiscente (GDL). Este servicio está dedicado al análisis químico y electrónico de superficies sólidas. También permiten conocer la composición en profundidad (desde la superficie hacia el interior) de los sólidos.

The surface analysis service consists of two untis: the X-ray Photoelectron Spectroscopy (XPS) and the Glow Discharge Luminescence. This service is devoted to the electronic and chemical analysis of solid surfaces. It also provides information about the compositional depth profile of solids (from their surface toward their bulk).

ESPECTROSCOPÍA DE FOTOEMISIÓN DE ELECTRONES / X-RAY PHOTOELECTRON SPECTROSCOPY

Las "Espectroscopías de Fotoelectrones" (XPS/ESCA y AES) son unas poderosas técnicas de análisis cuantitativo no destructivo, sensibles exclusivamente a las primeras capas de la super-

ficie de los sólidos (20-30 Å), lo que permiten obtener información sobre las propiedades químicas, físicas y electrónicas de las mismas.
El interés técnico de esta información es enorme en campos tales como corrosión, catálisis, tratamientos de superficies, fenómenos de flotación y adherencia, segregación de fases, etc.
La característica más importante de la Espectroscopía de Fotoelectrones (XPS/ESCA) es que permitir diferenciar distintos estados de oxidación y/o situaciones del entorno (coordinación) de los átomos en las muestras sólidas analizadas. El límite de detección es del 0.5% para cada especie química.
El servicio dispone actualmente de dos instrumentos independientes.

Typically, “photoelectron spectroscopies” are a powerful set of non-destructive analysis techniques, exclusively sensitive to the more superficial few atomic layers (20-30 Å), allowing to obtain valuable information about their chemical, physical and electronic properties.
The technical interest of the resulting information is huge in fields such as catalysis, corrosion, surface treatments,, floating and adhesion phenomena, or segregation processes, among others. The most remarkable characteristic of X-Ray Photoelectron Spectroscopy (XPS/ESCA) is that it allows to discriminate, for a given element, between different oxidation states or chemical surroundings (coordination).

INSTRUMENTAL DISPONIBLE / AVAILABLE EQUIPMENT

Espectrómetro de Fotoelectrones VG ESCALAB 210, compuesto de:
Photoelectron Spectrometer VG ESCALAB 210, consisting on:

- Cámara de análisis, analizador hemiesférico multicanal VG ESCALAB 210, manipulador de cuatro ejes, y fuentes de excitación de rayos X (dual, Alkα y MgKα, acromático), de luz ultravioleta y de haces de electrones, lo que permite realizar análisis superficiales mediante técnicas de XPS, UPS y REELS, así como estudios angulares.
  Analysis Chamber, equipped with a hemispheric multichannel analyser VG ESCALAB 210, a four axis manipulator, a dual X-ray source (achromatic Al Kα, Mg Kα), a UV lamp, and a electron gun, allowing to perform surface analysis by XPS, UPS and REELS, including angular resolved studies.
- Dos Precámaras de tratamientos, con vacío residual de 10^{-8} y 10^{-9} mbar respectivamente, en las que es posible someter a las muestras a tratamientos diversos como: calentamientos a alta temperatura (T<800ºC) bajo atmósfera controlada, desbastado iónico con gases inertes o reactivos, exposición a plasmas, iluminación con laser, deposición de metales, óxidos y compuestos sencillos, exfoliación in situ, etc.
  Two prechambers for different treatments, with ultimate vacuum levels of 10-8 and 10-9 mbar respectively, where samples can be subjected to diverse treatments and transferred to the analysis chamber without exposure to the atmosphere. The possible treatments include heating at high temperature (< 800C) under controlled atmosphere, ion sputtering with inert or reactive gases, exposure to plasma, laser treatments, deposition of metals, oxides or simple compounds, exfoliation, etc.

Espectrómetro de Fotoelectrones SPECS, compuesto de:
Photoelectron Spectrometer SPECS, consisting on:

- Cámara de análisis, dotada de analizador hemiesférico multicanal PHOIBOS 100, manipulador de tres ejes, y fuentes de excitación de rayos X (dual, Alkα y MgKα).
  Analysis Chamber, equipped with a hemispheric multichannel analyser PHOIBOS 100, three axis manipulator and dual X-ray source (achromatic Al Kα, Mg Kα).
- Precámara de tratamiento de alta Presión y alta Temperatura (HPHT Cell). En esta Cámara es posible someter a las muestras a tratamientos térmicos en presencia de gases hasta una presión de 20 atm y 800 ºC, tanto en estático como en dinámico (simultáneamente).
  Pre-chamber for High Pressure/High Temperature treatments (HPHT Cell).Samples can be subjected to treatments in the presence of gases up to 20 bar and 800ºC (simultaneously). These treatments can be performed either under static or flowing gas conditions. After treatments, samples can be transferred to the analysis chamber without exposure to the atmosphere.
- Una cámara de inserción rápida dotada de sistema de aparcamiento/ desgasificado, que permite evacuar las muestras a temperatura reducida (T < 150ºC). También es posible la realización de tratamientos de desbatado iónico o la incorporación de otros sistemas (iluminación con luz Uv-Vis, evaporación de metales, u otros compuestos, etc.)
  A Fast entry chamber, equipped with a parking and degassing system, allowing the samples to be evacuated at moderate temperature (T < 150ºC). It is also possible to sputter the samples under an accelerated ion beam (0.5- 5.0 kV) using inert or reactive gases. Incorporation of some other equipment (Visible light illumination, metal evaporators) is also contemplated.

Responsables Científicos/ Scientific Responsibles: Dr. Juan Pedro Espinós Manzorro y Dr. Juan Pedro Holgado Vázquez
Personal Técnico/Technical Assistant: Ldo. David Benítez

SERVICIO DE ESPECTROMETRÍA DE EMISIÓN ÓPTICA POR DESCARGA LUMINISCENTE/ GLOW DISCHARGE OPTICAL EMISSION SPECTROMETRY SERVICE (GD-OES)

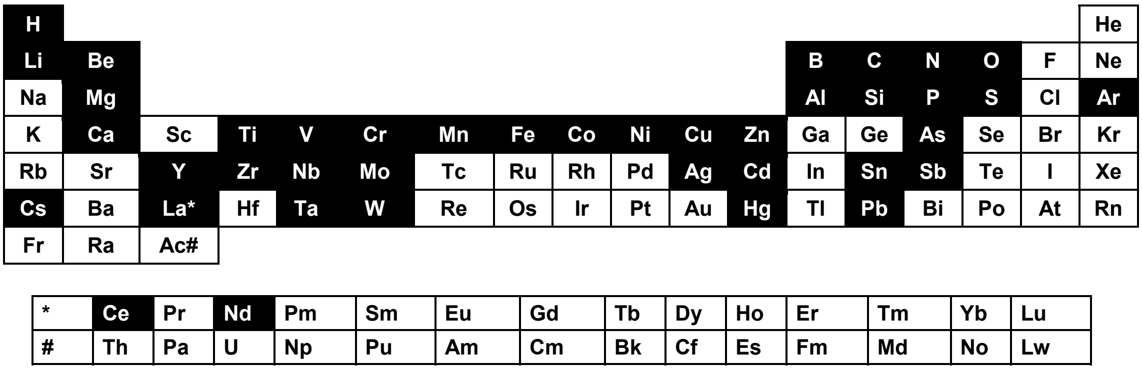
La técnica de Espectrometría por Descarga Luminiscente constituye una potente herramienta para el análisis rápido de sólidos, tanto en masa como en superficie. Además se pueden determinar concentraciones elementales en función de la profundidad lo que permite realizar perfiles de concentración sobre materiales avanzados: metales tratados, materiales recubiertos, multicapas, superficies pintadas, capas finas, procesos de corrosión y oxidación, etc.. La descarga luminiscente es un plasma autosustentado que se genera en un gas encerrado a baja presión (1 kPa aproximadamente) entre dos electrodos que se en-cuentran a una diferencia de potencial del orden de 1 kV. La diferencia de potencial puede lograrse tanto mediante la aplicación de corriente continua (DC), como mediante radiofrecuencia (RF), pudiéndose medir tanto muestras conductoras como no conductoras.

Glow discharge optical emission spectrometry (GDOES) has emerged as a major technique for surface and depth profile analysis, owing to the unique combination of fast sputtering rate, high depth resolution, excellent sensitivity and multi-element capability. Glow discharge is a selfsustained plasma that is generated in a gas enclosed to low pressure (1 kPa) between two electrodes at a potential difference of 1 kV. This potential difference can be achieved by the application of a direct current (DC.) or by radio frequency (RF), which offers the advantage that both conducting and non-conducting samples can be analyzed.

INSTRUMENTAL DISPONIBLE / AVAILABLE EQUIPMENT

- Espectrómetro de descarga luminiscente LECO GDS 750A equipado con dos policromadores holográficos de 3600 y 1800 líneas, óptica a vacío que permite el análisis en el UV y 43 fotomultiplicadores que permiten analizar los elementos resaltados en negro en la tabla mostrada abajo. Puede trabajar en modo de funcionamiento en DC y RF.

  Glow Discharge Spectrometer LECO GDS 750ª equipped with two holographic diffraction gratings of 1800 lines/mm and 3600 lines/mm, optics in vacuum and 43 photomultipliers giving the ability to detect the elements highlighted in the table below. It is equipped with a RF and a DC sputter source.



H																	He
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	La*	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	Ac#															

*	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
#	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lw

Responsable Científico/ Scientific Responsible: Dr. Miguel Angel Centeno Gallego

SERVICIO DE MECANIZADO/ MECHANICAL WORKSHOP

Se trata de un servicio horizontal fundamental para el Instituto y unidades externas adscritas al mismo, puesto que, además del mantenimiento del material y equipamiento científico, permite su mejora y adaptación a los distintos experimentos en curso, y de acuerdo con las necesidades de los investigadores y/o los proyectos que se llevan a cabo.

The Machining workshop is a basic and essential service that provides technical support to the maintenance, change, fitting and development of simple scientific equipments, according with the current requirements of the experiments and projects carried out by the researchers at the ICMS.

INSTRUMENTAL DISPONIBLE / AVAILABLE EQUIPMENT

Además de otras herramientas menores para cortar, soldar, doblar, taladrar, etc., el taller de mecanizado cuenta con los siguientes equipos:
Besides other minor tolos for cutting, soldering, folding, drilling, etc, this workshop is equipped with:

- Torno de control numeric computerizado, modelo HASS TM1
  A computer numeric control turing machine, model HASS TM1
- Taladro vertical, modelo ERLO TSAR32
  A vertical drill, model ERLO TSAR32
- Un par de tornos manuales o semiautomáticos, modelos PINACHO TURN180 y SUPER 11 CD EMCO
  A couple of turning machines: models PINACHO TURN180 and SUPER 11 CD EMCO

Responsable/ Responsible: Ing. Enrique Jiménez Roca
Personal Técnico: Juan Carlos Sánchez Martín

ACTIVIDADES DIVULGATIVAS Y FORMATIVAS
OUTREACH AND TEACHING ACTIVITIES

DOCENCIA / TEACHING

CURSOS DE POSTGRADO / POSTGRADUATE COURSES

MÉTODOS FÍSICOS DE ANÁLISIS DE CAPAS FINAS Y SUPERFICIES DE SÓLIDOS

Curso de Postgrado del CSIC
Programa 2010

Métodos Físicos de Análisis de Capas Finas y Superficies de Sólidos

Sevilla, del 28 de Junio al 2 de Julio de 2010

Este curso de postgrado pretende familiarizar a los asistentes con algunos de los métodos físicos de análisis más utilizados en la actualidad para la caracterización de capas finas y superficies. El curso, de una semana de duración, constará de clases teóricas y sesiones prácticas. Será impartido por profesores de la Universidad de Sevilla e investigadores del CSIC, en las instalaciones y con el equipamiento científico disponible en el Instituto de Ciencia de Materiales de Sevilla y el Centro Nacional de Aceleradores.

Está dirigido a científicos e ingenieros especializados en temas de análisis, diagnóstico e investigación en materiales y superficies. También se considera especialmente adecuado para alumnos de tercer ciclo de ingenierías de materiales.

Temáticas

Aplicaciones Tecnológicas de las Películas Delgadas
Técnicas de Preparación de Películas y Recubrimientos (CVD, PVD)
Espectroscopías de Fotoemisión (XPS, UPS)
Microscopías Electrónicas de Transmisión y Barrido (TEM y SEM) Espectroscopías Electrónicas (Auger, REELS, EDX, PEELS)
Difracción de Rayos X
Absorción de Rayos X (EXAFS, XANES)
Dispersión de Iones (ISS, RBS)
Microscopías de Aproximación de puntas (AFM, STM)

Directores:

Dr. Juan Pedro Espinós Manzorro
Instituto de Ciencia de Materiales de Sevilla
jpespinos@icmse.csic.es

Dr. Guillermo Munuera Contreras
Instituto de Ciencia de Materiales de Sevilla
Dpto. Química Inorgánica

Instituto de Ciencia de Materiales de Sevilla
c/ Américo Vespucio, 49. 41092 (Sevilla)
Telf: 954 48 95 27 • Fax: 954 46 06 65
http://www.icmse.csic.es/cursocapas.htm
CUOTA DE INSCRIPCIÓN: 300 €

Hay disponible un número limitado de becas para alumnos de tercer ciclo (adjuntar curriculum vitae y una carta de presentación de un investigador cualificado)

Organizado por el Instituto de Ciencia de Materiales de Sevilla
Directores: Dr. Juan Pedro Espinós y Dr. Guillermo Munuera
Fecha de Celebración: 27 junio al 1 de julio de 2011
Horas lectivas: 25 de teoría + 15 de prácticas
Dirigido a: Grado de Doctor, Estudiante de Doctorado o Especialista de Empresa

Este curso de postgrado pretende familiarizar a los asistentes con algunos de los métodos físicos de análisis más utilizados en la actualidad para la caracterización, de materiales en general, y de capas finas y superficies en particular. El curso, de carácter intensivo y una semana de duración, consta de clases teóricas y sesiones prácticas. Estas últimas, desarrolladas con grupos de reducidos de alumnos, se realizarán con el equipamiento científico disponible en el Instituto de Ciencia de Materiales de Sevilla, el Centro Nacional de Aceleradores y el Servicio de Espectroscopía de Fotoelectrones de la Universidad de Sevilla.

El contenido y enfoque de los temas y otras actividades del curso son eminentemente prácticos, estando dirigido a científicos e ingenieros especializados en temas de análisis, diagnóstico, investigación en superficies, etc. También se considera especialmente adecuado para alumnos de tercer ciclo relacionados con la temática tratada.

Teoría**:**

Aplicaciones Tecnológicas de las Películas Delgadas | Dr. Juan Pedro Espinós Manzorro
Espectroscopía de Fotoemisión de Rayos X: Composición Superficial | Dr. Guillermo Munuera Contreras
Espectroscopía de Fotoemisión de Rayos X: Estado Químico en la Superficie de Sólidos | Dr. Agustín R. González-Elipe
Determinación de Perfiles de Composición a partir del Análisis de Forma de Pico en XPS: Método de Tougaard | Dr. Francisco Yubero Valencia
Deposición de Láminas Delgadas mediante Métodos Basados en la Utilización de Plasmas| Dr. José Cotrino Bautista

Microscopía Electrónica de Transmisión: Fundamentos y Aplicaciones Generales | Dra. Concepción Real Pérez
Microscopía Electrónica: Análisis PEELS y EFTEM| Dra. Cristina Rojas Ruiz
Microscopía Electrónica de Barrido| Dra. María del Carmen Jiménez de Haro
Microscopías Efecto Túnel y de Fuerzas Atómicas | Dr. José Jesús Benítez Jiménez
Métodos de Determinación de Espesores de Capas Finas | Dr. Juan Pedro Espinós Manzorro
La Difracción de Rayos X: Generalidades | Dr. Angel Justo Erbez
Análisis de Texturas: Difracción de Rayos X y Espectroscopía Raman | Dr. Juan Carlos González González
Absorción de Rayos X: Orden a Corto Alcance en Superficie y Láminas Delgadas| Dr. Juan Pedro Holgado Vázquez
Retrodispersión Rutherford: Perfiles de Composición | Dr. Miguel Angel Respaldiza (CNA)

Prácticas:
Microscopías Electrónicas de Transmisión y Barrido | Dra. Cristina Rojas Ruiz | Lda. Carmen Jiménez de Haro | Lda. Olga Montes
XPS/ISS/REELS | Dr. Juan Pedro Espinós | Dr. Francisco Yubero | Dr. Guillermo Munuera
Difracción y Fluorescencia de Rayos X | Dr. Angel Justo | Ldo. José M. Martínez
Absorción de Rayos X | Dr. Juan Pedro Holgado | Ldo. Victor González
Retrodispersión Rutherford | Dr. Javier García
Microscopía de Fuerzas Atómicas | Dra. Carmen López Santos | Dra. Ana Borrás

APLICACIÓN DE LA RADIACIÓN SINCROTRÓN A LA CARACTERIZACIÓN DE MATERIALES

Curso de Postgrado del CSIC
Programa 2006-07

Aplicación de la Radiación Sincrotrón a la Caracterización de Materiales

Sevilla, del 9 al 11 de Abril de 2007

Organizado por el Instituto de Ciencia de Materiales de Sevilla
Directores: Dra. Adela Muñoz Páez y Dr. Alfonso Caballero Martínez
Fecha de Celebración: 19 al 21 de octubre de 2011
Horas lectivas: 20 horas
Dirigido a: Licenciados o alumnos de los últimos cursos

Curso de Postgrado de 3 días de duración que tratará de las aplicaciones de la radiación sincrotrón al estudio espectroscópico de sólidos. El creciente interés de nuestro país por las técnicas que hacen uso de las fuentes de radiación sincrotrón nos ha movido a organizar este curso que pretende dar una visión general de las técnicas espectroscópicas más utilizadas en el análisis de los sólidos, las cuales hacen uso de este tipo de radiación de características notables. El curso es intensivo para facilitar su realización por personas con domicilio fuera de Sevilla. El número de alumnos estará limitado a un máximo de 30 para asegurar una amplia e informal interacción entre el profesorado y los asistentes.

El curso está dirigido a científicos e ingenieros implicados en problemas de análisis de materiales, investigación en estado sólido, etc., así como alumnos de tercer ciclo que cursen su doctorado en disciplinas afines.

Interacción de la Radiación con la Materia Condensada | Dra. Asunción Fernández Camacho
La Radiación Sincrotrón, Principios, Instrumentación | Dr. José Manuel Quesada, Universidad de Sevilla
Dispersión de Rayos X: de los Sistemas Heterogéneos a las Capas Delgadas | Dra. Mari Cruz García Gutiérrez, IEM, Madrid
Espectroscopía de Absorción de Rayos X | Dr. Jesús Chaboy Nalda, ICMA Zaragoza
Demostración práctica de los métodos de Análisis de Espectroscopía EXAFS| Dr. Juan Pedro Holgado
Espectroscopía de Fotoelectrones: Fotoemisión | Dr. Juan Pedro Espinós
Fotoemisión a Altas Presiones | Dr. Alfonso Caballero Martínez
Difracción de Rayos X con Radiación Sincrotrón | Dr. Carlos Frontera, ICMB, Barcelona
Macromolecular Crystallography for Industry at the Advanced Photon Source, Argonne National Laboratory | Dr. Stephen R. Wasserman, Eli Lilly and Company
Espectroscopía de Absorción de Rayos X de Baja Energía | Dr. Agustín R. González Elipe
Application of NEXAFS to absorbed species and their reactions | Dr. Richard Lambert, Universidad de Cambridge-ICMS
Microscopía de Rayos X: Principios y Aplicaciones | Dra. Gema Martínez Criado, ESRF, Grenoble, Francia
Eperimentos con Resolución Temporal | Dr. Victor López Flores, Universidad de Estraburgo, Bélgica
La Fuente de Luz Sincrotrón "ALBA". Estado de la Fuente y Puesta a Punto de las líneas | Dra. Inmaculada Peral, ALBA, Barcelona

DETERMINACIÓN DE ESTRUCTURAS EN SÓLIDOS REALES: TÉCNICA DE RESONANCIA MAGNÉTICA NUCLEAR

Curso de Postgrado del CSIC
Programa 2007-08

Determinación de Estructuras en Sólidos Reales: Técnica de Resonancia Magnética Nuclear

Sevilla, del 8 al 12 de septiembre de 2008

PROFESORES

Dra. Mª Dolores Alba
Dr. Miguel Angel Avilés
Dra. Ana Isabel Becerro
Dra. Teresa Blasco
Dr. Miguel Angel Castro
Dr. Pablo Chain
D. Juan I. Corredor
Dr, Laurence Delevoye
Dr. Alberto Escudero
Dr. Pedro Nieto
Dr. Jesús Sanz
Dª Esperanza Pavón

Este curso pretende suministrar los conocimientos básicos para el estudio de los sólidos reales a través de una técnica que informa acerca del orden local de los átomos de la red. Para ello, se hará una breve introducción teórica de los sólidos reales, haciendo hincapié en aquellos aspectos estructurales que demandan el empleo de técnicas instrumentales que aporten información a corto alcance. Además, se darán los principios básicos en los que se basa la resonancia magnética nuclear que irán acompañados de una colección de problemas.

HORARIO

Lunes-Jueves: 9:00-13:00 y 15:30-19:00
Viernes: 9:00-13:00

DIRIGIDO A

Alumnos de tercer ciclo e investigadores interesados en el área de RMN y Química del Estado Sólido

DIRECTORA

Dra. **María Dolores Alba Carranza**
alba@icmse.csic.es

SECRETARIA

Dª Margarita Adorna
Dª Ana García Martín
D. José Carlos Rivero

Instituto de Ciencia de Materiales de Sevilla
c/ Américo Vespucio, 49, 41092 (Sevilla)
Telf: 954 48 95 46 • Fax: 954 46 06 65
http://www.icmse.csic.es/cursormn.htm
CUOTA DE INSCRIPCIÓN: 150 €

Organizado por el Instituto de Ciencia de Materiales de Sevilla
Directores: Dra. María Dolores Alba Carranza
Fecha de Celebración: 5 al 8 de septiembre de 2011
Horas lectivas: 15 horas teórica + 15 horas prácticas
Dirigido a: Licenciados o alumnos de los últimos cursos

Este curso pretende suministrar los conocimientos básicos para el estudio de los sólidos reales a través de una técnica que informa acerca del orden local de los átomos de la red. Para ello, se hará una breve introducción teórica de los sólidos reales, haciendo hincapié en aquellos aspectos estructurales que demandan el empleo de técnicas instrumentales que aporten información a corto alcance.

Además, se darán los principios básicos en los que se basa la resonancia magnética nuclear que irán acompañados de una colección de problemas. Por último, se plantearán las dificultades mostradas por esta técnica en su aplicación al estado sólido en función de la naturaleza del núcleo a estudiar. Las secciones prácticas incluirán el uso del equipo para resolver casos prácticos sencillos y el empleo del paquete informático apropiado para el procesado y tratamiento matemático de los espectros.

Introducción | Dra. María Dolores Alba Carranza
Conceptos Básicos | Ldo. Juan Isidro Corredor
Secuencia de Pulso Básica en RMN | Dr. Laurent Delevoye
Herramientas Matemáticas Básicas para RMN | Dr. Laurent Delevoye
Estado Sólido: Componentes Anisotrópicas| Dr. Alberto Escudero
RMN de Sólido de Núcleos con Espín ½ Abundantes | Dra. Esperanza Pavón González
RMN de Sólido de Núcleos con Espín ½ y Bajo γ | Dra. María Dolores Alba Carranza
RMN de No-Sólido No-Líquido | Dr. Pedro Nieto
RMN de Sólido de Núcleos con Espín ½ poco Abundantes | Dr. Jesús Sanz
RMN de Sólido de Núcleos con Espín mayor de ½ | Dra. Teresa Blasco
Profesores de Seminarios: Dr. Pablo Chaín, Dr. Laurent Delevoye, Dr. Juan Isidro Corredor, Dra. Carolina Pazos, Dra. Esperanza Pavón
Profesor de Prácticas: Dr. Miguel Angel Avilés Escaño y Dr. Juan Isidro Corredor

MÁSTER / MASTER

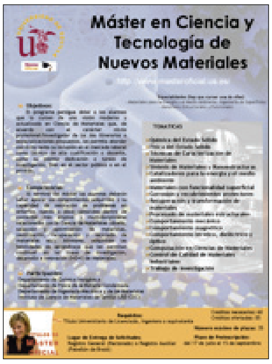
MÁSTER EN ESTUDIOS AVANZADOS EN QUÍMICA

Organizado por la Universidad de Sevilla
Coordinadora: Dra. Mª Angeles Alvarez Rodríguez
Fecha de Celebración: Curso Académico 2010-11
Créditos necesarios: 60
Dirigido a: Licenciados en Química, Física, así como, los Titulados en Ingeniería afines (Ingenieros Químicos, de Materiales, etc.)
Especialidades: Materiales para la Energía y el Medio Ambiente. Ingeniería de Superficies, Materiales Estructurales y Funcionales.
Mención de Calidad

Seminario-Laboratorio de espectroscopia Avanzada (Créditos Europeos: 8) |Dr. Ernesto Carmona (IIQ) | Dra. María Dolores Alba | Dr. Antonio M. Gil (UNSE) | Dra. Maria Angeles Pradera (UNSE) | Dr. José M. Fernández-Bolaños (UNSE)

Química de Polímeros. Biomateriales (Créditos Europeos: 4) | Dr. Manuel Bueno Martínez (USE) | Dr. Juan A. Galbis Pérez | Dr. Manuel Mancera Clavería (USE)
Catálisis Homogénea y Heterogénea (Créditos Europeos: 4) | Dr. Guillermo Munuera | Dr. Juan Cámpora (IIQ) | Dr. Antonio Pizzano (IIQ)
Química de Polímeros. Biomateriales (Créditos Europeos: 4) | Dr. Manuel Bueno Martínez (USE) | Dr. Juan A. Galbis Pérez | Dr. Manuel Mancera Clavería (USE)
Catálisis Homogénea y Heterogénea (Créditos Europeos: 2) | Dr. José Antonio Odriozola Gordón | Dr. Juan Cámpora (IIQ) | Dr. Antonio Pizzano (IIQ)
Laboratorio de Espectroscopía Avanzada (Créditos Europeos: 10) | Dra. María Dolores Alba Carranza

Máster en Ciencia y Tecnología de Nuevos Materiales


Máster en Ciencia y Tecnología de Nuevos Materiales

Organizado por la Universidad de Sevilla
Coordinador: Dr. José Antonio Odriozola Gordón
Fecha de Celebración: Curso Académico 2011-12
Créditos necesarios: 60
Dirigido a: Licenciados en Química, Física, así como, los Titulados en Ingeniería afines (Ingenieros Químicos, de Materiales, etc.)
Especialidades: Materiales para la Energía y el Medio Ambiente. Ingeniería de Superficies, Materiales Estructurales y Funcionales.
Mención de Calidad

Química del Estado Sólido (Créditos Europeos: 5) | Dra. María Dolores Alba Carranza | Dr. Miguel Angel Castro | Dra. Pilar Malet
Fisica del Estado Sólido (Créditos Europeos: 5) | Dra. Angela Gallardo López | Dra. Josefa Borrego | Dr. Manuel Jiménez Melendo
Técnicas de Caracterización de Materiales (Créditos Europeos: 8) | Dr. Antonio Ramírez de Arellano | Dr. Julián Martínez Fernández | Dr. Juan M. Montes (UNSE)
Síntesis de Materiales y Nanoestructuras (Créditos Europeos: 7) | Dra. Asunción Fernández Camacho | Dr. Francisco J. Gotor | Dr. Juan Pedro Espinós | Dr. Manuel Ocaña
Catalizadores para la Energía y el Medio Ambiente (Créditos Europeos: 5) | Dr. Alfonso Caballero | Dr. José Antonio Navío | Dr. Miguel Angel Centeno
Materiales con Funcionalidad Superficial (Créditos Europeos: 5) | Dr. Angel Barranco | Dr. Agustín R. González-Elipe | Dr. Francisco Yubero
Corrosión y Recubrimientos Protectores (Créditos Europeos: 5) | Dr. Antonio Paúl (UNSE) | Dr. Juan Carlos Sánchez López | Dr. L. Soria Conde (UNSE) | Dr. Enrique Herrera (UNSE)
Recuperación y Transformación de Materiales (Créditos Europeos: 5) | Dr. José Antonio Odriozola | Dr. Luis Pérez Maqueda | M. Isabel Domínguez Leal
Procesado de Materiales Estructurales (Créditos Europeos: 5) | Dr. Alfonso Bravo León | Dr. Julián Martínez Fernández | Dr. José A. Rodríguez Ortiz (UNSE)

Comportamiento Mecánico (Créditos Europeos: 5) | Dr. Gómez García
Comportamiento Magnético (Créditos Europeos: 5) Dr. Javier Blázquez Gámez | Dr. Victorino Franco García
Comportamiento Térmico, Dieléctrico y Óptico (Créditos Europeos: 5) | Dra. M. Carmen Gallardo Cruz | Dr. Francisco Javier Romero Landa
Computación en Ciencia de Materiales (Créditos Europeos: 5) | Dra. Regla Ayala Espinar | Dr. Antonio Córdoba Zurita (UNSE) | Dr. Felipe Gutiérrez Mora
Metodología de Proyectos (Créditos Europeos: 5) | Dr. Julián Martínez Fernández

OTROS / OTHER

Master Física Avanzada

Relatividad Especial y General
Dr. Diego Gómez García (5 créditos)
Organizado por la Universidad de Sevilla

Master of Crystallography and Crystallization

X-Ray Absorption Spectroscopies
Dra. Adela Muñoz Páez (4 horas)
Organizado por la Universidad Internacional Menéndez Pelayo - CSIC

Máster “Biotecnología Avanzada”

Módulo de Nanotecnología
Dra. Aránzazu Díaz Cuenca, Dr. José Jesús Benítez Jiménez
Lugar: La Rábida, Huelva
Organizado por la Universidad de Málaga y la Universidad Internacional de Andalucía

Máster “Estudios de Género y Desarrollo Profesional”

Perspectiva de género en la construcción del conocimiento científico
Dra. Asunción Fernández Camacho
Lugar: Sevilla, España
Organizado por la Universidad de Sevilla

Máster “Cristalografía y Cristalización”

Fundamentos de difracción y técnicas de imagen
Dra. Asunción Fernández Camacho
Lugar: Sevilla, España
Organizado por el CSIC y la Universidad Internacional Menéndez Pelayo

Escuela de Verano de la Universidad de Teruel

Nuevos desarrollos con funcionalización superficial de materiales (cerámicos)
Dr. Agustín R. González-Elipe
Lugar: Teruel, España
Organizado por la Universidad de Zaragoza

XVIII Escuela de Verano "Nicolás Cabrera"

Surface Functionalization of Materials for Added Value
Dr. Juan Carlos Sánchez López
Lugar: Madrid, España
Organizado por el Instituto Nicolás Cabrera y Consolider FUNCOAT

Experto en gestión de programas internacionales de I+D+i

Dra. Asunción Fernández Camacho
Lugar: Sevilla, España
Organizado por la Consejería de Economía, Innovación y Ciencia de la Junta de Andalucía y la Universidad Internacional de Andalucía

La Difracción de Rayos X. Introducción al Análisis de Difractogramas

Dra. María Dolores Alba Carranza, Esperanza Pavón González
Lugar: Sevilla, España
Organizado por BRUKER, con la colaboración del Servicio General de Investigación "Laboratorio de Rayos X" del CITIUS de la Universidad de Sevilla

Aplicación de Métodos de Refinamiento y Ajuste al Estudio de Difractogramas. Cuantificación de Fases Cristalinas

Dra. María Dolores Alba Carranza, Esperanza Pavón González
Lugar: Sevilla, España
Organizado por BRUKER, con la colaboración del Servicio General de Investigación "Laboratorio de Rayos X" del CITIUS de la Universidad de Sevilla

Asimismo, el personal del ICMS ha impartido cursos regulares de primer y segundo ciclos de las correspondientes Licenciaturas y/o Grados en Química, Física y Farmacia e Ingeniería de Materiales en la Universidad de Sevilla.

CONFERENCIAS INVITADAS IMPARTIDAS POR PERSONAL DEL ICMS
INVITED CONFERENCES BY PERSONNEL OF THE ICMS

Arcillas: estructura, propiedades y aplicaciones
María Dolores Alba Carranza
Universidad de Alcalá de Henares
Madrid, España, 4 de Abril

Microrreactores aplicados a la industria química
José Antonio Odriozola Gordón
Curso de Extensión Universitaria, Departamento de Ingeniería Química de la Universidad Federal de Pernambuco.
Recife, Brasil, del 4 al 6 de Abril

Superparamagnetic nanoparticles: analysis of their dipolar interactions
Victorino Franco
University of South Florida
Tampa, Estados Unidos de América, 6 de Abril

Oxidación de CO con catalizadores de oro: Hacia la tecnología de microrreactores
Miguel Angel Centeno Gallego
Conferencia en el Seminario Científico Energy and Environment: An Overview of some Catalytic Processes and After Treatment Technologies, dentro del ciclo Catálisis. Química Verde, Energía y Medio Ambiente de la Universidad de Málaga
Málaga, España, 27 Abril

Surface characterisation with REFELEXAFS of surface modified materials
Adela Muñoz Páez
Material Sciences Department, Universidad de Oxford
5 Junio

Hydrogen production in microchannel reactors
José Antonio Odriozola Gordón
Conferencia invitada en: International Conference “Nanostructured catalysts and catalytic processes for the innovative energetics and sustainable development”, devoted to the year of Spain in Russia and of Russia in Spain
Novosibirsk, Rusia, 5-8 Junio

Caracterización de Catalizadores mediante Espectroscopías de Electrones: XPS y Auger
José Antonio Odriozola Gordón
Escuela de Verano de la Sociedad Española de catálisis, SECAT’2011
Zaragoza, España, 28 Junio

Liquides ioniques: utilisation en synthèse inorganique
Svetlana Ivanova
Université Louis Pasteur

Estrasburgo, Francia, 7 de Julio

Characterization by TEM techniques with nano-scale resolution of nanostructured-multifunctional thin films prepared by magnetron sputtering
T. Cristina Rojas Ruiz
18th International Symposium on Metastable, Amorphous and Nanostructured Materials
Gijón, España, 1 de Julio

Diffusion cationique dans l'oxide de zirconium par dynamique moleculaire: une nouvelle methode
Diego Gómez García
Université de Nantes
Nantes, Francia, septiembre

Nanostructured Protective Coatings
Juan Carlos Sánchez López
XVIII Summer School Nicolás Cabrera: "Surface Functionalization of Materials for Added Value Applications"
Miraflores de la Sierra, Madrid, 12-16 septiembre

Tribological behaviour of amorphous carbon-based coatings
Juan Carlos Sánchez López
Specialist Meeting on Carbon 2011
Puerto Vallarta, México, 26-28 septiembre

Protection of surfaces exposed to wear by nanoengineered coatings
Juan Carlos Sánchez López
IV International Conference on Surfaces, Material and Vacuum
Puerto Vallarta, México, 26-30 septiembre

Redescubriendo el oro: nuevas aplicaciones en el siglo XXI
Miguel Angel Centeno Gallego
Conferencia en la Semana de la Ciencia y la Tecnología en el CICcartuja.
Sevilla, España, 15 Noviembre

Supported Nanostructures: From Thin films to Supported nanowires
Agustín R. González-Elipe
Institut de Ciències Fotòniques - ICFO
Barcelona, España, 14 Diciembre

CONFERENCIAS Y SEMINARIOS IMPARTIDOS EN EL ICMS CONFERENCES AND SEMINAR IN THE ICMS

CICLO DE CONFERENCIAS / CONFERENCES

25 de marzo |**Template-assisted fabrication and characterization of polymer nanopillar arrays for optoelectronic applications**
Lluis Marçal
Universitat Rovira i Virgili

28 de marzo |**Novel materials based on modified and synthetic Clays**
Josef Breu
Universität Bayreuth

1 de abril | **Reacciones de moléculas orgánicas y biomoléculas sobre superficies de monocristales**
José Ángel Martín Gago
Instituto de Ciencia de Materiales de Madrid

14 de julio | **Structural relaxation in glasses and supercooled liquid**
Jiri Malek
University of Pardubice

ESTANCIAS Y VISITAS DE PERSONAL DEL ICMS EN OTROS CENTROS PERSONNEL OF THE ICMS IN OTHER LABORATORIES

Université Louis Pasteur		
Estrasburgo, Francia	**Svetlana Ivanova**	[4 días]
	Francisca Romero Sarriá	[3 días]
	José Antonio Odriozola Gordón	[3 días]
	Miguel Angel Centeno Gallego	[3 días]
Université de Nantes		
Nantes, Francia	**Diego Gómez García**	[1 semana]
CLS (Canadian Light Synchrotron)		
Saskatoon, Canadá	**Juan Carlos Sánchez López**	[1 semana]
ICMCB-CNRS, Institut de Chimie de la Matière Condensée de Bordeaux		
Burdeos, Francia	**Victorino Franco**	[1 semana]

Institute of Geotechnics (Academia Eslovaca de Ciencias)		
Kosice, Eslovaquia	**Francisco J. Gotor Martínez**	[10 días]
	M. Jesús Sayagués de Vega	[10 días]
	José Manuel Córdoba Gallego	[10 días]
Institute of General and Inorganic Chemistry, Bulgarian Academy of Sciences		
Sofia, Bulgaria	**Svetlana Ivanova**	[10 días]
Facultad de Ciencias Físicas y Matemáticas, Departamento de Ciencia de los Materiales		
Santiago de Chile, Chile	**M. Jesús Diánez Millán**	[14 días]
	José Manuel Criado Luque	[14 días]
ICMCB-CNRS, Institut de Chimie de la Matière Condensée de Bordeaux		
Burdeos, Francia	**Javier S. Blázquez**	[14 días]
Walther-Meissner-Institut (Academia de Ciencias de Baviera)		
Garching, Alemania	**Juan Poyato Ferrera**	[1 mes]
ICMCB-CNRS, Institut de Chimie de la Matière Condensée de Bordeaux		
Burdeos, Francia	**Rafael Caballero-Flores**	[1 mes]
Department of Industrial Engineering, University of Salermo		
Salermo, Italia	**Julie J. Murcia**	[3 meses]
Material Sciences Department, Universidad de Oxford		
Oxford, Gran Bretaña	**Adela Muñoz Páez**	[3 meses]
Institute for Biomaterials at the Department of Materials Science and Engineering, University of Erlangen-Nuremberg		
Nuremberg, Alemania	**M. Lourdes Ramiro Gutiérrez**	[3 meses]
Faculty of Science and Technology. University of Twente		
Enschede, Holanda	**Sebastián Murcia López**	[3 meses]
Chemistry Department, Brookhaven National Laboratory		
New York, EE.UU.	**Tomás Ramírez Reina**	[3 meses]
Instituto de Nanociencia de Aragón		
Zaragoza, España	**Sonia Rodríguez Liviano**	[3 meses]
University of South Florida (USF)		
Tampa, Estados Unidos de América	**Rafael Caballero-Flores**	[3 meses]
	Victorino Franco	[2 meses]

Institute for Chemical and Bioengineering ICB) and Department of Chemistry and Applied Biosciences (D-CHAB) del ETH

Zurich, Suiza	**Rosa Pereñiguez Rodríguez**	[6 meses]

Estancias y Visitas de Investigadores en el ICMS Personnel of the Other Laboratories in the ICMS

Centro de Investigaciones Energéticas, Medioambientales y Tecnológicas (CIEMAT)

Madrid, España	**José Herrero Rueda**	[2 días]

Instituto Nacional del Carbón, INCAR-CSIC

Oviedo, España	**Conchi O. Anía**	[3 días]

Universidad de Bayreutz

Bayreutz, Alemania	**Josef Breu**	[1 semana]

University of Oxford

Oxford, Reino Unido	**Richard Todd**	[1 semana]

CIDIAS, Universidad de Las Palmas de Gran Canaria

Las Palmas de Gran Canaria, España	**José Miguel Doña Rodríguez**	[1 semana]

University of South Florida (USF)

Tampa, Estados Unidos de América	**Hariharan Srikanth**	[1 semana]

Institute of Geotechnics (Academia Eslovaca de Ciencias)

Kosice, Eslovaquia	**Peter Balaz**	[11 días]
	Martin Fabian	[11 dias]
	Zdenka Bujnakova	[11 dias]

Bulgarian Academy of Sciences

Sofia, Bulgaria	**Tatyana Tabakova**	[14 días]

Facultad de Ciencias Físicas y Matemáticas, Departamento de Ciencia de los Materiales, Universidad de Chile

Santiago de Chile, Chile	**Eduardo Donoso**	[14 días]
	Rodrigo Espinoza González	[14 días]

Instituto de Química Inorgánica. Academia de Ciencias Checa

Praga, República Checa	**Petra Pulisova**	[14 días]
	Eva Kleinova	[14 días]

Walther-Meissner-Institut (Academia de Ciencias de Baviera)		
Garching, Alemania	**Anton Lerf**	[14 días]
Universidad Pública de Navarra		
Pamplona, España	**Alberto Navajas León**	[15 días]
Instituto de Biociencias de la Universidad Estatal Paulista “JULIO DE MESQUITA FILHO”, UNESP		
Botucatu, Brasil	**Rafael Innocenti Viera da Silva**	[15 días]
Universidad de Pardubice		
Pardubice, Republica Checa	**Sarka Botkova**	[1 mes]
	Jiri Malek	[1 mes]
CEMHTI-CNRS. Conditions Extrêmes et Matériaux : Haute Température et Irradiation		
Orleans, Francia	**Mathieu Allix**	[1 mes]
Laboratoire de Chimie du Gaz Naturel, Faculté de Chimie		
Argel, Argelia	**Baya Djebarri**	[2 meses]
ENSICAEN, L'Ecole Nationale Supérieure d'Ingénieurs de Caen		
Caen, Francia	**Bastien Lorenzatti**	[4 meses]
	Badrouin Marecar	[4 meses]
University de Casablanca-Mohammedia		
Casablanca, Marruecos	**Moctar Abba**	[6 meses]
School of Metallurgy and Materials Engineering, University of Tehran		
Teherán, Irán	**Saeed Sheibani**	[6 meses]

Otras Actividades / Other Activities

Feria de la Ciencia / Fair of Science

La IX Feria de la Ciencia (12 al 14 de mayo de 2011, en Sevilla) constituye un punto de encuentro donde se desarrollaron actividades de divulgación de la Ciencia y la Tecnología, realizando demostraciones y experimentos para facilitar la comprensión de contenidos científicos. El Instituto de Ciencia de Materiales de Sevilla presentó la actividad: “Luz y Materia”. Se presentaron demostraciones sobre la difracción de la luz, el color en los sólidos, la emisión de luz, el color en nanotecnología y el color por dispersión.
Coordinadora: Asunción Fernández Camacho. Participaron un total de 16 monitores.

The VII Fair of Science (12 to 14 May 2011, in Seville) constituted a meeting point where many activities for spreading of science and technology were carried out. Demonstrations and experiments where presented to facilitate the understanding of scientific aspects. The Materials Science Institute of Seville presented the activity: “Luz y Materia”
Coordination: Asunción Fernández Camacho.

SEMANA DE LA CIENCIA Y LA TECNOLOGÍA / SCIENCE AND TECHNOLOGY WEEK

Jornadas de puertas abiertas (Semana del 14 al 17 de Noviembre de 2011, en Sevilla). La Semana de la Ciencia y la Tecnología está dirigida a todos los públicos. Este evento de carácter europeo está diseñado para demostrar cómo la ciencia y la tecnología nos afectan y cómo éstas pueden ser utilizadas para mejorar nuestras vidas y el mundo que nos rodea.

Actividad visitas guiadas.- Coordinadores Dr. A. Ruiz Conde y Dr. P.J. Sánchez Soto
15-17 de Noviembre 2011. Visita de 6 Institutos de Educación Secundaria:
IES Virgen de Valme / IES Juan de Mairena / IES Federico Mayor Zaragoza/ IES Los Alcores / IES Catedrático Pulido / Colegio Juan Nepomuceno Rojas

Actividad charlas
15 de Noviembre de 2011. Dr. Miguel Angel Centeno Gallego
Titulo: "Redescubriendo el oro: nuevas aplicaciones en el siglo XXI"
17 de Noviembre de 2011. Dra. Asunción Fernández Camacho
Un viaje por el nanomundo y los nanomateriales a través del microscopio electrónico

Actividad Café con Ciencia
7 de noviembre de 2011. Dña. Gisela M. Arzac. Coloquio con estudiantes de 3º y 4º de bachillerato y un profesor/a. Institutos participantes: IES Gerena, IES Galileo Galilei. Tema: “Un viaje por el nanomundo y los nanomateriales a través del microscopio electrónico”

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