Instituto de Ciencia de Materiales de Sevilla

Memoria de Actividades

Annual Report

Consejo
Superior de
Investigaciones
Científicas

Universidad
de Sevilla

Junta de
Andalucía

2010

Consejo Superior de Investigaciones Científicas
Universidad de Sevilla
Junta de Andalucía

INSTITUTO DE CIENCIA DE MATERIALES DE SEVILLA

Memoria de Actividades
Annual Report
2010

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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
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COMISIÓN MEMORIA-ICMS

Hernán R. Míguez García – Manuel Ocaña Jurado – Pedro José Sánchez Soto

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El ICMS en 2010
ICMS in 2010

Presentación Presentation

A través de esta Memoria 2010, 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 (USE), 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 130 personas, 49 de las cuales son científicos permanentes.
El recientemente implantado Plan Estratégico 2010-2013 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 padecemos en la actualidad, 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.

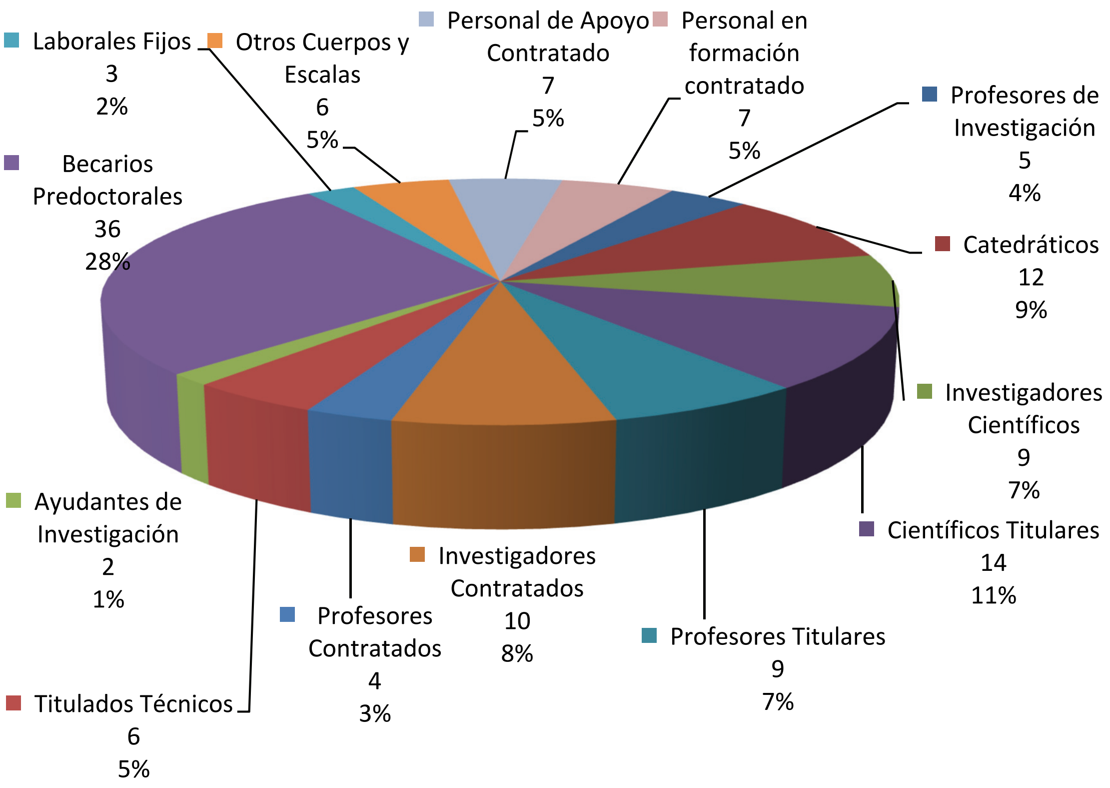
Through this Report 2010, the Institute of Materials Science of Seville is trying to communicate the best of its scientific activities for the period. Our Institute, a joint Center of the Spanish Research Council (CSIC) and the University of Seville (USE), also funded by the Junta de Andalucia, is included 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 120 people, 50 of which are permanent scientific staff. The recently implemented 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.

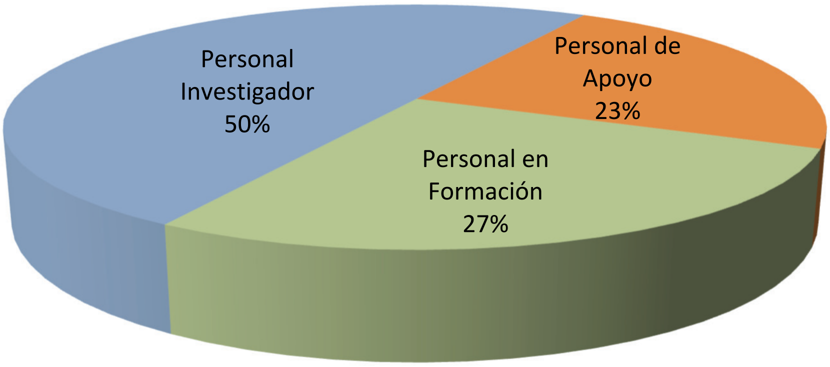
Dr. **Alfonso Caballero Martínez**
Director del Instituto de Ciencia de Materiales de Sevilla

Datos Estadísticos del ICMS
Statistical Data of ICMS

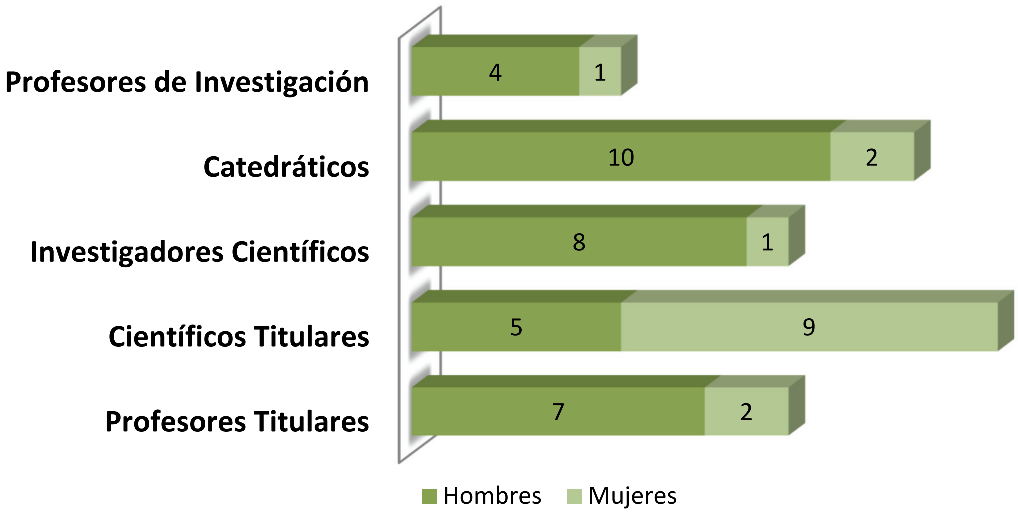
RECURSOS HUMANOS / HUMAN RESOURCES

Distribución del personal por categorías
Distribution of by cathegories

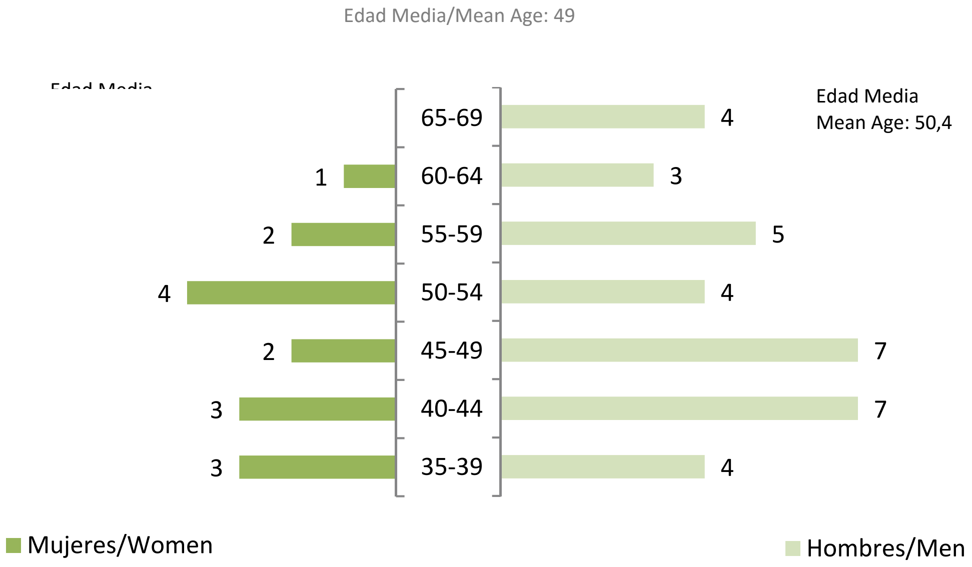




Distribución del personal científico de plantilla
Scientific staff by cathegories

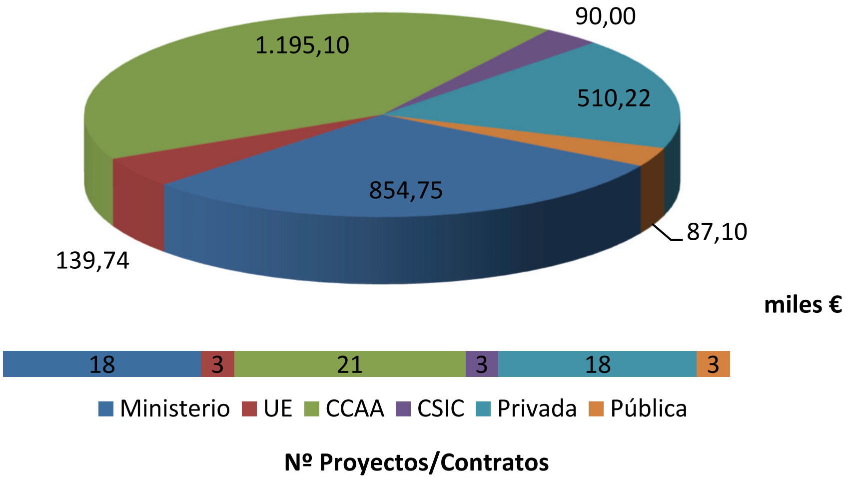


Distribución del personal investigador por edad
Scientific staff by age

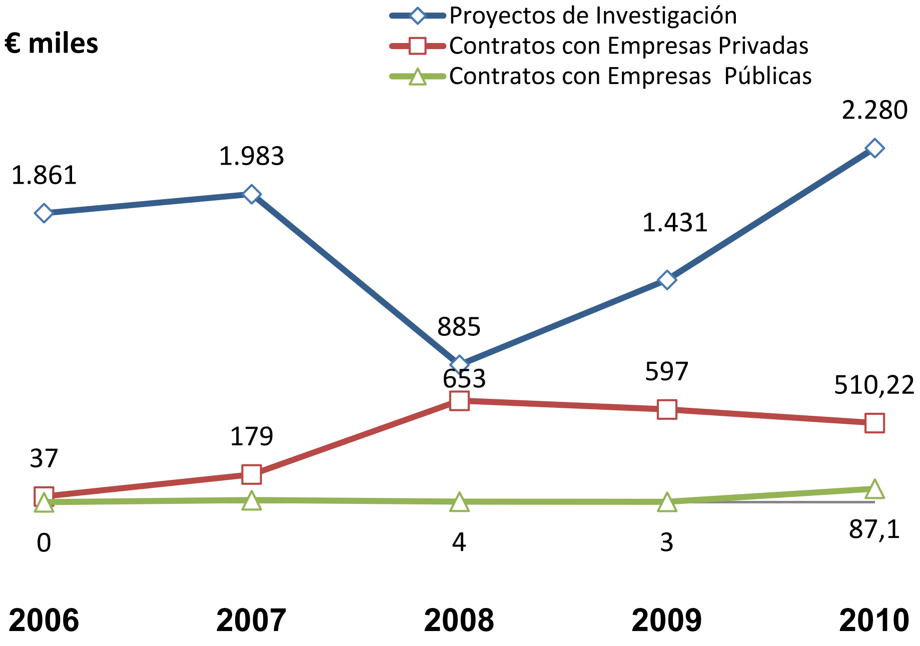


FINANCIACIÓN / FUNDING

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



Evolución 2006-2010 de la Financiación del ICMS (PCO)
Evolution of the funding of the ICMS in the period 2006-2010



PRODUCCIÓN CIENTÍFICA / SCIENTIFIC PRODUCTION

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 (*)
JOURNAL OF THE AMERICAN CHEMICAL SOCIETY	1	9,023
SMALL	1	7,336
CHEMISTRY OF MATERIALS	2	6,4
ANALYTICAL CHEMISTRY	1	5,874
CHEMICAL COMMUNICATIONS	3	5,787
JOURNAL OF CATALYSIS	1	5,415
JOURNAL OF MATERIALS CHEMISTRY	2	5,101
NANO RESEARCH	1	5,078
NANOMEDICINE-NANOTECHNOLOGY BIOLOGY AND MEDICINE	1	4,882
ACTA BIOMATERIALIA	1	4,824
CLINICAL MICROBIOLOGY AND INFECTION	1	4,784
APPLIED CATALYSIS B-ENVIRONMENTAL	6	4,749
JOURNAL OF PHYSICAL CHEMISTRY C	7	4,524
ANALYTICA CHIMICA ACTA	1	4,311
LANGMUIR	3	4,269
NANOSCALE	1	4,109
GEOCHIMICA ET COSMOCHIMICA ACTA	1	4,101
APPLIED PHYSICS LETTERS	1	3,841
ANALYTICAL AND BIOANALYTICAL CHEMISTRY	1	3,841
POLYMER	1	3,829
MOLECULAR BIOSYSTEMS	1	3,825
ACTA MATERIALIA	2	3,791
PHYSICAL REVIEW B	1	3,774
OPTICS EXPRESS	1	3,753
PLASMONICS	1	3,544
PHYSICAL CHEMISTRY CHEMICAL PHYSICS	1	3,454
APPLIED CATALYSIS A-GENERAL	2	3,384
SENSORS AND ACTUATORS B-CHEMICAL	1	3,37
CHEMPHYSCHEM	1	3,34
JOURNAL OF NANOPARTICLE RESEARCH	2	3,253
CHEMICAL ENGINEERING JOURNAL	2	3,074

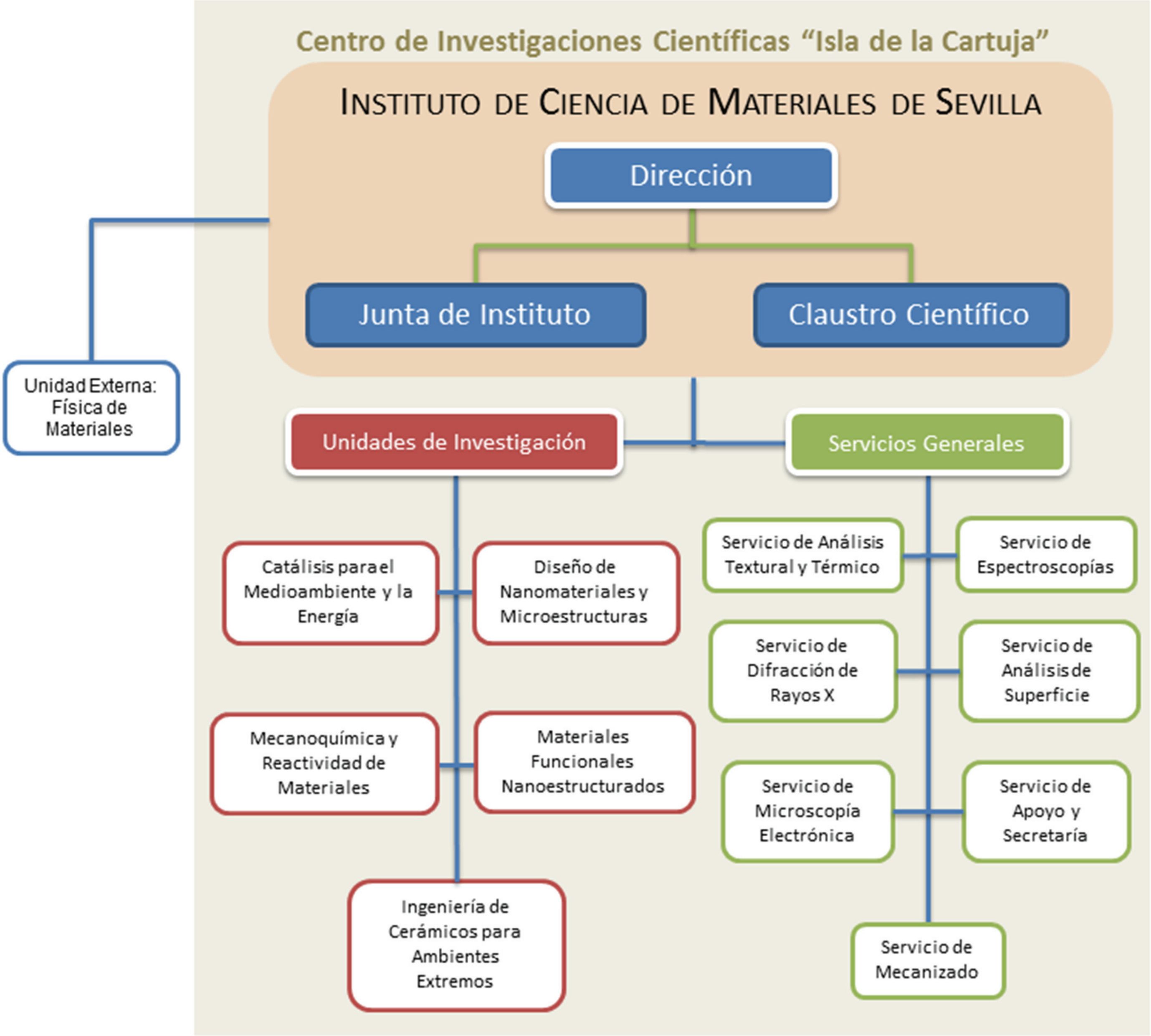
JOURNAL OF COLLOID AND INTERFACE SCIENCE	1	3,068
CATALYSIS TODAY	5	2,993
ACS APPLIED MATERIALS & INTERFACES	2	2,925
JOURNAL OF MOLECULAR CATALYSIS A-CHEMICAL	1	2,872
CHEMISTRY AND PHYSICS OF LIPIDS	1	2,861
JOURNAL OF PHYSICAL CHEMISTRY A	2	2,732
POLYMER DEGRADATION AND STABILITY	1	2,594
JOURNAL OF THE EUROPEAN CERAMIC SOCIETY	3	2,575
MATERIALS CHEMISTRY AND PHYSICS	1	2,356
APPLIED CLAY SCIENCE	2	2,303
JOURNAL OF SOLID STATE CHEMISTRY	1	2,261
JOURNAL OF BIOMEDICAL MATERIALS RESEARCH PART B-APPLIED BIOMATERIALS	1	2,22
SOLAR ENERGY	1	2,172
JOURNAL OF THE AMERICAN CERAMIC SOCIETY	5	2,169
SURFACE & COATINGS TECHNOLOGY	3	2,141
JOURNAL OF THE OPTICAL SOCIETY OF AMERICA B-OPTICAL PHYSICS	1	2,097
JOURNAL OF APPLIED PHYSICS	5	2,079
INDUSTRIAL & ENGINEERING CHEMISTRY RESEARCH	1	2,072
COMPOSITE STRUCTURES	1	2,036
SURFACE SCIENCE	1	2,011
THIN SOLID FILMS	1	1,935
JOURNAL OF MATERIALS SCIENCE	1	1,859
APPLIED SURFACE SCIENCE	2	1,795
APPLIED PHYSICS A-MATERIALS SCIENCE & PROCESSING	1	1,765
JOURNAL OF THERMAL ANALYSIS AND CALORIMETRY	2	1,752
CLAYS AND CLAY MINERALS	1	1,752
JOURNAL OF ARCHAEOLOGICAL SCIENCE	2	1,71
APPLIED OPTICS	1	1,707
WEAR	1	1,635
COMPTES RENDUS CHIMIE	1	1,6
ARCHAEOMETRY	1	1,581
JOURNAL OF MICROENCAPSULATION	1	1,515
IEEE SENSORS JOURNAL	1	1,473
JOURNAL OF VACUUM SCIENCE & TECHNOLOGY A	1	1,291
SURFACE AND INTERFACE ANALYSIS	1	1,249
JOURNAL OF CULTURAL HERITAGE	1	1,162
VACUUM	1	1,051

ENVIRONMENTAL PROGRESS & SUSTAINABLE ENERGY	1	0,86
INTERNATIONAL JOURNAL OF MATERIALS RESEARCH	1	0,86
MATERIALES DE CONSTRUCCION	2	0,6465
JOURNAL OF SURFACE INVESTIGATION-X-RAY SYNCHROTRON AND NEUTRON TECHNIQUES	1	0,279
REVISTA DE METALURGIA	1	0,25
BOLETÍN DE LA SOCIEDAD ESPAÑOLA DE CERÁMICA Y VIDRIO	1	0,204
TRANSACTIONS OF THE INDIAN CERAMIC SOCIETY	1	0,159

(*) Factor de Impacto correspondiente al año 2010
Journal Citation Reports of 2010

COMPOSICIÓN Y ESTRUCTURA
STRUCTURE AND ORGANISATION

Organigrama / Organization Chart



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"Una manera de hacer Europa"
MINISTERIO DE CIENCIA E INNOVACIÓN

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 - Fondos FEDER
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 manométrico 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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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:	J.A. Odriozola, 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 baterias. 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

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:	1-12-2007/30-11-2010
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 H2(+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.

Diseño de sistemas fotocatalíticos con alta actividad en el visible para aplicaciones ambientales Design of photocatalytic systems highly active in the visible for environmental applications

Código/Code:	FQM-1406 (Proyecto de Excelencia)
Periodo/Period:	01-01-2007 / 31-12-2010
Organismo Financiador/Financial source:	Junta de Andalucía
Importe total/Total amount:	82.000 €
Investigador responsable/Research head:	Gerardo Colón Ibáñez
Componentes/Research group:	José Antonio Navío Santos, Manuel Macías Azaña, Carmen Hidalgo López, Marina Maicu

RESUMEN / ABSTRACT

La Fotocatálisis ha demostrado ser una técnica muy eficiente en la oxidación de una gran variedad de sustratos en cortos tiempos de reacción. Es conocido que los catalizadores más utilizados, solo pueden ser activados por radiaciones menores de 390 nm, constituyéndose en una limitación para su empleo a mayor escala por el impedimento de usar luz solar. El objetivo principal de este proyecto se basa en el desarrollo en nuestro laboratorio de sistemas basados en TiO_2 de alta eficiencia fotocatalítica en UV, capaz 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. El bloque central de la actividad de este proyecto consistirá en el desarrollo de sistemas de óxidos de Ti y Zn dopados, de forma que podamos obtener sistemas cuyo umbral de absorción esté en la región del visible.

Así, desde el punto de vista de la mejora en las eficiencias de los procesos fotocatalíticos, es evidente que el diseño y desarrollo de fotocatalizadores alternativos al TiO_2 es de un interés considerable. Se pretende la obtención de materiales altamente eficientes en procesos fotocatalíticos heterogéneos (en fase líquida y gaseosa) mediante la incorporación de distintos dopantes y la inmovilización de estos sistemas en distintos soportes. Para ello se abordarán distintas rutas de síntesis de polvo, y métodos de deposición. La evaluación la actividad fotocatalítica de los catalizadores se abordará estudiando procesos de fotooxidación de distintos compuestos orgánicos tóxicos (fenol y pigmentos orgánicos).

The heterogeneous photocatalysis has demonstrated to be a promising and efficient technology for the oxidation of a large variety of toxic substrates in relatively short reaction times. It is widely known that the most used photocatalysts can be only activated by means of photons with wavelengths lower than 390 nm, being an important limitation for large scale use. The main objective of this project is based on previous development in our group of highly UV photoactive TiO_2 powders able to completely remove different toxic species for the environment. Our challenge is to overcome the problems and limitations of the UV range in the solar spectrum. The core of our activity will be the development of new oxidic photoactive doped systems based on Ti and Zn, which could provide a shift in the absorption edge toward the visible range.

Thus, under the point of view of the enhancement in the photon efficiencies of the photocatalytic processes, it is evident that the designing and development of alternative photocatalysts is of great interest. We intend the obtention of highly efficient materials that can be used for the degradation of contaminants in water and gas effluents by the incorporation of cationic/anionic dopants and the immobilization in different adequate supports.The evaluation of the photocatalytic activity will be performed for the photooxidation of a great variety of toxic organic compounds and using solar simulation lamps.

Reformado Catalítico de Glicerina

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:	Bobadilla Baladrón, Luis F., Cruz Torres, Sylvia A., Domínguez Leal, M. Isabel, Penkova, Anna D., Romero Sarria, Francisca, Alvarez Moreno, Andrea

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.

Desarrollo de catalizadores de Ni nanoestructurados: Obtención de hidrógeno a partir de CH_4 y ánodos de pilas de combustible SOFT (CATANIC)

Código/Code:	P07-FQM-02520 (Proyecto de Excelencia)
Periodo/Period:	01-02-2008 / 31-01- 2011
Organismo Financiador/Financial source:	Junta de Andalucía
Importe total/Total amount:	241.668 €
Investigador responsable/Research head:	Juan Pedro Holgado Vázquez
Componentes/Research group:	Alfonso Caballero Martínez, Rosa Pereñíguez Rodríguez, Victor Manuel González de la Cruz, Fátima Ternero Fernández, Juan Pedro Espinós Manzorro, Angel Baranco Quero

RESUMEN / ABSTRACT

El presente proyecto plantea el desarrollo de materiales catalíticos para el reformado de metano y de ánodos de celdas de combustible de óxido sólido (SOFCs). Si bien los materiales considerados como “state of the art” para ambas aplicaciones tienen formulaciones casi idénticas y deben cumplir unas condiciones de trabajo similares, tradicionalmente han existido pocos trabajos que aborden ambos problemas de forma conjunta. No obstante, esta aproximación puede aportar ventajas interesantes en términos de poder correlacionar de forma más completa las relaciones entre las características fisicoquímicas y sus propiedades funcionales como catalizadores de reformado y/o ánodos SOFCs.

The main objective This Project intends the development of catalytic materials for reforming of methane and anodes of solid oxide fuel cells (SOFCs). Although “state of the art” materials for such applications have almost identical formulations, and operate under similar conditions, traditionally the research work have been done separately, and few works can be found where a joint approach has been performed. Nevertheless, this combined scheme could improve substantially the results, leading to a better r correlation between physicochemical characteristics and functional properties as reforming catalysts and/or SOFCs anodes.

OTROS PROYECTOS / OTHER PROJECTS

Investigación básica de Nanomateriales Innovadores Avanzados: Aplicaciones a la Solución de Desórdenes Neurológicos

Código/Code:	2010/00000222
Periodo/Period:	09-09-2009 / 30-06-2011

Organismo Financiador/Financial source: Fondo de Cooperación Interanacional en Ciencia y Tecnología. Unión Europea – Mexico (FONCICYT)
Importe total/Total amount: 12.518,89 €
Investigador responsable/Research head: José Antonio Odriozola Gordón

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

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: 2.996,83 €
Investigador responsable/Research head: Francisca Romero Sarria

Thermal stability against reduction of La1-xA´xCo0.5Mn0.5O3 (A´=Er, Y) perovskite type oxides catalysts

Periodo/Period: 1-03-2009 / 1-03-2013
Entidad Financiadora/Financial source: CONICYT. Comisión Nacional de Investigación Científica y Tecnológica del Gobierno de Chile
Importe total/Total amount: 2.996,83 €
Investigador responsable/Research head: Gina Angel Pecci Sánchez
Investigador responsable ICMS
Research head ICMS: Miguel Angel Centeno Gallego

Transferencia / Technological Transfer

Convenios y Contratos / Contracts and Agreements

Estudio de las causas del proceso de corrosión de un sistema tubular de acero inoxidable

Periodo/Period: 26-05-2010 / 26-06-2010
Organismo Financiador/Financial source: APLEAN, S.L.
Importe total/Total amount: 600 €
Investigador responsable/Research head: Alfonso Caballero Martínez

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

Periodo/Period:	15-04-2010 / 30-06-2011
Organismo Financiador/Financial source:	ACERINOX, S.A.
Importe total/Total amount:	33.240,60 €
Investigador responsable/Research head:	José Antonio Odriozola Gordón
Componentes/Research group:	Alicia Corrales Miralles

Reformado catalítico de Glicerina

Periodo/Period:	1-10-2008 / 30-06-2011
Organismo Financiador/Financial source:	Befesa Gestión de Residuos Industriales
Importe total/Total amount:	330.600 €
Investigador responsable/Research head:	José Antonio Odriozola Gordón

Procesado de bioetanol y otros alcoholes en sistemas compactos. II

Periodo/Period:	1-03-2010 / 31-12-2010
Organismo Financiador/Financial source:	DIGEMA Technologies, S.L.
Importe total/Total amount:	104.663,23 €
Investigador responsable/Research head:	José Antonio Odriozola Gordón
Componentes/Research group:	Ara Muñoz Murillo, Sara Oraá Díaz-Santos

Desarrollo de catalizadores para pilas de combustible

Periodo/Period:	1-08-2010 / 31-01-2011
Organismo Financiador/Financial source:	ENDESA INGENIERÍA, S.L.
Importe total/Total amount:	6.490 €
Investigador responsable/Research head:	José Antonio Odriozola Gordón
Componentes/Research group:	Sara Oraá Díaz-Santos

PATENTES / PATENTS

Procedimiento de preparación de nanopartículas de aleaciones Ni-Sn y su uso en reacciones de reformado

Inventores: José Antonio Odriozola Gordón, Luis F. Bobadilla Baladrón, Francisca Romero Sarria, Miguel Angel Centeno Gallego
Ámbito Geográfico: Internacional
PATENTE SOLICITADA. N. de solicitud: PCT/ES2010/000234
Fecha Solicitud/Licencia: 27/mayo/2010
Entidad Titular: Universidad de Sevilla

PUBLICACIONES / PUBLICATIONS

ARTÍCULOS PUBLICADOS EN REVISTAS SCI / PAPERS IN SCI JOURNALS

Room-Temperature Reaction of Oxygen with Gold: An In situ Ambient-Pressure X-ray Photoelectron Spectroscopy Investigation
Peng Jiang, Soeren Porsgaard, Ferenc Borondics, Mariana Köber, Alfonso Caballero, Hendrik Bluhm, Flemmming Besenbacher and Miquel Salmeron
J. Am. Chem. Soc., **132** (9) (2010) 2858–2859
DOI: 10.1021/ja909987j

The interaction of O_2 with gold foil and gold nanoparticles grown by thermal deposition on TiO_2(110) was studied by in situ ambient pressure X-ray photoelectron spectroscopy at room temperature. No spontaneous dissociation of O_2 was observed either on Au foil or on Au nanoparticles up to 1 Torr of O_2. X-ray irradiation, however, is very effective in promoting gold oxidation on both surfaces in the presence of O_2. Our results help reconcile recent conflicting experimental observations regarding the activation of molecular oxygen, which is a crucial issue in Au catalyzed oxidation reactions.

In situ spectroscopic detection of SMSI effect in a Ni/CeO_2 system: hydrogen-induced burial and dig out of metallic nickel
Alfonso Caballero, Juan P. Holgado, Victor M. Gonzalez-delaCruz, Susan E. Habas, Tirma Herranz and Miquel Salmeron
Chem. Commun., **46** (2010) 1097-1099
DOI: 10.1039/B920803H

In situ APPES technique demonstrates that the strong metal support interaction effect (SMSI) in the Ni-ceria system is associated with the decoration and burial of metallic particles by the partially reduced support, a phenomenon reversible by evacuation at high temperature of the previously absorbed hydrogen.

Sunlight highly photoactive Bi2WO6–TiO2 heterostructures for rhodamine B degradation
G. Colón, S. Murcia López, M. C. Hidalgo and J. A. Navío
Chem. Commun., **46** (2010), 4809-4811
DOI: 10.1039/C0CC00058B

Highly efficient Bi_2WO_6–TiO_2 heterostructures are synthesized by means of a hydrothermal method; they have high photoactivity for the degradation of rhodamine B under sunlike irradiation. An interesting synergetic effect between TiO_2 and Bi_2WO_6 leads to an improved charge carrier separation mechanism, causing the excellent photocatalytic performance.

Gold supported on metal-doped ceria catalysts (M = Zr, Zn and Fe) for the preferential oxidation of CO (PROX)
O.H. Laguna, F. Romero Sarria, M.A. Centeno and J.A. Odriozola

Journal of Catalysis, 276 (2) (2010) 360-370
DOI: 10.1016/j.jcat.2010.09.027

The doping CeO_2 with Zr, Zn and Fe was studied. Doping with Zr or Fe resulted in solid solution, while doping with Zn resulted in the surface segregation of ZnO. The formation of oxygen vacancies is enhanced with Zr, remains constant with Zn and disappears on doping with Fe.

Study of the stabilization of zinc phthalocyanine in sol-gel TiO_2 for photodynamic therapy applications
Tessy Lopez, Ema Ortiz, Mayra Alvarez, Juan Navarrete, Jose A. Odriozola, Fernando Martinez-Ortega, Edgar A. Páez-Mozo, Patricia Escobar, Karla A. Espinoza and Ignacio A. Rivero
Nanomedicine: Nanotechnology, Biology and Medicine, **6** (6), (2010), 777-785
DOI: 10.1016/j.nano.2010.04.007

Mechanism of PDT cytotoxicity photosensitizer (PS) administration (step I) leading to photophysic reactions represented by modified Jablonski diagram (step II) (vibrational levels omitted).

Complete n-hexane oxidation over supported Mn–Co catalysts
S. Todorova, H. Kolev, J.P. Holgado, G. Kadinov, Ch. Bonev, R. Pereñíguez and A. Caballero
Applied Catalysis B: Environmental, 94 (2010) 46-54
DOI: 10.1016/j.apcatb.2009.10.019

Two series of Co–Mn samples were prepared by impregnation of silica with aqueous solutions of $Co(NO_3)_2{\cdot}6H_2O$ and/or $Mn(NO_3)_2{\cdot}6H_2O$. Cobalt oxide was the predominant phase in one of the series and manganese was used as the promoter. The major component in the second series was manganese oxide and Co was the promoter. The prepared samples were characterized by powder X-ray diffraction (XRD), scanning electron microscopy (SEM), temperature-programmed reduction (TPR), and X-ray photoelectron spectroscopy (XPS) and tested in the reaction of complete n-hexane oxidation. The catalytic activity of both single component cobalt and manganese samples was similar, however, a combination between the two elements changed significantly the activity and this depended on the method of preparation. Catalysts prepared by a common solution of Co- and Mn nitrates manifested a considerable increase in activity as a result of very low crystallinity of the supported metal oxide phases, partial enrichment of the surface with cobalt and uniform distribution of oxide agglomerates on the support.

Doping level effect on sunlight-driven W,N-co-doped TiO_2-anatase photo-catalysts for aromatic hydrocarbon partial oxidation
Anna Kubacka, Belén Bachiller-Baeza, Gerardo Colón and Marcos Fernández-García
Applied Catalysis B: Environmental, 13 (2010) 274-281
DOI: 10.1016/j.apcatb.2009.09.039

A series of nanosized W,N-co-doped anatase TiO_2 catalysts with different dopant contents has been prepared by a microemulsion method and examined in the sunlight selective photo-oxidation of toluene and styrene. The activity results have been correlated with structural, electronic, and surface examinations of the catalysts done with the help of XRD–Rietveld, N2 physisorption and NH_3 chemisorption–calorimetry, XPS, Infrared, and UV–visible spectroscopies. Irrespective of the reaction, a consistent reaction rate enhancement with respect to titania (nano-TiO_2, P25) references and W-doped TiO_2 systems is observed for single-phase anatase W,N-co-doped samples. This is likely linked with the decrease of the band gap energy decrease and results from a combined W–N cooperative effect on structural properties of the anatase network. W,N simultaneous presence also makes a drastic effect on selectivity, maximizing the yield to partial oxidation products. This appears related with surface properties of the materials.

N- and/or W-(co)doped TiO_2-anatase catalysts: Effect of the calcination treatment on photoactivity
Anna Kubacka**,** Gerardo Colón and Marcos Fernández-García
Applied Catalysis B: Environmental,95 (2010) 238-244
DOI: 10.1016/j.apcatb.2009.12.028

A series of nanosized W,N-codoped and single-doped N- and W-anatase-TiO_2 catalysts have been prepared by a microemulsion method and calcined at different temperatures. The activity in the sunlight selective photo-oxidation of toluene and styrene has been correlated with structural, electronic, and surface examinations of the catalysts done with the help of XRD-Rietveld, N_2 physisorption, X-ray photoelectron, infrared, electron paramagnetic resonance (EPR) and UV–vis spectroscopies. Irrespective of the reaction, W,N-codoped nanocatalysts showed an enhanced photoactivity with respect to bare anatase and single-doped N-TiO2 and W-TiO_2 materials. A strong W–N synergistic interaction appears to play a decisive role in driving the excellent photoactivity performance of W,N-codoped materials by affecting (i) electronic properties, particularly maximizing the anatase band gap decrease and enhancing the subsequent visible light photon absorption, and (ii) surface properties, in turn related to the formation of OH radicals upon light excitation. The maximum photoactivity is reached by calcination at 450 °C and is concomitantly observed with a near complete selectivity to partial oxidation products. Higher calcination temperatures yielded solids with significantly inferior photocatalytic performance. The properties of the W–N interaction are discussed as a function of the calcination temperature.

Photocatalytic degradation of phenolic compounds with new TiO_2 catalysts
Araña, J; Dona-Rodriguez, JM; Portillo-Carrizo, D; Fernandez-Rodriguez, C; Perez-Pena, J; Diaz, OG; Navio, JA; Macias, M
Applied Catalysis B: Environmental,100 (2010) 346-354
DOI: 10.1016/j.apcatb.2010.08.011

New TiO_2 catalysts have been synthesised by means of a sol-gel method in which aggregates have been selected before thermal treatment. Sieving and calcination temperature have been proved to be key factors in obtaining catalysts with greater photoactivity than that of Degussa P-25. These new catalysts have been characterized by means of transmission electron microscopy (TEM), BET surface area, diffuse reflectance spectroscopy (DRS). UV-vis spectroscopy, Fourier transformed infrared (FTIR) and X-ray diffraction (XRD). The different parameters studied were compared to those obtained from two commercial catalysts (Degussa P-25 and Hombikat-UV100). The photocatalytic efficiency of the new catalysts was evaluated by the degradation of various phenolic compounds using UV light (maximum around 365 nm, 9 mW). The catalyst sieved and calcinated at 1023 K, ECT-1023t, showed phenol degradation rates 2.7 times higher than those of Degussa P-25. Also in the degradation of different phenolic compounds, this catalyst showed a higher activity than that of the commercial one. The high photoactivity of this new catalyst has been attributed to the different distribution of surface defects (determined from FTIR studies) and its increased capacity to yield H_2O_2.

Synthesis and characterization of a $LaNiO_3$ perovskite as precursor for methane reforming reactions catalysts

Rosa Pereñíguez, Víctor M. González-DelaCruz, Juan P. Holgado and Alfonso Caballero
Applied Catalysis B: Environmental, 93 (2010) 346-353
DOI: 10.1016/j.apcatb.2009.09.040

The objective of the present work has been the study of the physicochemical and catalytic properties of a Ni/La_2O_3 catalyst obtained by reduction of a lanthanum nickelite, $LaNiO_3$, with perovskite structure. The perovskite, obtained by means of a spray pyrolysis method, provides a Ni/La_2O_3 system active in different methane reforming reactions. The catalyst was characterized by scanning electron microscopy (SEM), X-ray diffraction (XRD), X-ray absorption spectroscopy (XAS), X-Ray photoemission spectroscopy (XPS), temperature-programmed reduction and oxidation (TPR, TPO) and catalytic activity tests. Although not evidenced by XRD data, XAS and TPR measurements show the presence of an amorphous NiO phase in the original sample, together with the crystalline $LaNiO_3$ phase. Upon reoxidation treatment of the reduced Ni/La_2O_3 catalyst, the $LaNiO_3$ structure is partly recovered which provides a convenient way to regenerate a waste catalyst (reoxidation and new reduction in hydrogen). The catalyst is active in several reactions of methane with oxygen, water and CO_2, showing a remarkable stability specially under dry reforming of methane (DRM) reaction conditions. This quite great catalytic performance has been explained by the high resistance of the nickel particles to be oxidized, as detected by in situ XAS. In the presence of water, as in steam reforming of methane (SRM) reaction conditions, these metallic particles are gradually oxidized, which explains the linear decreasing of the catalytic performance observed for the SRM reaction.

Synthesis of biodiesel from the methanolysis of sunflower oil using PURAL® Mg–Al hydrotalcites as catalyst precursors

A. Navajas**,** I. Campo**,** G. Arzamendia**,** W.Y. Hernández**,** L.F. Bobadilla**,** M.A. Centeno**,**

J.A. Odriozola and L.M. Gandía
Applied Catalysis B: Environmental,100 (2010) 299-309
DOI: 10.1016/j.apcatb.2010.08.006

A series of commercial Mg–Al hydrotalcites have been used as catalyst precursors for the methanolysis of sunflower oil. The solids were characterized by low Mg/Al molar ratios in the 0.5–2.3 range. Additionally, a solid consisting mainly of $Mg(OH)_2$ but containing some Al (4.2 wt.%) was also employed. The as-received materials were inactive for biodiesel synthesis so calcination and rehydration in boiling water were considered as activation treatments. Among the calcined solids, only the material consisting of MgO was significantly active, achieving about 50% oil conversion after 24 h at 60 °C, methanol/oil molar ratio of 12 and 2 wt.% of catalyst. The effects of the calcination temperature in the 350–700 °C range have been investigated; calcination at 500 °C led to the best catalytic performance. In the case of the rehydrated materials, only the solids with the highest Mg/Al molar ratios recovered a well-ordered layered double hydroxide structure. These samples showed an improved catalytic activity compared with their calcined counterparts. A good correlation between catalytic activity and the basic properties determined using Hammett indicators and benzoic acid titration has been found. Rehydrated hydrotalcites were slightly more selective to biodiesel (75%) at intermediate levels of oil conversion than the calcined counterparts (66%). It has been verified that no Mg or Al leaching in the reaction mixture took place; however, the rehydrated samples deactivated significantly. In the case of MgO, after washing and calcination, the recycled catalyst gave 68% of the original oil conversion.

In Situ Characterization of the Dynamic Gold−Support Interaction over Ceria Modified Eu3+. Influence of the Oxygen Vacancies on the CO Oxidation Reaction

Willinton Y. Hernández, Francisca Romero-Sarria, Miguel A. Centeno and Jose A. Odriozola
J. Phys. Chem. C, 114 (24) (2010), 10857–10865
DOI: 10.1021/jp1013225

Gold-supported ceria and europium-doped ceria catalysts were prepared by the deposition−precipitation method. The influence of the pretreatment atmosphere and temperature on the concentration of oxygen vacancies and gold dispersion on the Au/CeEu(10) catalyst under actual reaction conditions was investigated by “in situ” X-ray diffraction and Raman analysis. By Raman spectroscopy, a preferential interaction of the gold with the support across the oxygen vacancies was established and correlated with the gold dispersion. The increase in the concentration of oxygen vacancies in the presence of hydrogen induces changes in the gold crystallite size by breaking-off and migration of gold nanoparticles toward the oxygen vacancies on the CeEu(10) support. The activity of the Au/CeEu(10) solid in the CO oxidation reaction was significantly improved when the catalyst was preactivated in a reducing atmosphere. This trend could be associated with the redispersion of gold together with the increase in the concentration of oxygen vacancies in the support.

Study of nanostructured Ni/CeO_2 catalysts prepared by combustion synthesis in dry reforming of methane

Víctor M. Gonzalez-Delacruz, Fátima Ternero, Rosa Pereñíguez, Alfonso Caballero and Juan P. Holgado
Applied Catalysis A: General, 384 (2010) 1-9
DOI: 10.1016/j.apcata.2010.05.027

This work reports the study of several catalysts of Ni–CeO_2 active for dry methane reforming process ($CH_4 + CO_2 \rightarrow 2CO + 2H_2$). The use of Ni as active phase is highly preferred, due to its availability, high activity and low cost, although its main lack is the coke formation on the surface of Ni metal particles, resulting in a severe deactivation. Here we report a new synthesis method that allows a simple, effective and fast way to prepare Ni–CeO_2 catalysts, in a wide range of metallic loadings, resulting in all the cases in well-formed NiO crystallites with sizes in the range of 12–18 nm. The use of CeO_2 as a support has been based on its massive use in TWC catalysts formulations, where it is recognized to activate CH4 and lower hydrocarbon dissociation. Moreover, CeO_2 has been reported to have an intrinsic activity in the CH_4 reforming reaction. Besides the metallic loading, several factors that control the preparation method of the catalyst have been varied, in order to optimize their performance. Most of the catalysts prepared show activity and selectivity values close to thermodynamic ones, maintaining a good stability on long periods of time and severe conditions. Nevertheless, formation of some carbon nano-fibers has been observed, which could result in a drawback for their application at large scale.

Characterisation and photocatalytic properties of titania–silica mixed oxides doped with Ag and Pt

B. Llano, G. Restrepo, J.M. Marín, J.A. Navío and M.C. Hidalgo
Applied Catalysis A: General, 387 (2010) 135-140
DOI: 10.1016/j.apcata.2010.08.021

TiO_2–SiO_2 mixed oxides have been synthesised and modified by Ag and Pt deposition. Due to the effect of the silica on the mixed oxide, the prepared materials presented high surface areas and stabilised anatase as the only crystalline phase after calcination at 700 °C. Even using the same photodeposition experimental conditions, the yield for metal deposition depended highly on the metal considered, being much lower for Ag deposition. XPS studies permitted to estimate metal dispersion and oxidation state of the different samples, being both factors of high importance regarding photocatalytic improvement by metal deposition.

AISI 304 austenitic stainless steel monoliths: Modification of the oxidation layer and catalytic coatings after deposition and its catalytic implications

L.M. Martínez**,** O. Sanz**,** M.A. Centeno and J.A. Odriozola
Chemical Engineering Journal, 162 (2010) 1082-1090
DOI: 10.1016/j.cej.2010.07.005

Monolithic CeO_2 and Au/CeO_2 catalysts were prepared using austenitic stainless steel (AISI 304) as metallic substrate. Both monolithic and powdered catalysts were characterized before and after CO oxidation reaction by N_2 adsorption–desorption, XRD, SEM, TEM and GD-OES. Catalyst deposition on the stainless steel surface results in modifications of the catalyst, the oxide scale and the oxide scale/alloy interface through the interaction between the coating and the steel oxidation layer. Besides this, oxidation of the alloy is also detected. The extension and nature of these modifications depends on the catalyst nature, and on the reaction conditions. As a result of these modifications CO oxidation on Au/CeO_2 catalysts is enhanced and gold surface dynamics is modified.

Computational fluid dynamics study of heat transfer in a microchannel reactor for low-temperature Fischer–Tropsch synthesis

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Chemical Engineering Journal, 160 (2010) 915-922

DOI: 10.1016/j.cej.2009.12.028

A three-dimensional computational fluid dynamics (CFD) study of heat transfer in a microchannel reactor for the low-temperature Fischer–Tropsch synthesis (FTS) is presented. The microreactor studied is a steel block with 80 square microchannels of 1 mm of side arranged in cross-flow configuration for the transport of syngas and cooling water. Syngas space velocities in the 5000–30,000 h^{-1} (STP) range have been considered. The microreactor exhibited good isothermicity under most simulated conditions. The FTS can be conducted with very low-temperature change between 483 and 523 K within a wide range of CO conversions using boiling water as coolant. To this end the pressure has to be set at the appropriate value between about 5 and 35 atm. The pressure would have to be reduced as the CO conversion increases which might have a negative effect on the FTS selectivity to middle distillates. However, adjusting the cooling water flow rate in the range 0.25–250 g min^{-1} allows maintaining the FTS temperature at suitable values while avoiding the use of low pressures. Relatively high values of the overall heat transfer coefficient in the 20–320 W m−2 K^{-1} range have been obtained. A significant effect of the buoyancy forces on the thermal performance of the microreactor has been found.

Iron-modified ceria and Au/ceria catalysts for Total and Preferential Oxidation of CO (TOX and PROX)

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Catalysis Today, 157 (2010) 155-159

DOI: 10.1016/j.cattod.2010.04.011

Iron-modified ceria supports containing different molar percentages of Fe (0% 10% 25% and 50%) were synthesized by thermal decomposition of the metal propionates The formation of a Ce-Fe oxide solid solution is evidenced through XRF XRD BET and Raman spectroscopy For Iron contents above 25% the formation of alpha-Fe_2O_3 was detected pointing out the formation of the isolated oxides The catalytic activity of the Fe-modified catalysts in the Total Oxidation of CO reaction (TOX) is higher than for the bare CeO_2 material The synergy between Ce and Fe shows a maximum for 10% Fe content (CeFe10) catalyst that shows the highest CO conversion per atom of Fe incorporated Gold catalyst was also prepared on CeFe10 and its catalytic activity compared with Au/CeO_2 catalyst The addition of iron to the gold catalyst resulted in an enhancement of the catalytic activity for CO oxidation especially at low temperature This Au/CeFe10 catalyst was also active and selective with excellent stability in the Preferential Oxidation of CO (PROX) showing a higher CO conversion than the Au/CeO_2 catalyst at temperatures below 150 C being hardly affected by the presence of CO_2 and H_2O in the gas stream.

Modified cryptomelane-type manganese dioxide nanomaterials for preferential oxidation of CO in the presence of hydrogen

W.Y. Hernandez, M.A. Centeno, F. Romero-Sarria, S. Ivanova, M. Montes, J.A. Odriozola

Catalysis Today, 157 (2010) 160-165

DOI: 10.1016/j.cattod.2010.03.010

Transition metal (Cu Co Ni and Zn)-modified cryptomelane-type manganese dioxide nanomaterials were synthesized by the milling method The obtained solids have been characterized by means of Xray diffraction (XRD) scanning electron microscopy and transmission electron microscopy (SEM and TEM) N_2 adsorption-desorption measurements at 77 K Raman spectroscopy and temperature programmed reduction (TPR-H_2) showing similar structural and textural properties All the solids were active in the preferential oxidation of CO in the presence of hydrogen (PROX) being the modified with copper the most active The catalytic activity correlates fairly well with the TPR results finding higher CO conversion for the material with higher reducibility (OMS-Cu) The O_2 selectivity measured as ($[CO]_{in}$-$[CO]_{out}/_2[O\text{-}_2]_{in}$-$[O\text{-}_2]_{out}$) x 100 is very similar for all synthesized materials.

Operando XAS and Raman study on the structure of a supported vanadium oxide catalyst during the oxidation of H_2S to sulphur

J.P. Holgado**,** M.D. Soriano**,** J. Jiménez-Jiménez**,** P. Concepción**,** A. Jiménez-López, A. Caballero, E. Rodríguez-Castellón and J.M. López Nieto

Catalysis Today, 155 (2010) 296-301

DOI: 10.1016/j.cattod.2010.02.050

The modification of crystalline phases of a vanadium oxide supported on mesoporous zirconium phosphate during the partial oxidation of H_2S to sulphur has been studied by using an operando Raman-GC approach and XAS in reaction conditions. The catalyst, mainly presenting crystalline V_2O_5, is transformed during the oxidation of H_2S at 200 °C, presenting crystals of V_4O_9, which is identified by the presence of a band at ca. 900 cm^{-1} in the Raman spectra (using a 785 nm line of an Argon ion laser) and by the presence of a pre-edge at 5469.8 eV (and a main-edge at 5482.2 eV) in XANES spectra. At the same time, it is observed a high conversion of H2S to sulphur (the main reaction product) and SO_2 (as minority). Both activity and selectivity depend on the time on stream. In this way, the selectivity to SO_2 decreases from ca. 5 to 1% with the time on stream. This change could be explained on the basis of the nature of V-species: the initial presence of V^{5+}–O–V^{5+} pairs and the appearance of V^{5+}–O–V^{4+} pairs at high time on stream.

Study of nanoporous catalysts in the selective catalytic reduction of NOx
María José Orellana Rico, Ramón Moreno-Tost, Antonio Jiménez-López, Enrique Rodríguez-Castellón, Rosa Pereñíguez, Alfonso Caballero and Juan Pedro Holgado
Catalysis Today, 158 (2010) 78-88
DOI: 10.1016/j.cattod.2010.04.016

Two SBA-15 type materials were synthesized using a low-cost route, a pure silica SBA-15 and an Al containing SBA-15 (with a Si/Al ratio of 10), where Al was added by a post-synthesis modification. The later solid was achieved without any significant loss in the textural properties of SBA-15, besides improving its properties as support of catalysts. Copper impregnated catalysts were prepared through the incipient wetness impregnation of the two supports. With both supports, the copper weight loading were 1, 3 and 6 wt%. The copper incorporation kept the support mesoporous structures, obtaining a better dispersion of the active phase in the containing aluminium support. All the catalysts showed a moderated catalytic activity in the SCR of NO with propane in presence of an excess of oxygen in the whole studied interval of temperatures and a much better performance was observed when using NH_3 instead of propane. The changes of the active phases were studied by operando XAS spectroscopy. Factor analysis of in operando XANES results with sample SiAl_6 indicate that no Cu^0 was detected, but only Cu^{1+} and Cu^{2+}. The temperature where the Cu^{1+}/Cu^{2+} ratio is maximum occurs at the reaction temperature where the observed catalytic NO conversion is also maximum.

Supported nickel catalysts with a controlled molecular architecture for the catalytic reformation of methane
Dirk Hufschmidt, L.F. Bobadilla, F. Romero Sarria, M.A. Centeno, J.A. Odriozola, M. Montes and E. Falabella
Catalysis Today, 149 (2010) 394-400
DOI: 10.1016/j.cattod.2009.06.002

In this work a lanthanum and nickel catalyst having perovskite structure, grown on a γ-alumina carrier, is being presented. The structure of the catalyst was confirmed by XRD. The behaviour of this material under the conditions of steam reforming has been studied and the influence of the temperature, the space velocity and the steam/carbon ratio on the conversion of methane and the product distribution in the process was determined. In all cases at higher temperatures conversions of more than 90% and high selectivities were achieved. The experiments to determine the stability of the catalyst demonstrated that no deactivation in experimental runs of more than 17 h occurred. Additionally a study of the catalyst after the reaction showed that only lowly structured carbonaceous species were formed on the catalyst surface, which is not expected to inhibit strongly the initial catalytic activity.

Gas phase photocatalytic oxidation of toluene using highly active Pt doped TiO_2

G. Colón, M. Maicu, M.C. Hidalgo, J.A. Navío, A. Kubacka and M. Fernández-García
Journal of Molecular Catalysis A: Chemical, 320 (2010) 14-18
DOI: 10.1016/j.molcata.2009.12.009

Platinum doped TiO_2 materials were studied for the gas phase photocatalytic degradation of toluene. Platinum deposition was achieved by photodeposition method over TiO_2 prepared by means of a sol–gel route. The effect of sulphuric acid pretreatment on the further platinisation process has been extensively studied. From the wide structural and surface analysis of the catalysts an interesting synergetic effect has been demonstrated. The previous sulphate treatment over TiO_2 leads to improved dispersion of the Pt which presents a lower aggregation and homogeneous cluster size. This fact, together with the adequate control of anatase structural and surface parameter due to the sulphate treatment, renders a good photocatalytic performance for toluene oxidation reaction. The highest reaction rates and CO_2 selectivities have been obtained for $Pt–S–TiO_2$ samples.

Catalytic nanomedicine: Functionalisation of nanostructured cryptomelane
Tessy López, Emma Ortiz, Mayra Alvarez, Joaquin Manjarrez, Mario Montes, Paloma Navarro and José Antonio Odriozola
Materials Chemistry and Physics, 120 (2010) 518-525
DOI: 10.1016/j.matchemphys.2009.11.049

Nanostructured cryptomelanes (KMn_8O_{16}) were synthesized from manganese sulphate and manganese acetate precursors by the reflux method. The respectively obtained samples, CRYSO4 and CRYAc, were functionalised with hydroxyl, ammonium, sulphate and phosphate groups in order to modify the biocompatibility and surface properties of cryptomelane. Characterization by FTIR and XRD confirmed bond formation of CRY–NH, $\mathrm{CRY{=}S{=}O}$, CRY–NH, and $\mathrm{CRY{=}PO_4}$. In both functionalise samples ($CRYSO_4$-F and CRYAc-F), IR bands occurred at 1399 cm^{-1}, corresponding to the sulphate species, and 1106 cm^{-1}, related to phosphate vibrations; along with the OH and NH characteristic vibration bands in the high energy region. Biocompatibility of functionalised samples was tested by implantation of cryptomelane reservoir in the basolateral amygdala and caudal nucleus of Wistar rats using stereotactic surgery. The brains of the rats were processed in order to evaluate any damage associated with the implant. The results showed that functionalised cryptomelanes did not cause tissue damage or inflammation while not functionalised cryptomelanes caused cell death.

Chemical and electronic characterization of cobalt in a lanthanum perovskite. Effects of strontium substitution
José L. Hueso, Juan Pedro Holgado, Rosa Pereñíguez, Simon Mun, Miquel Salmeron and Alfonso Caballero
Journal of Solid State Chemistry, 183 (2010) 27-32
DOI: 10.1016/j.jssc.2009.10.008

Two different cobaltites, $LaCoO_3$ and $La_{0.5}Sr_{0.5}CoO^{3-\delta}$, have been prepared and characterized by means of high energy Co K-edge and low energy O K-edge X-ray absorption spectroscopy (XAS). Even though half of the La(III) is substituted by Sr(II), little or no changes can be detected in the formal oxidation state of cobalt atoms. The presence of strontium cations induces two main effects in the chemical and electronic state of the perovskite. The charge balance with Sr(II) species is reached by the formation of oxygen vacancies throughout the network, which explains the well-known increase in the reactivity of this substituted perovskite. O K-edge XAS experiments show that the Sr(II) species induce the transitions of d electrons of cobalt cations from low to high spin configuration. We propose that this change in spin multiplicity is induced by two cooperative effects: the oxygen vacancies, creating five coordinated cobalt atoms, and the bigger size of Sr(II) cations, aligning the Co–O–Co atoms, and favoring the overlapping of π-symmetry cobalt and oxygen orbitals, reducing the splitting energy of eg and t2g levels.

The Effect of Water on Particle Size, Porosity and the Rate of Drug Release From Implanted Titania Reservoirs

Lopez, T; Ortiz, E; Alexander-Katz, R; Odriozola, JA; Quintana, P; Gonzalez, RD; Lottici, PP; Marino, LG

Journal of biomedical Materials Research Part B-Applied Biomaterials, 93B (2010) 401-406

DOI: 10.1002/jbm.b.31595

The implantation of controlled drug release devices represents a new strategy in the treatment of neurodegenerative disorders Sol-gel titania implants filled with valproic acid, have been used for this purpose to treat induced epilepsy in rats The kinetics of the drug release depend on. (a) porosity, (b) chemical interactions between valproic acid and surface hydroxyl groups of titania, (c) particle size, and (d) particle size agglomerates The concentration of water used in the hydrolysis reaction is an important variable in the degree of porosity, hydroxylation, and structural defects of the nanostructured titanium oxide reservoir The titanium n-butoxide/water ratio was systematically varied during the sol-gel synthesis, while maintaining the amount of valproic acid constant. Characterization studies were performed using DTA-TGA, FTIR, Raman, TEM, SEM, BET, and in vitro release kinetic measurements The particle agglomerate size and porosity were found to depend on the amount of water used in the sol-gel reaction.

Structure and microstructure of EB-PVD yttria thin films grown on Si (111) substrate

Mária Hartmanová, Matej Jergel, Juan Pedro Holgado and Juan Pedro Espinos

Vacuum, 85 (2010) 535-540

DOI: 10.1016/j.vacuum.2010.09.003

Structure and microstructure of yttria thin films grown by electron beam physical vapour deposition on a stationary Si (111) substrate at room temperature (RT), 500° and 700 °C, were investigated by the grazing-incidence X-ray diffraction and scanning electron microscopy, respectively. X-ray photoelectron spectroscopy provided information on the surface contamination from the atmosphere and the Y oxidation state. A strong effect of the deposition temperature and the vapour flux incidence angle was found. The film deposited at RT is polycrystalline with very fine grains of the body-centered cubic (bcc) crystallographic symmetry.

An increase of deposition temperature results in a rapid growth of bcc grains with an improved crystalline structure. Moreover, the based-centered monoclinic phase appears for the deposition temperature of 700 °C. Preferred grain orientation (texture) with two main components, (400) and (622), was observed in the films deposited at 500 °C whereas no texture was found for 700 °C. The microstructure exhibits the columnar feather-like structure of different degrees of perfection which can be explained by the shadowing effects caused by an oblique vapour flux incidence angle. Surface morphology of the films is governed by a combination of the triangular and four-sided (square) columns. All films were found to be dense with a little porosity between the columns.

Physicochemical Characterization and Use of Wastes from Stainless Steel Mill
Dominguez, MI; Romero-Sarria, F; Centeno, MA; Odriozola, JA
Environmental Progress & Sustainable Energy, 29 (2010) 471-480
DOI: 10.1002/ep.10435 (C) 2010 American Institute of Chemical Engineers Environ Prog

Several types of wastes are produced during the manufacture of stainless steel (slags, refractory bricks, and dust). Most of these wastes are not recycled but stored in security deposits or landfills depending on their environmental danger This article reports the study of the physicochemical and mineralogical properties of stainless steel wastes. Their possible uses are also discussed.

Determination of the local structure of a highly dispersed Pd-Nanosystem located on a titanium dioxide carrier
Kriventsov, VV; Novgorodov, BN; Yakimchuk, EP; Kochubey, DI; Zyuzin, DA; Simakova, IL; Chistyakov, AV; Zhmakin, VV; Bukhtenko, OV; Tsodikov, MV; Kozitsyna, NY; Vargaftik, MN; Moiseev, II; Maksimovskii, EA; Nechepurenko, SF; Navio, JA; Nikitenko, SG
Journal of Surface Investigation-X-Ray Synchrotron And Neutron Techniques, 4 (2010) 636-639
DOI: 10.1134/S1027451010040166

This work is devoted to a structural study of a highly dispersed Pd nanosystem, which is stabilized in the TiO_2 matrix, by XAFS spectroscopy. Nanocomposite was prepared from bimetallic PdCo(mu-OOCMe)(4)(NCMe) precursor followed by processing in several ways: calcination in air and in argon and microwave irradiation. The local structure of Pd catalysts formed by different methods was studied. Possible structural models were considered in detail.

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

Washcoating of metallic monoliths and microchannel reactors
L. C. Almeida, F.J. Echave, O. Sanz, M. A. Centeno, J. A. Odriozola, M. Montes

Studies on Surface Science and Catalysis 175, 2010, 25-3

Synthesis of ionic liquid template zeolite structures
A. Morano, S. Ivanova, F. Romero-Sarria, M. A. Centeno, J. A. Odriozola
Studies on Surface Science and Catalysis 175, 2010, 597-600

New class of acid catalysts for methanol dehydration
S. Ivanova, X. Nitsch, F. Romero-Sarria, B. Louis, M. A. Centeno, A.C. Roger, J. A. Odriozola
Studies on Surface Science and Catalysis 175, 2010, 601-604

Highly porous hydrotalcite-like film growth on anodised aluminium monoliths
F.J. Echave, O. Sanz, L.Costa, J. A. Odriozola, M. Montes
Studies on Surface Science and Catalysis 175, 2010, 639-642

Ethyl Acetate combustión catalyzed by oxidized brass micromonoliths
O. Sanz, S.A. Cruz, J.C. Millán, M. Montes, J. A. Odriozola
Studies on Surface Science and Catalysis 175, 2010, 661-664

LIBROS Y OTRAS PUBLICACIONES / BOOKS AND OTHER PUBLICATIONS

Estudio del efecto de la modificación superficial de monolitos metálicos en el anclaje de catalizadores
L.M. Martínez T., O. Sanz, A. Paúl, J.A. Odriozola
En: Tratamientos Térmicos, abril 2010, nº 119, pp. 29-34. *Editorial Capitole Press*
ISSN: 1132-0346

CONGRESOS Y REUNIONES INTERNACIONALES / INTERNATIONAL CONGRESS AND MEETINGS

COMUNICACIONES EN CONGRESOS Y REUNIONES / COMMUNICATIONS IN CONGRESS AND MEETINGS

11th International Conference on Microreaction Technology, IMRET 11
8-10 Marzo [Kyoto, Japón]

“Fischer-Tropsch Synthesis in microchannels”, L. C. Almeida, F. J. Echave, M. A. Centeno, G. Arzamendi, L.M. Gandía, E.F. Souza-Aguiar, J. A. Odriozola, M. Montes. Comunicación oral

"Design and testing of a microchannel reactor for the PROX reaction", S. Cruz, O. Sanz, R. Poyato, O. Laguna, F. J. Echave, L.C. Almeida, M.A. Centeno, G. Arzamendi, L.M. Gandia, E.F. Souza-Aguiar, M. Montes, J.A. Odriozola. Comunicación oral

COST Action CM0903-UBIOCHEM I (Utilisation of Biomass for Fuels and Chemicals)

13-15 Mayo [Córdoba, España]

"One step catalytic conversion of alcohols into fuel components", A.V. Chystyakov, M.V.Tsodikov, G.I. Konstatinov, F.A. Yandieva,Gekhaman, A.E. Moiseev, J.A. Navio. Poster

"Catalysts for the steam reforming of glycerol: Influence of the preparation method and gold presence", L.F. Bobadilla, S.A. Cruz, R. Innocenti, S. Ivanova, M.J. Saeki, M.A. Centeno, F. Romero-Sarria, J.A. Odriozola. Poster

6th European Meeting on Solar Chemistry& Photocatalysis: Environmental Applications (SPEA6)

13-16 Junio [Praga, República Checa]

"Tuning the Features of Au Nanoparticles on TiO_2 by the control of the Photodeposition Parameters**",** Julie J. Murcia Mesa, Jose Antonio Navio Santos, Gerardo Colon Ibáñez, Maria Carmen Hidalgo Lopez. Comunicación oral

"Sunlight Highly Photoactive Bi_2WO_6-TiO_2 Heterostructures for Rhodamine B Degradation**",** Sebastián Murcia López, Maria Carmen Hidalgo Lopez, Jose Antonio Navio Santos, Gerardo Colon Ibañez. Poster

"Characterization and Photocatalytic Properties of Titania-Silica Mixed Oxides Doped with Ag and Pt**",** J.M.Doña-Rodriguez, J.Araña, C. Fernández-Rodriguez, D. Portillo-Carrizo, J.Pérez-Peña, O.González-Díaz, J.A.Navio, M. Macias. Poster

"Characterization of New Highly Photoactive Catalysts**",** J.M.Doña-Rodriguez, J.Araña, C. Fernández-Rodriguez, D. Portillo-Carrizo, J.Pérez-Peña, O.González-Díaz, J.A.Navio, M. Macias. Poster

"Assessment of Synthesis Conditions of Bare TiO2 Doped and Si, V, Se Codoped Using Sol-gel Method**",** L.Galeano, J.M.Marín, G.Restrepo, M.C. Hidalgo, J.A.Navio. Poster

European Conference On X-ray Spectrometry

20-25 Junio [Coimbra, Portugal]

“Determination of state and local structure of active component of nanostructured precious metal supported catalysts by XAFS**”,** V.V. Kriventsov, I.E. Beck, I.L. Simakova, A. Simakov, E. Smolentseva, B.N. Novgorodov, E.P. Yakimchuk, D.I. Kochubey, D.P. Ivanov, A.V. Chistyakov, V.V. Gmakin, M.V. Tsodikov, J.A. Navio, S.GNikitenko, V.I. Bukhtiyarov. Comunicación oral

9th International Symposium of the Romanian Catalysis Society”, RomCat 2010

24 Junio [Iasi, Rumania]

“CO oxidation on gold catalysts: towards microreactor technology**”,** M.A. Centeno. Conferencia Invitada

10th International Symposim on the Scientific Bases for the Preparation of Heterogeneous Catalysts

11-15 Julio [Louvain-la-Neuve, Bélgica]

“Washcoating of metallic monoliths and microchannel reactors**”,** L.C. Almeida, F.J. Echave, O.Sanz, M.A. Centeno, J.A. Odriozola, M. Montes. Conferencia Invitada

“Synthesis of ionic liquid templated zeolite structures**”,** A. Morano, S. Ivanova, F. Romero-Sarria, M.A. Centeno, J.A. Odriozola. Comunicación oral

“New class of acid catalyst for metanol dehydration”, S. Ivanova, X. Nitsch, F. Romero-Sarria, B. Louis, M.A. Centeno, A.C. Roger, J.A. Odriozola. Poster

“Ethyl acetate combustion catalyzed by oxidized brass micromonoliths”, O. Sanz, S. Cruz, J.C. Millán, M. Montes, J.A. Odriozola. Poster

“Highly porous hydrotalcilte-like film growth on anodized aluminium monoliths”, F.J. Echave, O. Sanz, L. Costa, J.A. Odriozola, M. Montes. Poster

XVIII-th International Synchrotron Radiation Conference (SR-2010)

19-23 Julio [Novosibirsk, Rusia]

“XAFS study of active component formation of nano-structured precious metals supported catalysts**”,** V.V. Kriventsov, I.E. Beck, I.L. Simakova, A. Simakov, E. Smolentseva, B.N. Novgorodov, E.P. Yakimchuk, D.I. Kochubey, D.P.Ivanov, A.V. Chistyakov, K.B. Golubev, M.V. Chudakova, M.V. Tsodikov, J.A. Navio, V.I. Bukhtiyarov. Comunicación oral

XXII Congreso Iberoamericano de Catálisis

5-10 Septiembre [Viña del Mar, Chile]

“Evidencias del Efecto SMSI (Strong Metal-Support Interaction) En Sistemas Ni/CeO_2: Aplanamiento Y Enterramiento De Las Partícula**”,** A. Morano, S. Ivanova, F. Romero-Sarria, M.A. Centeno, J.A. Odriozola. Comunicación oral

“Oxidación de CO con Catalizadores Au/TiO_2 y Au/TiO_2-Y: Papel De Las Vacantes De Oxígeno En El Reacción**”,** Rafael S. Avellaneda, Svetlana Ivanova, Francisca Romero-Sarria, Miguel A. Centeno, José A. Odriozola. Comunicación oral

“Oxidación de CO Empleando Catalizadores De Au/TiO_2 Depositados Sobre Monolitos De Acero Ferrítico**”,** V.G. Milt; S. Ivanova; O. Sanz; M.I. Domínguez; J.A. Odriozola; M.A. Centeno. Comunicación oral

“Oxidación parcial de H_2S a azufre sobre catalizadores de vanadio soportado. raman y exafs-xanes en condiciones operando**”,** D. Soriano, J.P. Holgado, J. Jiménez, P. Concepción, A. Jiménez-Lopez, A. Caballero, E. Rodríguez-Castellón, J.M. López Nieto. Comunicación oral

“Oxidación total de co sobre catalizadores Au/CeZn**”,** Oscar Hernando Laguna, Miguel Angel Centeno, Francisca Romero Sarria, José Antonio Odriozola. Comunicación oral

“Preparación de soportes estructurados de Al_2O_3/al con porosidad a la carta**”,** Oihane Sanz, Francisco Javier Echave, Jose Antonio Odriozola, Mario Montes. Comunicación oral

“Au/$CePO_4$: Un catalizador para la oxidación de CO a baja temperatura**”,** F. Romero-Sarria, M. I. Domínguez, M. A. Centeno, J. A. Odriozola. Poster

“Catalizadores nanoestructurados de Ni para el reformado de metano con CO_2**”,** M. García-Diéguez, I.S. Pieta, M.C. Herrera, M.A. Larrubia, R. Pereñíguez, J. P. Holgado, A. Caballero, L.J. Alemany. Poster

“Catalizadores para el reformado con vapor de glicerina: influencia del método de presencia de oro”, L. Bobadilla, R. Innocenti, S. Ivanova, M. J. Saeki, F. Romero-Sarria, M. A. Centeno, J. A. Odriozola. Poster

“Efecto de los dopantes Ag y pt en las propiedades estructurales y fotocatalíticas de óxidos mixtos TiO_2-SiO_2”, B. Llano, J.M. Marín, G. Restrepo, L.A. Ríos, J.A. Navío, M.C.Hidalgo. Poster

“Eliminación de CO con mediante catalizadores a base de Au y Ce soportados sobre óxidos de manganeso”, Miguel A. Peluso, Willinton Y. Hernández, Jorge E. Sambeth, Horacio J. Thomas, Miguel A. Centeno, José A. Odriozola. Poster

“Estudio ”in operando” sobre catalizadores $LaNi_{1-x}Co_xO_3$ (x=0, 0.5 y 1) para la reacción de reformado seco de metano”, Rosa Pereñíguez, Víctor M. González–DelaCruz, Mónica García-Diéguez, Mª Ángeles Larrubia, Luis J. Alemany, Alfonso Caballero, Juan P. Holgado. Poster

“Influencia de la incorporación de Zr en el sistema Cu/CeO_2 soportado en SBA-15 para la reacción de oxidación preferencial de CO”, Álvaro Reyes Carmona, Ana Arango Díaz, Elisa Moretti, Aldo

Talon, Maurizio Lenarda, Juan Pedro Holgado Vázquez, Alfonso Caballero Martínez, Antonio Jiménez López, Enrique Rodríguez Castellón. Poster

CONGRESOS Y REUNIONES NACIONALES / NATIONAL CONGRESSES AND MEETINGS

COMUNICACIONES EN CONGRESOS Y REUNIONES / COMMUNICATIONS IN CONGRESS AND MEETINGS

9th Novel Gas Conversion Symposium, NGCS 9

30 Mayo-3 Junio [Lyon, Francia]

"New class of acid catalyst for methanol dehydration to DME", S. Ivanova, X. Nitsch, F. Romero-Sarria, B. Louis, M.A. Centeno, A.C. Roger, J.A. Odriozola. Comunicación oral

"New class of acid catalyst for methanol dehydration to DME", S. Ivanova, X. Nitsch, F. Romero-Sarria, B. Louis, M.A. Centeno, A.C. Roger, J.A. Odriozola. Comunicación oral

"Microchannel reactor for methane steam reforming", S.A. Cruz, O. Sanz, R. Poyato, D: Hufschmidt, L.C. Almeida, F. Romero-Sarria, M.A. Centeno.G. Arzamendi, L.M. Gandia, E.F. Souza-Aguiar, M. Montes, J.A. Odriozola. Comunicación oral

XI Congreso Nacional de Materiales

23-25 Junio [Zaragoza, España]

"Desarrollo y diseño de recubrimientos de TiO_2 opticamente transparentes con actividad fotocatalítica**",** José Antonio Navío, M. Carmen Hidalgo López, Marina Maicu, Gerardo Colón. Comunicación oral

"Recubrimientos de TiO_2 y TiO_2/SiO_2 en gránulos de poliéster. Aplicaciones Fotocatalíticas en fase gas**",** José Antonio Navio, J.M.Marin, L.A. Rios, Gloria Restrepo. Comunicación oral

FORMACION / TRAINING

TESIS DOCTORALES/ DOCTOR DEGREE THESIS

Título: **Estudio e influencia de itrio y otros modificadores superficiales en el comportamiento de catalizadores soportados en TiO_2**
Autor: Rafael Sánchez Avellaneda
Directores: José Antonio Odriozola, Miguel Angel Centeno, Francisca Romero-Sarria
Calificación: Sobresaliente "Cum Laude"
Centro: Universidad de Sevilla

Título: **Estudio de la actividad fotocatalítica de sistemas basados en TiO_2, sulfatado y no sulfatado, y modificado con Pt, Au y Pd**
Autor: Marina Maicu
Directores: José Antonio Navío, Gerardo Colón Ibáñez, M. Carmen Hidalgo
Calificación: Sobresaliente "Cum Laude"
Centro: Universidad de Sevilla

Título: **Obtención de H_2 mediante reformado de CH_4 sobre sólidos con estructura perovskita: $LaNi_{1-x}Co_xO_3$**
Autor: Rosa Pereñíguez Rodríguez
Directores: Alfonso Caballero, Juan Pedro Holgado
Calificación: Sobresaliente "Cum Laude"
Centro: Universidad de Sevilla

Título: **Estudio de la degradación de M-cresol, ácido ftálico y 2,4-diclorofenol mediante fotocatálisis heterogénea**
Autor: Elisenda Pulido Melián
Directores: Gerardo Colón, José Miguel Doña Rodríguez, Oscar M. González Díaz
Calificación: Sobresaliente "Cum Laude"
Centro: Universidad de Sevilla
Título: **Aplicaciones de la Técnica "Spark Plasma Sintering" a la Obtención de Materiales y Dispositivos de Interés en Catálisis**
Autor: Sylvia Andrea Cruz Torres
Directores: José Antonio Odriozola Gordón
Calificación: Sobresaliente "Cum Laude"
Centro: Universidad de Sevilla

Título: **Relación estructura de defectos – actividad catalítica en sistemas sólidos tipo $Au/Ce_{1-x}EuxO_{2-x}/2$ y MnO_x. Aplicación en la reacción de oxidación preferencial de CO en presencia de H_2.**
Autor: Willinton Yesid Hernández Enciso
Directores: José Antonio Odriozola Gordón, Miguel Angel Centeno Gallego
Calificación: Sobresaliente "Cum Laude"
Centro: Universidad de Sevilla

FORMACIÓN DE GRADUADOS / MASTER DEGREE THESIS

Título: **Efecto de la morfología de Co_3O_4 en la reacción de oxidación total de CO**
Autor: Andrea Álvarez Moreno
Directores: M.A. Centeno, Svetlana Ivanova
Grado: Trabajo Fin de Master
Centro: Universidad de Sevilla
Año Académico: 2009-2010

Título: **CO preferential oxidation over microchannel reactor (CuO/CeO_2)**
Autor: Manuel Ngassa Happi
Directores: J.A. Odriozola, F. Romero Sarria
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: 2009-2010

Título: **Evaluación de un reactor de microcanales (catalizador de CuO_x/CeO_2) en la oxidación preferencial de CO (PROX)**
Autor: Sara Oraá Díaz-Santos
Directores: J.A. Odriozola, Juan Francisco Rodríguez Romero, Oscar Hernando Laguna Espitia
Grado: Proyecto Fin de Carrera (Desarrollo Práctico Industrial) Ingeniería Industrial
Centro: Universidad de Castilla-La Mancha. Ciudal Real
Año Académico: 2010-2011
Título: **Desarrollo de catalizadores Au/TiO_2, sintetizados por fotodeposición para aplicaciones en fotocatálisis**
Autor: Julie Joseane Murcia Mesa
Directores: J.A. Navío
Grado: Trabajo Fin de Master
Centro: Universidad de Sevilla
Año Académico: 2009-2010

Título: **Actividad fotocatalítica de heteroestructuras Bi_2WO_6-TiO_2, bajo condiciones simuladas de iluminación solar**
Autor: Sebastián Murcia López
Directores: J.A. Navío
Grado: Trabajo Fin de Master
Centro: Universidad de Sevilla
Año Académico: 2009-2010

EQUIPAMIENTO CIENTÍFICO AVAILABLE EQUIPMENT

- 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

Nuevos procesos de bio-ceramización aplicables a estructuras vegetales jerarquizadas New Bio-ceramization processes applied to vegetable hierarchical structures

Código/Code:	STRP 033277 TEM-PLANT
Periodo/Period:	01-10-2006 / 30-09-2010
Organismo Financiador/Financial source:	Unión Europea
Importe total/Total amount:	314.000 €
Investigador responsable/Research head:	Martínez Fernández, J.
Componentes/Research group:	Ramírez de Arellano-López, A., Jiménez, M., Marrero, M., Clauss, M., Bravo, A., Quispe, J.J.

RESUMEN / ABSTRACT

El Proyecto TEM PLANT se centra en el desarrollo y aplicación de procesos avanzados para transformar estructuras jerarquizadas vegetales en dispositivos biomédicos innovadores con comportamientos anisotrópicos inteligentes y características biomédicas avanzadas, diseñadas para la sustitución de huesos y ligamentos. Las bioestructuras naturales normalmente poseen propiedades superiores a sus análogos sintéticamente fabricados con iguales composiciones de fase, ya que están sumamente organizadas desde las escalas molecular, a la nano, micro y macroscópica, siempre de una forma jerarquizada, con unas arquitecturas complejas pero extremadamente funcionales capaces de adaptarse constantemente a los cambios mecánicos necesarios. El proyecto TEM-PLANT combina la biología, química, ciencia de materiales, nanotecnología y tecnologías de producción, en nuevos y complejos procesos de transformación que originen materiales para implantes óseos o sustitutos de ligamentos. Partiendo de la materia prima vegetal adecuadamente seleccionada, se originarán precursores carbonosos, sobre los cuales se realizará procesos de infiltración en fase líquida o vapor de silicio y calcio, electroforesis y mineralización/deposición superficial, produciendo estructuras cerámicas inertes/reabsorbibles de carburo de silicio/apatita.

Los experimentos de implantación in vivo demuestran la excelente biocompatibilidad de este nuevo material, y cómo es colonizado por el tejido óseo anfitrión debido a su porosidad jerárquicamente interconectada única. Este proyecto desarrollará materiales ligeros y resistentes para la sustitución de huesos con una estructura-morfología adecuada para una funcionalidad mecánica óptima, lo que abriría las puertas a una amplia nueva generación de aplicaciones biomédicas.

TEM-PLANT project focuses on the development and application of breakthrough processes to transform plant-derived hierarchical structures into templates for the exploitation of innovative biomedical devices with smart anisotropic performances and advanced biomechanical characteristics, designed for bone and ligament substitution. The TEM-PLANT project primary addresses the nano-biotechnologies area and will push the current boundaries of the state-of-the-art in production of hierarchical structured biomaterials. By combining biology, chemistry, materials science, nanotechnology and production technologies, new and complex plant transformation processes will be investigated to copy smart hierarchical structures existing in nature and to develop breakthrough biomaterials that could open the door to a whole new generation of biomedical applications for which no effective solution exists to date.

Starting from suitably selected vegetal raw material, ceramization processes based on pyrolysis will be applied to produce carbon templates, which will be either infiltrated by silicon to produce inert SiC ceramic structures or exchanged by electrophoresis deposition to produce bioresorbable ceramics. For ligament yielding two processes will be developed: pH-controlled and electrophoresis-controlled fibration to generate fibrous collagenous cords with high tensile strength and wear-resistance.

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:	Becerro, A.I.
Componentes/Research group:	Alba, M.D., Trillo, J.M., Castro, M.A., Alvero, R.

RESUMEN / ABSTRACT

En las placas convergentes de la corteza terrestre se produce el transporte de material desde la superficie de la Tierra hacia su interior; este proceso, denominado subducción, es uno de los procesos fundamentales que tienen lugar en la Tierra y que determina la evolución dinámica, química y térmica de la misma. Está relacionado con una gran variedad de características de la superficie, desde la tectónica de placas a los terremotos y volcanes, pasando por la evolución química de la atmósfera terrestre. A pesar de la importancia señalada, existen aún numerosos aspectos de la subducción que se desconocen, principalmente los que se refieren a las propiedades físicas y relaciones entre fases de los componentes de los slabs, la cinética de las transformaciones de fases, las interacciones físicas y químicas del slab con el manto y los efectos de la deshidratación del slab y de la hidratación del manto.

El Consorcio c2c tiene como objetivo integrar los conocimientos de diversos subcampos científicos dentro de las Ciencias de la Tierra y la metodología y experiencia de varios Institutos de Ciencia de Materiales para avanzar en el conocimiento de los aspectos mencionados en el párrafo anterior. El Consorcio estudiará los cambios en las propiedades químicas y físicas de los materiales componentes del slab a medida que estos se someten a presión y se calientan como respuesta a su hundimiento en el interior de la Tierra. Se estudiará, asimismo, su interacción con los minerales terrestres circundantes y se cuantificará el flujo de materiales tanto desde el punto de vista de las zonas de subducción individuales como en una escala global.

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 are poorly understood to date, mainly in the following fields: Physical properties and phase relations of slab-related compositions, kinetics of phase transformations, chemical and physical interactions of the slab with the ambient mantle and dynamic effects of slab dehydration and mantle hydration.

The c2c Consortium aims to integrate research from different subfields within the Earth Sciences and to integrate methodology and experience from institutes in materials research to advance the knowledge and data base of properties that help to address the problems raised above. The Consortium will study the changing chemical and physical properties of slab material as it is compressed and heated in response to sinking into the interior, its interactions with the surrounding “unperturbed” Earth, and will quantify material fluxes, both for individual subduction zones and on the global scale.

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

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.

Materiales compuestos de matriz cerámica y fase de baja dimensionalidad orientados a la gestión de residuos Ceramic composites and low-dimensional phases to waste management

Código/Code:	CTQ2007-63297 (Plan Nacional)
Periodo/Period:	01-10-2007 / 30-09-2010
Organismo Financiador/Financial source:	Ministerio de Educación y Ciencia
Importe total/Total amount:	176.660 €
Investigador responsable/Research head:	Castro Arroyo, M.A.
Componentes/Research group:	Alba, M.D., Alvero, R., Becerro, A.I., Chain, P., Escudero, A., Naranjo, M., Trillo, J.M.

RESUMEN / ABSTRACT

El objetivo central del Proyecto es la obtención de materiales compuestos a partir de silicatos laminares de alta carga expansibles particularmente diseñados conteniendo fases de baja dimensionalidad con actividad eficaz respecto de la retención e inmovilización de residuos tóxicos y peligrosos. El aspecto esencialmente innovador surge, de una parte, de la confluencia de los estudios que el E.I. venía realizando con investigadores de la Universidad de Cambridge (Reino Unido) con los resultados del último proyecto nacional desarrollado. De otra, de la acción de reunificación de los investigadores que participan en un proyecto único, de carácter multidisciplinar, en la frontera de la química básica de los silicatos con la gestión de residuos e interpretación del fenómeno de subducción en el manto inferior de la Tierra. La hipótesis según la cual la eficacia en la eliminación de contaminantes tóxicos y radioactivos por aluminosilicatos laminares viene controlada por la disposición estructural y por la composición de las fases de baja dimensionalidad originada durante los tratamientos se ha elaborado a partir de los resultados obtenidos por el E.I. en la última década de trabajo. La metodología prevista no se limita a la síntesis de los materiales compuestos y a su caracterización, pues incorpora una medida del potencial que representarían en el tratamiento de residuos, esencialmente basados en algunos contaminantes orgánicos y cationes pesados, tóxicos y radiactivos. El desarrollo del proyecto incidirá sobre las relaciones del E.I. con los Grupos de la Universidad de Bayreuth (Alemania) y Cambridge (Reino Unido), las cuales han conducido a numerosas publicaciones conjuntas, antecedentes de la presente solicitud. El carácter multidisciplinar del proyecto junto con el marcado carácter académico y docente, se considera avales de la elevada capacidad formativa del Proyecto.

The main objective of this Project is obtaining composite materials from especially designed expansible and high layer charge laminar silicates containing low dimensional phases with effective activity for the retention and immobilization of toxic and dangerous wastes. The main innovating aspect of the Project arises, on one hand, from the confluence of the studies that the research team has performed with researchers from University of Cambridge (United Kingdom) within the development of the current national project. On the other hand, it arises from the action of reunification of the researchers who participate in a unique multidisciplinary project in the border of the basic chemistry of silicates in connection with the waste management. The proposed hypothesis, elaborated from the results obtained by the research team during the last decade, states that the effectiveness of the elimination of polluting agents by layered aluminosilicates is controlled by the structural disposition and the composition of the low dimensional phases originated during the treatments. Methodology is not limited to synthesis of the composite materials and its characterization, and it incorporates a measurement of the potential which they would represent in the treatment of wastes, essentially based on some organic polluting agents and heavy, toxic and radioactive cations. The development of the Project will affect the relations of the research team with Research Groups of the University of Bayreuth (Germany) and Cambridge (United Kingdom) and the multidisciplinary character of the Project and the noticeable academic and educational character of the team can be considered a guarantee of its high formative capacity.

Inertización de residuos tóxicos y radioactivos en una matriz de silicatos Inmobilization of toxic and radioactive wastes by silicates

Código/Code:	P06-FQM-02179 (Proyecto de Excelencia)
Periodo/Period:	28-2-2007 / 1-3- 2010
Organismo Financiador/Financial source:	Junta de Andalucía
Importe total/Total amount:	107.991 €
Investigador responsable/Research head:	Castro Arroyo, M.A.
Componentes/Research group:	Alba, M.D., Alvero, R., Becerro, A.I., Chain, P., Escudero, A., Naranjo, M., Pavón, E., Trillo, J.

RESUMEN / ABSTRACT

El presente Proyecto pretende emplear silicatos laminares expansibles de alta carga, diseñados bajo procedimientos que permitan controlar la cantidad y distribución de los centros tetraédricos activos, en un conjunto de tratamientos químicos suaves, en contacto con elementos tóxicos seleccionados, en colaboración con las empresas BEFESA y ENRESA, que permitan su encapsulamiento e inmovilización posterior. Durante la realización del mismo se plantea, en un primer período, analizar el efecto que las variables experimentales involucradas en el procedimiento de síntesis ejercen sobre la distribución de los centros activos de los materiales. En un segundo período, los precursores obtenidos se tratarán bajo condiciones hidrotermales, en condiciones subcríticas, con disoluciones conteniendo elementos tóxicos y radioactivos cuidadosamente seleccionados. Finalmente, se estimará el grado de retención de los elementos en las nuevas fases obtenidas. El Equipo Investigador (E.I.) responsable de la realización del Proyecto incorporará una metodología experimental desarrollada recientemente en su seno que incluye el empleo combinado de técnicas tales como la Resonancia Magnética Nuclear de Sólidos, la Difracción, y la Fluorescencia y Microfluorescencia de Rayos X, que suministrarán información acerca tanto del orden a largo alcance como del entorno local de los centros activos de los residuos, responsables de su peligrosidad. Ello deberá suministrar información directa, no disponible en la actualidad, acerca del mecanismo final de fijación, piedra angular del Proyecto. Los Resultados esperados aportarán, desde el punto de vista de la investigación desarrollada, información básica útil acerca de los mecanismos de interacción de iones metálicos con la red de silicatos laminares expansibles y su relación con el ordenamiento local de los átomos constituyente de éstos y, en segundo lugar, un conocimiento útil, de carácter aplicado, que permita desarrollar nuevos procedimientos adecuados de encapsulamiento de residuos industriales, en conexión con las colaboraciones actualmente desarrolladas con empresas del sector, lo cual marca el carácter innovador del mismo.

In The present Project tries to use high-charged silicates, which are designed under procedures that allow controling the quantity and distribution of the tetrahedral active centers. They will be submitted to a set of chemical soft treatments in order to inmobilize toxic elements. This project will be carried out in collaboration with BEFESA and ENRESA companies. Firstly, the effect that the experimental variables involved in the procedure of synthesis exert on the distribution of the active centers of the materials will be analyzed. In the second stage, the synthetic silicates will be treated under soft hydrothermal conditions with solutions containing carefully selected toxic and radioactive elements. Finally, the degree of retention of these elements in the new obtained phases will be estimated. The Research Team (R.T.) will incorporate an experimental methodology developed by itself that includes the combined employment of Nuclear Magnetic Resonance of Solids, X-ray Diffraction, X-rays Fluorescence and Microfluorescence, which will give information of the long range order and the local environment of the active centers of the residues, responsible of it dangerousness. It will have to give direct and not yet available information of the final mechanism of fixation, which is the main objective of this Project. The expected Results will bring basic useful information about the mechanisms of interaction of metallic ions with the framework of expansible aluminosilicates and its relation with the local arrangement of their atoms. Moreover, it will bring a useful knowledge allowing to develop new suitable procedures for immobilization of industrial waste, in collaboration with the companies of the sector, which marks the innovative character of the Project.

Bioener: Aplicación de tecnologías biomiméticas a sistemas energéticos

Código/Code:	P09-TEP-5152 (Proyecto de Excelencia)
Periodo/Period:	01-01-2010 / 31-12-2012
Organismo Financiador/Financial source:	Junta de Andalucía
Importe total/Total amount:	311.167,68 €
Investigador responsable/Research head:	Julián Martínez Fernández
Componentes/Research group:	Jiménez Melendo, M., De Arellano-López, A. R. Bravo León, A., Varela Feria, F. M.

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 electroquímico 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.

OTROS PROYECTOS / OTHER PROJECTS

Investigación y desarrollo de electrodos de difusión de gas para tratamiento de electroxidación avanzada de aguas residuales

Periodo/Period:	01-6-2009 / 30-05-2010
Organismo Financiador/Financial source:	CTA
Investigador responsable/Research head:	Alfonso Bravo León, Julián Martínez Fernández

Resistencia y desgaste mecánico de sistemas implantoprotésicos de óxido de circonio

Periodo/Period:	22-01-2009 / 22-07-2010
Organismo Financiador/Financial source:	CTA
Investigador responsable/Research head:	Manuel Jiménez Melendo

■ TRANSFERENCIA / TECHNOLOGICAL TRANSFER

CONVENIOS Y CONTRATOS / CONTRACTS AND AGREEMENTS

Investigación y desarrollo de electrodos de difusión de gas para el tratamiento de electrooxidación avanzada de aguas residuales

Periodo/Period:	01-06-2009 / 30-05-2010
Organismo Financiador/Financial source:	CYCLUS ID, SL
Importe total/Total amount:	16.203,74 €
Investigador responsable/Research head:	Julián Martínez Fernández

Valorización de los lodos de estaciones de tratamiento de agua potable

Periodo/Period:	01-12-2009 / 30-06-2010
Organismo Financiador/Financial source:	EMASESA
importe total/Total amount:	10.000 €
Investigador responsable/Research head:	Miguel Angel Castro Arroyo

Valorización de materiales mediante oxidación catalítica

Periodo/Period: 1-02-2010 / 31-01-2011
Organismo Financiador/Financial source: BEFESA
importe total/Total amount: 12.929 €
Investigador responsable/Research head: Miguel Angel Castro Arroyo

Caracterización de mecanismos de retención de actínidos en materiales silicatados

Periodo/Period: 1-03-2010 / 28-02-2011
Organismo Financiador/Financial source: ENRESA
importe total/Total amount: 64.482,76 €
Investigador responsable/Research head: Miguel Angel Castro Arroyo

Patentes / Patents

Procedimiento hidrotérmico de obtención de la calsilita

Inventores: Ana Isabel Becerro Nieto, Marco Mantovani, Alberto Escudero
Ámbito Geográfico: Internacional
PATENTE SOLICITADA. N. de solicitud: PCT/ES2010/070373
Fecha Solicitud/Licencia: 2/junio/2010
Entidad Titular: CSIC

Dispositivo portamuestras para el estudio de interfaces mediante difracción de Rayos X en modo transmisión

Inventores: Miguel Angel Castro Arroyo, Santiago Medina Carrasco, María Dolores Alba Carranza, María del Mar Orta Cuevas, Esperanza Pavón González, Carmen Millan Chacartegui
Ámbito Geográfico: Internacional
PATENTE SOLICITADA. N. de solicitud:
Fecha Solicitud/Licencia: 9/noviembre/2010
Entidad Titular: Universidad de Sevilla

Nanogalerías de organomicas, procedimiento de obtención y su aplicación en descontaminación

Inventores: María Dolores Alba Carranza, Miguel Angel Castro Arroyo, María del Mar Orta Cuevas, Esperanza Pavón González, M. Carolina Pazos Zarama
Ámbito Geográfico: Internacional
PATENTE SOLICITADA. N. de solicitud: PCT/ES2010/070859
Fecha Solicitud/Licencia: 21/diciembre/2010
Entidad Titular: Universidad de Sevilla

Impianti per sostituzioni osee “Load Bearing” ad architettura gerarchicamente organizzata derivante dalla trasformaziones di strutture vegetali

Inventores: Anna Tampieri, Simone Sprio, Andrea Ruffini, Julia Will, Peter Greil, Frank Mueller, Julián Martínez Fernández, Carmen Torres Raya, Francisco M. Varela Feria, Joaquín Ramírez Rico, Mari-Francoise Harmand
Ámbito Geográfico: Italia
PATENTE SOLICITADA. N. de solicitud: MI2010A00270
Fecha Solicitud/Licencia: 8/Noviembre/2010
Entidades Titulares: Consiglio Nazionalize Delle Ricerche (Italia), Friedrich-Alexander-Universiteit Erlangen-Nuernberg (Alemania), Universidad de Sevilla (España), Laboratoire D’Evaluation des Matériels implantables (Francia)

PUBLICACIONES / PUBLICATIONS

ARTÍCULOS PUBLICADOS EN REVISTAS SCI / PAPERS IN SCI JOURNALS

Bioactivation of biomorphous silicon carbide bone implants
Will J., Hoppe A., Muller F.A., Raya C.T., Fernández J.M., Greil P.
Acta Biomaterialia, 6 (2010) 4488-4494
DOI: 10.1016/j.actbio.2010.06.036

Wood-derived silicon carbide (SiC) offers a specific biomorphous microstructure similar to the cellular pore microstructure of bone. Compared with bioactive ceramics such as calcium phosphate, however, silicon carbide is considered not to induce spontaneous interface bonding to living bone. Bioactivation by chemical treatment of biomorphous silicon carbide was investigated in order to accelerate osseointegration and improve bone bonding ability. Biomorphous SiC was processed from sipo (Entrandrophragma utile) wood by heating in an inert atmosphere and infiltrating the resulting carbon replica with liquid silicon melt at 1450 °C. After removing excess silicon by leaching in HF/HNO3 the biomorphous preform consisted of β-SiC with a small amount (approximately 6 wt.%) of unreacted carbon. The preform was again leached in HCl/HNO3 and finally exposed to CaCl2 solution. X-ray photoelectron spectroscopy (XPS) and Fourier transform infrared analyses proved that oxidation of the residual carbon at the surface induced formation of carboxyl [COO-] groups, which triggered adsorption of Ca2+, as confirmed by XPS and inductively coupled plasma optical emission spectroscopy measurements. A local increase in Ca2+ concentration stimulated in vitro precipitation of Ca5(PO 4)3OH (HAP) on the silicon carbide preform surface during exposure to simulated body fluid, which indicates a significantly increased bone bonding activity compared with SiC.

Sc-45 Spectroscopy of Solids: Interpretation of Quadrupole Interaction Parameters and Chemical Shifts

Maria D. Alba, Pablo Chain, Pierre Florian and Dominique Massiot
Journal of Physical Chemistry C, 114 (2010) 12125-12132
DOI: 10.1021/jp1036525

The aims of the present study is to describe for the first time the Sc-45 MAS NMR spectra of X-2-Sc2SiO5 and C-Sc2Si2O7, to combine the spectroscopic information with the structures published from diffraction data, and to propose a rational interpretation of the chemical shifts and quadrupolar parameters. For that purposed, we have correlated the experimental quadrupole coupling parameters of Sc-45 determined for a number of scandium compounds to those found by a simple electrostatic calculation and we have found that the isotropic chemical shift of the Sc-45 is linearly correlated to the shift parameter, calculated by bond-valence theory. We also show that a simple point charge calculation can approximate the electric field gradient to a sufficiently good approximation that it provides a valuable mean to assign the NMR spectra.

Lanthanide sorption on smectitic clays in presence of cement leachates
Evgeny Galunin, María D. Alba, Maria J. Santos, Taufik Abrão and Miquel Vidal
Geochimica et Cosmochimica Acta, 74 (2010) 862-875
DOI: 10.1016/j.gca.2009.11.003

Due to their potential retention capacity, clay minerals have been proposed for use in the engineered barriers for the storage of high-level radioactive actinides in deep geological waste repositories. However, there is still a lack of data on the sorption of actinides in clays in conditions simulating those of the repositories. The present article examines the sorption of two lanthanides (actinide analogues) in a set of smectitic clays (FEBEX bentonite, MX80 bentonite, hectorite, saponite, Otay montmorillonite, and Texas montmorillonite). Distribution coefficients (K_d) were determined in two media: water and 0.02 mol L^{-1} Ca, the latter representing the cement leachates that may modify the chemical composition of the water in contact with the clay. The K_d values of the lanthanides used in the experiments (La and Lu) varied greatly (25–50 000 L kg^{-1}) depending on the ionic medium (higher values in water than in the Ca medium), the initial lanthanide concentration (up to three orders of magnitude decrease inversely with lanthanide concentration), and the examined clay (up to one order of magnitude for the same lanthanide and sorption medium). Freundlich and Langmuir isotherms were used to fit sorption data to allow comparison of the sorption parameters among smectites. The model based on the two-site Langmuir isotherms provided the best fit of the sorption data, confirming the existence of sorption sites with different binding energies. The sites with higher sorption affinity were about 6% of the total sorption capacity in the water medium, and up to 17% in the Ca medium, although in this latter site sorption selectivity was lower. The wide range of K_d values obtained regarding the factors examined indicated that the retention properties of the clays should also be considered when selecting a suitable clay for engineered barriers.

Effect of pressure on kaolinite illitization
Marco Mantovani, Alberto Escudero and Ana Isabel Becerro
Applied Clay Science, 50 (2010) 342-347
DOI: 10.1016/j.clay.2010.08.024

The illitization of kaolinite at increasing pressures was followed by hydrothermal experiments of kaolinite in KOH solution at 300 °C for 12 h and pressures between 500 and 3000 bar. XRD indicated a direct transformation of kaolinite into muscovite/illite with increasing pressure. However, the 27Al MAS NMR spectra showed, in addition to the muscovite/illite resonances, the presence of a signal at 61 ppm that should correspond to a secondary phase, not detected by XRD. A second series of experiments at 300 °C and 1000 bar for 1, 3 and 6 h was carried out to show direct evidence of such phase. The XRD patterns of the products clearly showed the crystallization of K–F zeolite, while the 27Al MAS NMR spectra of these samples displayed a signal at 61 ppm that must correspond, therefore, to Al in the K–F zeolite structure. In conclusion, kaolinite transformed into muscovite/illite when submitted to hydrothermal reaction in KOH solution with increasing pressure, with the formation of a secondary metastable phase called K–F zeolite, whose coherent diffraction domains were too small as to be detected by XRD.

Application of Micro-X-ray Fluorescence Analysis for the Characterization of Industrial Wastes

Maria D. Alba, Patricia Aparicio, Jose M. Benitez, Miguel A. Castro, Maria Diaz and M. Mar Orta

Industrial & Engineering Chemistry Research, 49 (2010) 2348-2352

DOI: 10.1021/ie901716w

The issue of how to improve product quality and product yield in a short period of time is becoming more critical in many industries. Thus, shorter delay times between laboratory analysis and process correction are important in process control. Elimination of sample handling and operator Manipulation is desirable. The present article proposes micro-X-ray fluorescence (mu XRF) as an economical control method for industrial product quality with a minimum time cost. Samples from different industrial processes have been chosen and analyzed by XRF and mu XRF, The results show that the two techniques give similar results and that mu XRF allows the waste to be classified and is able to detect problems in the production process.

Illization of kaolinite: The effect of pressure on the reaction rate

Mantovani, M; Becerro, AI

Clays and Clay Minerals, 58 (2010) 766-771

DOI: 10.1346/CCMN.2010.0580604

Studies of the paragenesis of authigenic illite in arkosic sandstones of various regions and ages have revealed that the illitization of kaolinite is an important reaction accounting for the formation of authigenic illite in sandstones during burial diagenesis. The illitization of kaolinite takes place at an intermediate burial depth of 3–4 km, where pressure can reach values of 100 MPa ({approx}1000 bars). The purpose of the present study was to analyze the effect of pressure on the rate of kaolinite illitization in alkaline conditions. Hydrothermal reactions were conducted on KGa-1b kaolinite in KOH solution at 300°C and under pressures of 500, 1000, and 3000 bars for 1 to 24 h. The visual examination of the X-ray diffraction (XRD) patterns indicated a notable influence of pressure on the reaction rate. Molar percentages of muscovite/illite formed at each time interval were calculated from the analysis of two diagnostic XRD peaks, representing the 060 reflections of kaolinite and muscovite/illite. The data were modeled to obtain the initial rate of conversion at each pressure. The results indicated that the initial rate of kaolinite to muscovite/illite conversion is one order of magnitude greater at 3000 bars than at 500 or 1000 bars. Comparison of these data with those in the literature show a faster conversion rate (several orders of magnitude) in an initially high-alkaline solution than in a near-neutral solution

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

Silicoaluminates as “Support Activator” Systems in Olefin Polymerization Processes
Vanessa Tabernero, Claudimar Camejo, Pilar Terreros, María Dolores Alba, Tomás Cuenca
Materials 2010, 3(2), 1015-1030

LIBROS Y OTRAS PUBLICACIONES / BOOKS AND OTHER PUBLICATIONS

Porous biomorphic SiC for medical implants processed from natural and artivicial precursors
J. Ramirez Rico, C. Torres-Raya, D. Hernández-Maldonado, C. García-Gañan, J. Martínez-Fernández, A.R. de Arellano-López
En: Advances in Bioceramics and Porous Ceramics II (Ed. Roger Narayan and Paolo Colombo). 2010. Pag. 203-214
ISBN: 978-0-470-34494-1

Compressive Strength Degradation in Zrb2-Sic and Zrb2-Sic-C Ultra High Temperature Composites
J. Ramirez Rico, Miguel Antonio Bautista, Julian Martinez Fernandez, M. Singh
En: Mechanical Properties and Performance of Engineering Ceramics and Composites IV
NY, EEUU. Wiley & Sons. 2010. Pag. 127-136
Editor American Ceramic Society
ISBN: 978-0-470-58425-5

CONGRESOS Y REUNIONES INTERNACIONALES / INTERNATIONAL CONGRESS AND MEETINGS

COMUNICACIONES EN CONGRESOS Y REUNIONES / COMMUNICATIONS IN CONGRESS AND MEETINGS

Clay in Natural & Engineered barriers for radiactive confinement

29 marzo-1 abril [Nantes, Francia]

“Chemical Interaction of radioactive waste with clay engineered barriers: stability of resulting immobilizer phase”, Galunin, E., Alba, M.D., Vidal, M. Comunicación oral
“Chemical interaction of tetravalente actinides simulators and the engineering barrier”, Chain, P., Alba, M.D., Castro, M.A., Pavón, E., Orta, M.M. Poster

SETAC Europe 20th Annual Meeting. Science and Technology for Environnmental Protection

23-27 Mayo [Sevilla, España]

“Monitoring a soil remediation strategy based on the addition of materials at pilot plant level”, González-Núñez, R., Orta, M.M., Alba, M.D., Castro, M.A., Diaz, M., Benítez, J., Rigol, A., Vidal, M. Poster

“Design and start-up of remediation soil pilot plant”, Diaz, M., Orta, M.M., Alba, M.D., Castro, M.A., Vidal, M., Rigol, A., Vidal, M., Cornejo, J., Benitez, J., Orta, M.A. Poster

12th International Ceramic Congress CIMTEC 2010

6-11 Junio [Montecatini, Italia]

“Creep and fracture of proton-conducting perovskite oxides”, Cristina Vaquero Aguilar, Manuel Jiménez Melendo. Poster

Trilateral Meeting on Clays

8-11 Junio [Madrid, España]

“Kaolinite illization at 300C with increasing pressure”, Mantovani, M., Escudero, A., Becerro, A.I. Poster

“Cation Absorption in high technological layer silicates”, Pavón, E., Castro, M.A., Alba, M.D., Orta, M.M., Pazos, M.C., Naranjo, M. Poster

III International congress on higher education in pharmaceutical sciences

8-11 Junio [Granada, España]

“Evaluación del desarrollo de competencias de comunicación y capacidad de análisis en alumnos del practicum de Farmacia”, Orta, M.M., Vega, J.M., Sánchez Burson, J., Mencia Jos, A., Alvarez de Sotomayor, M. Comunicación oral

SXNS-11 International conference on surface X-Ray and neutron scattering

13-17 Julio [Chicago, Estados Unidos de América]

“2D adsorption on graphite stearic acid and hidroxylated stearic acid”, Castro, M.A., Alba, M.D, Cerrillos, C., Clarke, S.M., Medina, S., Millán, C., Orta, M.M., Pavón, E., Phillips, T.K. Poster

5th Mid-European Clay Conference

25-29 Agosto [Budapest, Hungria]

“Synthesis and degradation mechanism of a swelling fluoromica”, Cota, A., Alba, M.D., Castro, M.A., Pavon, E., Naranjo, M., Orta, M.M. & Pazos, M.C. Poster

“Water uptake and mucoadhesion of chitosan/montmorillonite composite”, Salcedo, I., Aguzzi, C., Bonferoni, C., Sandri, G., Sanchez, R., Cerezo, P., Alba, M.D. Poster

“Aquocomplex structure in the interlayer space of swelling high-charged micas”, Pavón, E., Alba, M.D., Castro, M.A., Cota, A., Naranjo, M., Orta, M.M. & Pazos, M.C. Poster

“Technological characterization of peloids maturated with montmorillonite and sepiolite”, Aguzzi, C., Cerezo González, M.P., Sánchez, R., Salcedo, I., Machado, J., Alba, M.D., Viseras, C. Poster

11th International Conference on Ceramic Processing Science

29 Agosto-1 Septiembre [Zurich, Suiza]

“Processing and mechanical properties of proton-conducting barium cerate ceramics”, Cristina Vaquero Aguilar, Manuel Jiménez Melendo. Poster

International Congress on Ceramics, ICC3

14-18 Noviembre [Osaka, Japón]

“Microstructure and mechanical properties of Biomorphic SiC materials obtained from enzymatically treated Red Oak wood”, J. Ramirez-Rico, Carmen Torres-Raya, J. Martinez-Fernandez, R. Wimmer. Poster

CONGRESOS Y REUNIONES NACIONALES / NATIONAL CONGRESSES AND MEETINGS

COMUNICACIONES EN CONGRESOS Y REUNIONES / COMMUNICATIONS IN CONGRESS AND MEETINGS

XI Congreso Nacional de Materiales
23-25 Junio [Zaragoza, España]

"Fluencia de $BaCeO_3$ dopado con itrio e iterbio", Cristina Vaquero Aguilar; Manuel Jiménez Melendo. Poster

FORMACION / TRAINING

TESIS DOCTORALES/ DOCTOR DEGREE THESIS

Título:	**Síntesis y Reactividad de Silicatos Laminares de Alta Carga**
Autor:	Moisés Naranjo Muñoz
Directores:	Miguel Angel Castro Arroyo
Calificación:	Sobresaliente "Cum Laude"
Centro:	Universidad de Sevilla

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

PROYECTOS DE INVESTIGACIÓN / RESEARCH PROJECTS

Estudio de Órganos Históricos: Composición y Alteración de Tubos Metálicos Study of Historical Organs: Composition and Alteration of Metallic Pipes

Código/Code:	MAT2007-63234 (Plan Nacional)
Periodo/Period:	2007 / 2010
Organismo Financiador/Financial source:	Ministerio de Ciencia y Tecnología
Importe total/Total amount:	60.500 €
Investigador responsable/Research head:	Justo Erbez, A.
Componentes/Research group:	Iñigo, A., Herrera, L.K., Durán, A., Sigüenza, B., Justo Estebaranz, A., Poyato, J., Cea Galán, A.,

RESUMEN / ABSTRACT

El principal objetivo del proyecto es conocer la composición y microestructura de las aleaciones estaño-plomo de tubos de órganos históricos españoles y sus productos de corrosión. Dicho objetivo persigue conocer los factores que afectan a dicha corrosión, como son el efecto de los compuestos volátiles desprendidos de las maderas y otros materiales orgánicos utilizados en la construcción de órganos, vapor de agua y anhídrido carbónico.

Los trabajos se realizarán en materiales con diferentes grados de corrosión tomados en los propios instrumentos, incluyendo principalmente aleaciones y maderas.

Se prepararán aleaciones con distintas proporciones estaño-plomo y trazas de otros elementos (As, Bi) y enfriadas a velocidades diferentes. Estas aleaciones se someterán a ensayos de corrosión acelerada y se estudiará la influencia de la composición y velocidad de enfriamiento en el proceso.

Se compararán los resultados obtenidos en el laboratorio 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 and microstructure of tin-lead alloys from historical pipe organs from Spain and its products of corrosion. This objective pursues to know the factors that affect to this corrosion, like the effect of the volatile compounds from the wood and other organic materials used in the construction of pipe organs, water vapour and carbon dioxide.

The work will be carried out in materials with different grades of corrosion taken in the own instruments, including alloys and woods.

Alloys with different tin-lead ratios, traces of other elements (As, Bi) and cooled at various cooling rates will be prepared in the laboratory. These alloys will undergo corrosion tests, and the influence of the composition, microstructure and volatile compounds will be studied.

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.

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

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 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 / 31-12-2010
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 hidrogenación. 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.

Síntesis de materiales avanzados nanoestructurados por “mechanical alloying” Synthesis of nanostructured advanced materials by mechanical alloying

Código/Code:	TEP-2248 (Proyecto de Excelencia)
Periodo/Period:	01-04-2007 / 31-03- 2010
Organismo Financiador/Financial source:	Junta de Andalucía
Importe total/Total amount:	155.099 €
Investigador responsable/Research head:	Criado Luque, J.M.
Componentes/Research group:	Real, C., Gotor, F.J., Diánez, M.J., Pérez-Maqueda, L.A., Ortega, A., Alcalá, M.D., Sayagués, M.J., Córdoba, J.M., Sánchez, P.E., Roldán, M.A.

RESUMEN / ABSTRACT

En el presente proyecto se pretende optimizar la síntesis por “mechanical alloying” de una serie de materiales nanoestructurados constituidos por sistemas metálicos, cerámicos y composites cerámica/metal (CERMET) todos ellos de gran interés tecnológico desde el punto de vista de las siguientes aplicaciones: a) Superaleaciones de cobre endurecidas por materiales cerámicos multifásicos para la manufactura de componentes electrónicos de altas prestaciones; b) Aleaciones con memoria de forma del sistema Cu/Al/Zn; c) Materiales con constante dieléctrica colosal (cerámicas CCTO y composites PZN/Ni) y d) Catalizadores de TiO_2 dopados con nitrógeno para controlar la contaminación medioambiental. Los materiales obtenidos se caracterizarán por diversas técnicas, DRX, TEM, HRTEM y XPS. Asimismo se estudiarán las propiedades mecánicas, eléctricas o catalíticas de interés desde el punto de vista de las aplicaciones específicas propias de cada uno de los materiales obtenidos

It will be optimized the synthesis by mechanical alloying of a set of nanostructured metallic and ceramics materials of technological interest from the point of view of the following applications: a)copper superalloys hardened by multiphasic dispersed ceramic materials; b)Shaped memory alloys in the ternary system Cu/Al/Zn; c) Materials with colossal dielectric constant (CCTO and PZN/Ni ceramics) and d)TiO_2 catalysts doped with nitrogen for controlling the surrounding pollution. The obtained materials will be characterized by DRX, TEM, HRTM and XPS. The mechanical, electrical and catalytic properties will be studied according to the specific application of the obtained materials.

Cooperación Internacional y Otros International Cooperation and Others

Study of glazed ceramics from the Alcazar of Seville (X-XVth centuries)

Periodo/Period: 01-09-2010
Entidad Financiadora/Financial source: Proyecto AGLAE. Tiempo de Haz en el C2RMF/CNRS Paris
Investigador responsable/Research head: José Luis Pérez Rodríguez

Study of Metallica components of historical organ pipes by using IBA techniques

Periodo/Period: 01-09-2010
Entidad Financiadora/Financial source: Proyecto AGLAE. Tiempo de Haz en el C2RMF/CNRS Paris
Investigador responsable/Research head: Adrián Durán Benito y Angel Justo Erbez

Mechanochemical synthesis and properties of nanosized materials

Periodo/Period: 1-01-2010 / 31-12-2011
Entidad Financiadora/Financial source: CSIC/Academia Eslovaca de Ciencias (2009SK0002)
Investigador responsable/Research head: Francisco J. Gotor Martínez

Síntesis mecanoquímica de fotocatalizadores basados en la titania

Periodo/Period: 1-01-2009 / 31-12-2010
Entidad Financiadora/Financial source: CSIC/Academia de Ciencias Checa (2008CZ0021)
Investigador responsable/Research head: Luis A. Pérez Maqueda

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

Periodo/Period:	1-01-2009 / 31-12-2010
Entidad Financiadora/Financial source:	FONDECYT/CONYCIT. Ministerio de Tecnología Chileno
Investigador responsable/Research head:	E. Donoso Catalán

Reversible crystallization and structural relaxation in amorphous materials for phase change recording

Periodo/Period:	1-01-2008 / 31-12-2011
Entidad Financiadora/Financial source:	Ministerio de Educación Checo
Investigador responsable/Research head:	J. Málek

TRANSFERENCIA / TECHNOLOGICAL TRANSFER

PATENTES / PATENTS

Procedimiento de optimización para la explotación de canteras de mármol para pavimentos

Inventores: Sánchez-Soto P.J., Ruiz-Conde A., Garzón Garzón E., Morales Hernández L., García Rodríguez I.G.
Ámbito Geográfico: Nacional
PATENTE SOLICITADA. N. de solicitud: P201031096
Fecha Solicitud/Licencia: 17/julio/2010
Entidadades Titulares: CSIC y Universidad de Almería

Procedimiento de obtención de un material cerámico de forsterita

Inventores: Sánchez-Soto P.J., Ruiz-Conde A., Bono Barrón R., Raigón Pichardo M., Garzón Garzón E.
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PUBLICACIONES / PUBLICATIONS

ARTÍCULOS PUBLICADOS EN REVISTAS SCI / PAPERS IN SCI JOURNALS

Quantitative Characterization of Multicomponent Polymers by Sample-Controlled Thermal Analysis

Pedro E. Sánchez-Jiménez, Luis A. Pérez-Maqueda, José Crespo-Amoros, Juan López, Antonio Perejón, and José M. Criado
Analytical Chemistry, 82 (2010) 8875-8880
DOI: 10.1021/ac101651g

This paper explores the potential of sample-controlled thermal analysis (SCTA) in order to perform compositional analysis of multicomponent polymeric materials by means of thermogravimetric experiments. In SCTA experiments, the response of the sample to the temperature determines the evolution of the temperature by means of a feedback system; thus, what is controlled is not the temperature−time profile, as in conventional analysis, but rather the evolution of the reaction rate with time. The higher resolving power provided by the technique has been used for determining the composition of polymer blends composed of polyvinyl chloride (PVC) and different commercial plasticizers, a system where the individual components have very similar thermal stabilities, thereby rendering useless thermogravimetric experiments run under conventional conditions. Different SCTA procedures, such as constant rate thermal analysis (CRTA), which has received special attention, and high-resolution and stepwise isothermal analysis have been tested, and the results obtained have been compared with linear heating rate technique. It has been proven that CRTA can be used to effectively determine the exact composition of the blend.

Murillo's paintings revealed by spectroscopic techniques and dedicated laboratory-made micro X-ray diffraction

Duran, A; Siguenza, MB; Franquelo, ML; de Haro, MCJ; Justo, A; Perez-Rodriguez, JL
Analytica Chimica Acta, 671 (2010) 1-8
DOI: 10.1016/j.aca.2010.05.004

This paper describes one of the first case studies using micro-diffraction laboratory-made systems to analyse painting cross-sections. Pigments, such as lead white, vermilion, red ochre, red lac, lapis lazuli, smalt, lead tin yellow type I, massicot, ivory black, lamp black and malachite, were detected in cross-sections prepared from six Bartolome Esteban Murillo paintings by micro-Raman and micro-XRD combined with complementary techniques (optical microscopy, SEM-EDS, and FT-IR). The use of micro-XRD was necessary due to the poor results obtained with conventional XRD. In some cases, pigment identification was only possible by combining results from the different analytical techniques utilised in this study.

Kinetic model for thermal dehydrochlorination of poly(vinyl chloride)
Sanchez-Jimenez, PE; Perejon, A; Criado, JM; Dianez, MJ; Perez-Maqueda, LA
Polymer, 51 (2010) 3998-4007
DOI: 10.1016/j.polymer.2010.06.020

In this paper, a novel method for calculating degradation kinetics is presented. The method has been applied to the thermal dehydrochlorination of two different samples of PVC. It has been observed that this dehydrochlorination is complex and involves two different processes. A model that accounts for the entire dehydrochlorination is proposed. This model involves nucleation and growth and diffusion controlled mechanisms. The kinetic parameters are obtained from linear heating rate, isothermal and sample controlled thermal analysis experiments. Kinetic results obtained from the macroscopic thermal analysis measurements demonstrate the correlation between the kinetics of the thermal dehydrochlorination of PVC and the structure of this macromolecule.

Generalized Kinetic Master Plots for the Thermal Degradation of Polymers Following a Random Scission Mechanism
Sanchez-Jimenez, PE; Perez-Maqueda, LA; Perejon, A; Criado, JM
Journal of Physical Chemistry A, 114 (2010) 7868-7876
DOI: 10.1021/jp103171h

In this paper, the f(alpha) conversion functions for random scission mechanisms have been proposed to allow for the construction of generalized master plots suitable for these kinds of mechanisms. The master plots have been validated by their application to simulated data and to the thermal degradation of poly(butylene terephthalate), polyethylene, and poly(tetrafluoroethylene).

A new model for the kinetic analysis of thermal degradation of polymers driven by random scission
Sanchez-Jimenez, PE; Perez-Maqueda, LA; Perejon, A; Criado, JM
Polymer Degradation and Stability, 95 (2010) 733-739
DOI: 10.1016/j.polymdegradstab.2010.02.017

In this paper, a series of f(alpha) kinetic equations able to describe the random scission degradation of polymers is formulated in such a way that the reaction rate of the thermal degradation of polymers that go through a random scission mechanism can be directly related to the reacted fraction. The proposed equations are validated by a study of the thermal degradation of poly(butylene terephthalate) (PBT). The combined kinetic analysis of thermal degradation curves of this polymer obtained under different thermal pathways have shown that the proposed equation fits all these curves while other conventional models used in literature do not.

Mechanochemical synthesis of vanadium nitride
M.A. Roldan, V. López-Flores, M.D. Alcala, A. Ortega and C. Real
Journal of the European Ceramic Society, 30 (2010) 2099-2107
DOI: 10.1016/j.jeurceramsoc.2010.04.008

Vanadium nitride (VN) has been prepared by mechanosynthesis from vanadium metal under a pressurized nitrogen atmosphere in a short milling time. 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 final product, VN with 96% of purity, is obtained at room temperature with nanometric particle size and a very high microhardness after sintering. A relationship between microstructure and microhardness as well as a comparison between the VN obtained mechanical and thermal method is also presented.

Microstructural characterization of ceramic-intermetallic composites using TEM related techniques
M.J. Sayagués, M.A. Avilés, J.M. Córdoba, M.D. Alcalá and F.J. Gotor
Journal of the European Ceramic Society, 30 (2010) 1765-1774
DOI: 10.1016/j.jeurceramsoc.2010.01.039

TiC_xN_y/Ti–Ni and TiC_xN_y/Ti–Co composites formed by ceramic and intermetallic binder phases were produced by pressureless sintering at 1400 °C from powders synthesized by a mechanically induced self-sustaining reaction (MSR) process. Four different composites were characterized using high-resolution electron microscopic techniques, in both scanning (SEM, HRSEM) and transmission (TEM, HRTEM, ED, EDS and EELS) modes and using an energy filtered technique (EFTEM) associated with electron energy loss spectroscopy (EELS). The microcharacterization showed that the ceramic phase with an *fcc*-cubic structure displayed a short-range order in many crystals detected by diffuse scattering in the ED patterns. This was possibly due to a sequence of C, N, and vacancies of both atoms along certain directions in the structure. On the other hand, even though the binder phase was introduced as metal in the reaction process, it was formed by Ni–Ti or Co–Ti known intermetallic compounds ($NiTi_2$, Ni_3Ti, and Co_3Ti). An unknown Ni–Ti intermetallic structure with a Ni:Ti ratio close to 2:1 was only found in one of the synthesized composites and displayed a cubic structure with a lattice parameter, a, of about 8.7 Å.

Physical and geotechnical properties of clay phyllites
Garzon, E; Sanchez-Soto, PJ; Romero, E
Applied Clay Science, 48 (2010) 307-318
DOI: 10.1016/j.clay.2009.12.022

An experimental programme is presented with the aim of characterising - from physical, microstructural and geotechnical perspectives - the main properties of compacted clay phyllites. These clay phyllites are widely used as waterproofing material for roofs in the Alpujarra (Andalusia, Spain), as sealing liners in irrigation ponds, and as core material of small earthen zoned dams. An exhaustive physical-characterisation programme on the powder fraction has been followed using X-ray fluorescence (XRF), X-ray diffraction (XRD), transmission electron microscopy (TEM), scanning electron microscopy (SEM), chemical analysis by energy dispersive X-ray spectroscopy (EDX), thermal analysis, particle-size distribution analysis, consistency limits, and density of solid particles. From a microstructural standpoint, mercury intrusion porosimetry (MIP) tests, as well as nitrogen-adsorption tests, were carried out to characterise the pore network and surface area of the material in both natural and compacted states. The geotechnical characterisation programme on the compacted material was focused on the water-permeability and water-retention properties, the volume change on soaking (swelling or collapse), the compressibility on loading, the shear-strength properties, and the mechanical-penetration properties. In this way, an important physical and hydro-mechanical data base is provided, which could help in evaluating the suitability for using this material in a wide range of earthen constructions (liners, road subgrades, embankments, core material in zoned dams). It has been found that the material contains illite, chlorite and quartz as the main components, and feldspar, iron oxide and interstratified illite-smectite as minor ones. Despite the presence of active clay minerals, the compacted material did not display an important swelling on soaking at low stresses, as a consequence of its low specific surface and low water-retention ability. The material exhibited good compaction properties and, consequently, low water permeability plus a stiff response on loading. Nevertheless, despite the low porosity attained on the dry-side compaction, the material underwent some collapse on soaking at stresses greater than 100 kPa.

Mechanochemical preparation of $BaTiO_3$-Ni nanocomposites with high dielectric constant

Pedro E. Sánchez-Jiménez, Luis A. Pérez-Maqueda, María J. Diánez, Antonio Perejón and José M. Criado

Composite Structures, 92 (2010) 2236-2240

DOI: 10.1016/j.compstruct.2009.08.011

A mechanochemical procedure is proposed for an easy preparation of a $BaTiO_3$-Ni composite in a single step. $BaTiO_3$ and Ni powders available in the market are mixed by dry ball milling producing a decrease of particle size and an evenly distribution of both phases. In the sintered pellets the nickel particles are homogeneously distributed into the $BaTiO_3$ matrix and isolated from others Ni particles. The dielectric constant of the composite is considerably higher than that of the barium titanate. Moreover, the temperature of the ferroelectric <-> paraelectric transition of the $BaTiO_3$-Ni composite here prepared is much lower than the one of the pure $BaTiO_3$ single phase.

Spark Plasma Sintering of Ultrafine TiC_xN_{1-x} Powders Synthesized by a Mechanically Induced Self-Sustaining Reaction

Amparo Borrell, Adolfo Fernández, Ramón Torrecillas, José M. Córdoba, Miguel A. Avilés, Francisco J. Gotor
Journal of the American Ceramic Society, 93 (2010) 2252-2256
DOI: 10.1111/j.1551-2916.2010.03735.x
High-purity, nanometer-sized titanium carbonitride powders, TiC_xN_{1-x}, were obtained with a mechanically induced self-sustaining reaction (MSR) in a high-energy planetary ball mill from a mixture of titanium and different carbon precursors under a nitrogen atmosphere. A promising method for developing dense TiC_xN_{1-x} materials is the coupling of MSR with the spark plasma sintering (SPS) technique. The powders were sintered at different temperatures to provide a completely dense monolithic ceramic (> 99% theoretical density). In this work, the influence of the carbon precursor and SPS treatment on the material microstructures were studied, and the main mechanical properties of the end material were evaluated.

Study of the Dehydroxylation-Rehydroxylation of Pyrophyllite

Jose L. Perez-Rodriguez, Adrian Duran, Pedro E. Sánchez Jiménez, Maria L. Franquelo, Antonio Perejón, Jose Pascual-Cosp and Luis A. Pérez-Maqueda
Journal of the American Ceramic Society, 93 (2010) 2392-2398
DOI: 10.1111/j.1551-2916.2010.03750.x - (c) 2010 The American Ceramic Society

Pyrophyllite is a raw material of significant interest due to its large number of applications. Most of these applications require a thermal transformation of pyrophyllite; this thermal transformation implies the release of structural OH groups and the formation of new phases. In this paper, we report on the dehydroxylation of pyrophyllite and the reversibility of the process. A value of 224 +/- 16 kJ/mol for the dehydroxylation of pyrophyllite was obtained. In addition, it was observed that the partially or totally dehydroxylated pyrophyllite suffered a partial reversible rehydroxylation when cooled to room temperature. This rehydroxylation was substantiated by thermogravimetric measurements, while infrared spectroscopic studies showed that, during the rehydroxylation, the intensity of the OH band at 3675 cm-1 increased as two new bands at 3690 and 3702 cm-1 appeared. This rehydroxylation process was heavily influenced by the particle size of the pyrophyllite. Thus, smaller particles (< 1 µm) showed a larger rehydroxylation percentage (about 12%), while the larger ones (20-40 µm) showed a smaller percentage (about 1.6%). The extent of rehydroxylation also depended on the dehydroxylation temperature and reached a maximum value at 750 degrees C.

The Multistep Nature of the Kaolinite Dehydroxylation: Kinetics and Mechanism

Andres Ortega, Manuel Macías, Francisco J. Gotor
Journal of the American Ceramic Society, 93 (2010) 197-203
DOI: 10.1111/j.1551-2916.2009.03328.x

The thermal dehydroxylation of kaolinite has been reexamined using small sample weights, a homogeneous particle size distribution and high-vacuum conditions in order to reduce the influences of heat and mass-transfer phenomena. The controlled rate thermal analysis (CRTA) technique, which was specially developed to minimize the pressure and temperature gradients through the sample, was employed to carry out meaningful kinetic experiments. Two advanced isoconversional methods, the Vyazovkin and the Galwey methods, were used complementarily to determine the dependence of the activation energy on the degree of conversion. For this purpose, the Vyazovkin method has been adapted to CRTA experiments. It was demonstrated that there are at least two different stages, revealing the multistep nature of this reaction. The activation energy for the first step, which is assigned to nucleation and the growth of nuclei, decreases from 100 to 75 kJ/mol. The second stage corresponds to a diffusion process and the activation energy rises to 120 kJ/mol because of the metakaolinite formation, which closes the interlamellar channels and leaves isolated patches of kaolinite from which the water escapes with difficulty.

Mechanosynthesis of $Hf_{1-x}Zr_xB_2$ Solid Solution and $Hf_{1-x}Zr_xB_2$/SiC Composite Powders
Miguel A. Avilés, José M. Córdoba, María J. Sayagués, María D. Alcalá, and Francisco J. Gotor´
Journal of the American Ceramic Society, 93 (2010) 197-203
DOI: 10.1111/j.1551-2916.2009.03484.x - (c) The American Ceramic Society

The synthesis of solid solutions in the HfB_2-ZrB_2 system was conducted by mechanically induced self-sustaining reaction (MSR) processes under an inert atmosphere from elemental mixtures of Hf, Zr, and B. The stoichiometry of the $Hf_{1-x}ZrxB_2$ solid solution phase was controlled by adjusting the Hf/Zr/B atomic ratio in the starting mixture. Composite materials with SiC were achieved by adding the required amount of SiC to the Hf/Zr/B reactant mixture. The presence of up to 20 vol% of SiC did not inhibit the MSR process. Longer milling times were required to ignite the mixture. Small amounts of the refractory phases ZrC or HfC were observed in the composite powders. The chemical composition, structure, and microstructure of products were studied by X-ray diffraction, scanning and transmission electron microscopy, electron diffraction, and energy-dispersive X-ray spectroscopy. This complete characterization confirmed the formation of P6/mmm hexagonal diboride phases with a submicrometric microstructure. The determination of the chemical composition and lattice parameters ascertained the formation of solid solutions with good chemical homogeneity in the HfB_2-ZrB_2 system.

Identification of cellulose fibres belonging to Spanish cultural heritage using synchrotron high resolution X-ray diffraction
Herrera, L.K., Justo, A., Duran, A., de Haro, M. C. Jimenez, Franquelo, M.L., Perez Rodríguez, J.L.
Applied Physics A-Materials Science & Processing, 99 (2010) 391-398
DOI: 10.1007/s00339-010-5626-z

A complete characterisation of fibres used in Spanish artwork is necessary to provide a complete knowledge of these natural fibres and their stage of degradation. Textile samples employed as painting supports on canvas and one sample of unprocessed plant material were chosen for this study. All the samples were investigated by synchrotron radiation X-ray diffraction (SR-XRD). Flax and cotton have the Cellulose I structure. The values of the crystalline index (CI) were calculated for both types of fibres. The structure of Cellulose IV was associated with the unprocessed plant material. The information obtained by SR-XRD was confirmed by laboratory techniques including scanning electron microscopy (SEM) and Fourier transform infrared spectroscopy (FTIR).

A thermal study approach to roman age wall painting mortars

A. Durán, L.A. Pérez-Maqueda, J. Poyato and J.L. Perez-Rodriguez

Journal of thermal Analysis and Calorimetry, 99 (2010) 803-809

DOI: 10.1007/s10973-009-0667-2

Roman ancient mortars have been widely studied, in connection with both diagnosis and application required for restoring. Thermoanalytical experiments performed on mortars from Pompeii and Herculaneum provided a very good understanding of the technology employed. The mortars from Pompeii were obtained by the proper mixing of lime and marble grains while mortars of Herculaneum by lime and silicates compounds. The position of the endothermic peak of calcite decomposition showed important variations in the different samples studied, which was assigned to the different crystallinity and particle sizes. Experiments under CO2 flow confirmed the presence of magnesium calcium carbonates.

Nonisothermal calorimetric study of the precipitation processes in a Cu-1Co-0.5Ti alloy

Donoso, E; Zuniga, A; Dianez, MJ; Criado, JM

Journal of Thermal Analysis and Calorimetry, 100 (2010) 975-980

DOI: 10.1007/s10973-009-0642-y

The precipitation processes in a Cu-1.0 at.%Co-0.5 at.%Ti (Cu-1.5 at.%Co2Ti) alloy were studied using differential scanning calorimetry (DSC), transmission electron microscopy (TEM), and microhardeness measurements. The analysis of the calorimetric curves from room temperature to 900 K shows the presence of two exothermic reactions attributed to the formation of CoTi and Co2Ti particles in the copper matrix. On the basis of enthalpy calculations, it was found that the decomposition begins with the precipitation of CoTi, followed by the formation of Co2Ti particles. The activation energies calculated using the modified Kissinger method were lower than the ones corresponding to diffusion of cobalt and titanium in copper. Kinetic parameters were obtained by a convolution method based on the Johnson-Mehl-Avrami (JMA) formalism. The values obtained for the parameter n were indicative of a particle nucleation process from preexistent nuclei. Microhardness measurements and TEM micrographs confirmed the formation of the mentioned phases.

Hydraulic structures of the Roman Mithraeum house in Augusta Emerita, Spain

M.D. Robador, J.L. Perez-Rodriguez and A. Duran

Journal of the Archaeological Science, 37 (2010) 2426-2432

DOI: 10.1016/j.jas.2010.05.003

This paper deals with some of the hydraulic structures of Augusta Emerita (Merida, Spain), specifically those found in the Mithraeum House. In particular, we describe and characterise the hydraulic mortars and coatings of the viridarium water channel. The recipient of the channel was covered with two hydraulic mortars and a finishing coating. Hydrated lime was used as binder. Calcite grains with different morphology have been observed in the mortars studied. The siliceous aggregate was composed of quartz, mica and feldspars. Ceramic fragments, which were added to the mortar to improve its hydraulic properties, were composed of quartz, mica, iron oxides, anorthite and an amorphous phase; aluminium-iron silicates were used as raw materials for their manufacture. We discuss the interactions between the hydrated lime and the surface of the ceramics in the mortars.

Variscite source and source analysis: testing assumptions at Pico Centeno (Encinasola, Spain)

Carlos P. Odriozola, J.A. Linares-Catela, and V. Hurtado-Pérez
Journal of the Archaeological Science, 37 (2010) 3146-3157
DOI: 10.1016/j.jas.2010.07.016

The analysis of trade and their implications for understanding social interaction is a major research question of prehistoric research in Europe. Variscite is a rare mineral that offers an excellent opportunity to study trade and exchange patterns in prehistoric Europe through proveniencing of source material. In this paper we discuss the exploitation and exchange of variscite at Pico Centeno mining district during the Copper Age. XRF, XRD, and FTIR analyses of the mineral recovered at Pico Centeno mining district during archaeological survey provides a baseline mineral signature for the source and sub-sources, which were then compared to other Iberian sources and to 44 green beads from 8 megalithic tombs from two different regions, in order to test 'provenance postulate' and distribution models. Mineral sampled during survey at Pico Centeno mining district turned out to be pure variscite phases, while extremely varied for the studied green beads: variscite, muscovite, talc or chlorite. On testing 'provenance postulate' we have focused on compositional comparison of Pico Centeno's variscite with reference from various geological sources of Western Europe. We found that the concentrations of trace elements do not allow us to establish the origin of the beads, as traditionally claimed, due to the strong natural variability on minor and trace elements of the sources. Instead we found after FTIR analysis, that different proportions of phosphate species, which results in P/Al ratios higher than 1, arose during the genesis of the variscite deposits and resulted from the associated pH and nature of the host-rocks, modifying the concentrations of PO43−, H2PO4− and HPO42−. Thus, the P/Al atomic ratio should be an indication of provenance as it is established during mineral genesis. This issue has not been addressed in any of the other studied sources where this ratio seems to be ≈1.

Determination of pigments and binders in Pompeian wall paintings using synchrotron radiation - High-resolution X-ray powder diffraction and conventional spectroscopy-chromatography

Duran, A; De Haro, MCJ; Perez-Rodriguez, JL; Franquelo, ML; Herrera, LK; Justo, A
Archaeometry, 52 (2010) 286-307
DOI: 10.1111/j.1475-4754.2009.00478.x

The employment of synchrotron techniques complemented by conventional laboratory systems has allowed us to deepen and improve our knowledge of Roman wall painting procedures. The palette identified in wall paintings from Pompeii and Herculaneum from the second century bc includes goethite, hematite, cinnabar, glauconite, Egyptian blue, and other components such as calcite and aragonite. Proof of the use of organic binders is provided by FTIR and PY-GC/MS. Therefore, the possibility of the use of 'a secco' techniques cannot be ruled out. Pigments in wall paintings are usually found in small percentages and conventional X-ray diffractometers do not detect them. Synchrotron radiation - high-resolution X-ray powder diffraction has allowed identification with only a few micrograms of sample.

Microscopic and spectroscopic techniques for the study of paper supports and textile used in the binding of hispano-arabic manuscripts from Al-Andalus: A transition model in the 15th century

Espejo, T; Duran, A; Lopez-Montes, A; Blanc, R
Journal of Cultural Heritage, 11 (2010) 50-58
DOI: 10.1016/j.culher.2009.01.007 - (C) 2009 Elsevier Masson SAS

This work focuses on the study of paper and textiles used in the binding of a series of manuscripts that share some specific characteristics that lead us to speculate on the possibility of a transitional codicological typology from the Arabic to the Christian book in Al-Andalus during the 15th century. The books we analyzed belong to the collection of the Historical Archive of Malaga, the Archive of Sacromonte Abbey, in Granada, the School of Arabic Studies and the Library of RP. Escolapios, also in Granada. Paper physical study was performed by microscopic and spectroscopic techniques. A routine and objective method, Fourier Transform Infrared (FIR) spectroscopy, was employed and proved to be a useful technique for the characterization of cellulosic fibres, main component of paper from the boards and the envelope flap pasteboards, and the fabric lining from the cover. The results of our research will help us to date, identify and study the evolution of the techniques, proving that the materials and innovations of the Italian paper manufacturing processes were perfectly known in the south of modern day Spain, before the Christian Reconquest.

Seville City Hall Chapter Room ceiling decoration

Duran, A; Robador, MD; de Haro, MCJ; Herrera, LK; Gimena, P; Perez-Rodriguez, JL
Materiales de Construcción, 60 (2010) 83-95
DOI: 10.3989/mc.2010.45107

The present article describes a chemical and physical study of the colour, chemical composition and mineral phases of the decorative materials in the Seville City Hall Chapter House ceiling. The findings showed that the inner most layer of material, calcite, was covered with white lead, in turn concealed under a layer of gilded bole. The ceiling underwent re-gilding, also over bole, due in all likelihood to wear on the original gold leaf. In the nineteenth century, the entire ceiling with the exception of the inscriptions was whitewashed with calcite and white lead. Silver was employed on King John I's sword (coffer 27). Gold leaf was used to adorn the royal attributes:

crowns, belts, sceptres, swords and rosary beads. The high reliefs were likewise gilded. The pigments identified on the ceiling adornments included azurite, malachite, vermilion and gas black. A lime and ground dolomite mortar was used throughout.

Microstructural characterization of copper based alloys produced by reactive milling
Palma, R; Sepulveda, A; Zuniga, A; Donoso, E; Dianez, MJ; Criado, JM
Revista de Metalurgia, 46 (2010) 197-205
DOI: 10.3989/revmetalm.0854

The micro and nanostructure of Cu-Al, Cu-V and Cu-Ti alloys produced by reactive milling were analyzed using X-ray diffraction (XRD) and transmission electron microscopy (TEM). Samples with different milling times (t = 0, 10, 20 and 30 h) were considered. The grain size, dislocation density and residual microstrain were evaluated form the XRD data using the Williamson-Hall and Klug-Alexander methods. The evolution of texture as a function of milling time was also studied using XRD. It was found, using TEM, that the grain size and dispersoid size were nanometric in all three alloys considered.

Sintering by SPS of ultrafine TiC_xN_{1-x} powders obtained using mechanically induced self sustaining reaction
Borrell, A; Fernandez, A; Torrecillas, R; Cordoba, JM; Aviles, MA; Gotor, FJ
Boletín de la Sociedad Española de Cerámica y Vidrio, 49 (2010) 357-360

In this work high purity and nanometer character titanium carbonitride TiCxN1-x powders were obtained by mechanically induced self sustaining reaction (MSR) in a high-energy planetary ball mill, from a mixture of titanium with graphite or carbon nanofiber (CNFs) in a nitrogen atmosphere. A promising method for developing these materials is the coupling of the MSR with SPS sintering technique. The product is sintered at 1400 degrees C and 1700 degrees C, obtaining a completely dense monolithic ceramic (>99% t.d). In this work, the influence of SI'S treatment and carbon precursor on material microstructures was studied and the main mechanical properties of the end material were evaluated.

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

High temperature mechanical properties of Ti(C,N)-Co-Mo_2C cermets
A. Gallardo-López, A. Morales-Rodríguez, A. Domínguez-Rodríguez, J. M. Córdoba, M. A. Avilés and F. J. Gotor
Key Engineering Materials, 423 (2010) 83-88

High-temperature plastic deformation of fine-grained Y-doped $BaCeO_3$ polycrystals.
C. Vaquero-Aguilar, C. Real, M. Jiménez-Melendo

J.Physics: conference series, 240 (2010) 012032

Elemental, molecular and mineralogical characterization of polychromes in the Oratory Room of Granade's Madrash (Spain)
Julia Romero-Pastor, J.; Duran, A.; Rodriguez-Navarro, A.;Sebastian, E.; Cardell, C.
MACLA, 13 (2010) 185-186

Ciencia y tecnología al servicio del arte
Durán, A.
Cuadernos de Divulgación Científica y Encuentros con la Ciencia, CicCartuja. D.L. SE-7339-2010

LIBROS Y OTRAS PUBLICACIONES / BOOKS AND OTHER PUBLICATIONS

Types of mortars in wall paintings by the "Older Villach's Workshop" and their followers (15th Century)
Kriznar A., Ruiz-Conde A. and Sánchez-Soto P.J
En: Proceedings of the Second Historic Mortars Conference 2010, RILEM TC203-RHM (Ed. J. Válek, C. Groot and J.J. Hughes) RILEM Publications s.a.r.l.., Bagneux 2010, pp. 673-681

Análisis del proceso de restauración del órgano Cavaillé-Coll de la Iglesia de la Merced de Burgos
A. Justo-Estebaranz, L.K. Herrera, A. Durán, B. Sigüenza, M.C. Jiménez de Haro, O. Laguna, A. Justo
En: Restaurar la Memoria -ARPA 2008". Castilla y León Regional Government, Valladolid Local Government 2010, pp. 471-476

Estudio de los materiales en el manuscrito XVI del Archivo de la Abadía del Sacromonte de Granada
López Montes, A.Mª.; María del Rosario Blanc García, Mª.R.; Durán, A.
En: El comentario al libro de las frases (Sharh Al-Yumal) de Ibn Al-Fajjar Al Bayri, Junta de Andalucía (Consejería de Cultura), D.L. GR 1234-2010
ISBN: 978-84-9959-0288

CONGRESOS Y REUNIONES INTERNACIONALES / INTERNATIONAL CONGRESS AND MEETINGS

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

Trilateral Meeting on Clays
8-10 junio [Sevilla, España]
José Luis Pérez Rodríguez [Miembro del Comité Científico]

10th European Symposium on Thermal Analysis and Calorimetry ESTAC-10
22-27 agosto [Rotterdam, Holanda]
José Manuel Criado Luque [Miembro del Comité Científico]

III Conferencia Internacional. Trabajadores Autonómicos de la Cultura. Profesión y Actuación en el Patrimonio
10 Octubre [Sevilla, España]
José Luis Pérez Rodríguez [Miembro del Comité Científico]

COMUNICACIONES EN CONGRESOS Y REUNIONES / COMMUNICATIONS IN CONGRESS AND MEETINGS

Trilateral Meeting on Clays
6-11 junio [Madrid, España]

"Porous materials from acid leached ground vermiculite", Pérez-Rodríguez, J.L., Maqueda, C., Subrt, J. Poster

8th ECNP Short Course on Nanostructured Polymers and Nanocomposites
28-30 abril [Madrid, España]

"Kinetic Study of the Thermal Degradation of Polystyrene-Clay Nanocomposite", P.E. Sánchez-Jiménez, A. Perejón, J.M. Criado, L.A. Pérez-Maqueda. Poster

5th Mid-European Clay Conference

25-29 agosto [Budapest, Hungria]

“Intercalation and dynamics of hydrated Fe2+ in the vermiculites from Santa Olalla and Ojén (Spain)”, Lerf, A., Wagner, F.E., Poyato, J. & Pérez-Rodríguez, J.L. Comunicación oral

“Thermal behaviour of ground and unground leached vermiculite”, Perez-Rodriguez, J.L., Maqueda, C., Subrt, J. & Balek, V. Poster

“Sonication induced reduction reactions of the Ojén (Andalucía, Spain) vermiculite”, Poyato, J., Pérez-Rodríguez, J.L., Lerf, A. & Wagner, F.E. Poster

SEM and microanalysis in the study of historical technology materials and conservation (SEM 2010)

9-10 septiembre [Londres, Reino Unido]

“Characterization of pigments mixture and minority components in Murillo’s paintings by EDX”, M.C. Jiménez de Haro, M.L. Franquelo, A. Duran, J.L. Perez-Rodriguez. Poster

9th Solid State Chemistry 2010

11-15 septiembre [Praga, República Checa]

“Soft synthesis and crystallographic characterization of magnesium based double alkaline earth carbonates”, Diánez M.J., Criado, J.M., Pérez-Maqueda L.A. and Perejón A. Poster

“Study of the mechanism of Cu-Zn mechanical alloying. A new “mechanochemical equilibrium” phase diagram”, José Manuel Criado Luque. Poster

17th International Microscopy Congress

19-24 septiembre [Rio de Janeiro, Brasil]

“Study by XRD and HRTEM of the Mechanism of Phase Transition of Anatase during the Titania Grinding”, M.J. Diánez, J.M. Criado, L. A. Pérez- Maqueda, J. Subrt, N. Murafa, A. Perejón and E. Donoso. Poster

“Precipitation Processes in a Quasi-Binari Cu-1.5Co2Ti Alloy”, E. Donoso, M.J. Diánez and J.M. Criado. Poster

Second Historic Mortars Conference (HMC 2010)

22-24 septiembre [Praga, República Checa]

“Types of mortars in wall paintings by the “Older Villach’s Workshop” and their followers (15th Century)”, Kriznar A., Ruiz-Conde A. and Sánchez-Soto P.J. Poster

30th IPH Congress of International Paper Historians

7-10 octubre [Angouleme, Francia]

“Materials characteristics of the collection of Arabic manuscripts of the Granada province archive based on the scientific analysis of components”, I. Lazarova, A. Duran, M.C. Jimenez, T. Espejo. Comunicación oral

CONGRESOS Y REUNIONES INTERNACIONALES / INTERNATIONAL CONGRESS AND MEETINGS

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

50 Congreso de la Sociedad Española de Cerámica y Vidrio (SECV)

22-27 octubre [Madrid, España]
Pedro José Sánchez Soto [Miembro del Comité Organizador]

COMUNICACIONES EN CONGRESOS Y REUNIONES / COMMUNICATIONS IN CONGRESS AND MEETINGS

Jornadas sobre investigación y conservación del patrimonio cultural NET-HERITAGE, CSIC

17-18 marzo [Madrid, España]
“Ciencia y cultura escrita”, T. Espejo, A. Duran, et al. Poster

Congreso de la Sociedad Española de Mineralogía 2010

13-16 septiembre [Madrid, España]

"Elemental, molecular and mineralogical characterization of polychromes in the Oratory Room of Granada's Madrasah (Spain)", J. Romero-Pastor, A. Duran, A. Rodriguez-Navarro, E. Sebastian, C. Cardell. Poster

50 Congreso de la Sociedad Española de Cerámica y Vidrio (SECV)

27-29 octubre [Madrid, España]

"Estudio de la transformación cromática y de fases de un pigmento de limonita procedente de Perú", Romero P., González J.C., Bustamante A., Arjonilla M., Ruiz A. y Sánchez-Soto P.J. Poster

"Caracterización química, mineralógica y microtextural de talco procedente de Fuengirola (Málaga)", Raigón M., Sanromán C., Garzón E., Pascual J., Ruiz-Conde A. y Sánchez-Soto P.J. Poster

"Evolución térmica y propiedades cerámicas de un talco industrial que contiene clorita", Sánchez-Soto P.J., Ruiz-Conde A., Garzón E., Morales L., Pascual J. y Raigón M. Poster

FORMACION / TRAINING

TESIS DOCTORALES/ DOCTOR DEGREE THESIS

Título:	**Sistemas técnicos de producción cerámica en el Guadiana Medio durante la Edad del Cobre**
Autor:	Carlos P. Odriozola Lloret
Directores:	Victor Hurtado Pérez y Angel Justo Erbez
Calificación:	Sobresaliente "Cum Laude"
Centro:	Universidad de Sevilla

FORMACIÓN DE GRADUADOS / MASTER DEGREE THESIS

Título:	**Desarrollo de Cermets basados en soluciones sólidas mediante la aplicación de la técnica MSR**
Autor:	Ernesto Chicardi Augusto
Directore:	Francisco J. Gotor Martínez

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

PROYECTOS DE INVESTIGACIÓN / RESEARCH PROJECTS

Nueva tecnología de chips fotónicos sensores basados en colorantes orgánicos fabricados mediante procesos integrables a escala de oblea de silicio New Photonic systems on a chip based on dyes for sensor applications scalable at wafer fabrication (PHODYE)

Código/Code: STREP 033793 Action Line: IST-2005-2.5.1
Periodo/Period: 01-10-2006 / 31-10-2010
Organismo Financiador/Financial source: Unión Europea
Importe total/Total amount: 2.200.000 € (360.000 €)
Investigador responsable/Research head: Barranco, A. (Coord.)
Componentes/Research group: Glez-Elipe, A.R., Cotrino, J., Espinós, J.P., Yubero, F.

RESUMEN / ABSTRACT

PHODYE es un proyecto multidisciplinar para el desarrollo de una nueva tecnología de sensores basada en la integración de películas nanométricas de colorantes orgánicos en estructuras fotónicas (anillos resonadores, redes de difracción de orden cero, etc.). Los dispositivos a desarrollar deben mostrar una respuesta óptica diferente, en función de cambios en el medioambiente que los rodea, que puedan medirse cuantitativamente y reconocerse por simple inspección visual del dispositivo. Las películas activas se preparan mediante una nueva técnica de polimerización que emplea plasmas remotos y que ha sido desarrollada en el ICMSE muy recientemente. Esta técnica es compatible con los procesos de fabricación optoelectrónicos. Las películas activas reaccionan a cambios en la concentración de ciertos gases, temperatura e irradiación UV mostrando cambios de color y de emisión fluorescente. Esta tecnología puede permitir la fabricación de chips sensores con capacidad de detección simultánea de varios parámetros medioambientales, que puedan integrarse fácilmente en dispositivos de medida, redes de comunicaciones informáticas, etc. El bajo coste de fabricación en serie de estos dispositivos y su compatibilidad con ambientes peligrosos, donde el empleo de dispositivos eléctricos está contraindicado, los hace una solución única para un amplio rango de aplicaciones (hogares, hospitales, industria, ambientes explosivos, tráfico, etc.)

En PHODYE participa un consorcio formado por cuatro centros de investigación y tres compañías, cubriendo toda la cadena tecnológica que va desde la investigación en ciencia de materiales hasta la fabricación del dispositivo final. Así, los procesos de fabricación, empaquetado de las estructuras, prueba y validación son asumidos por los distintos socios del proyecto.

PHODYE is a multidisciplinary project that aims to develop a new sensing and recognition technology based on the integration of dye thin films with photonic structures (subwavelenghts gratings, resonant rings, etc). The developed devices should yield a distinct optical response according to changes in the environment that can be easily measured by a photonic chip or recognized directly by the human eye. The dye thin films will be prepared by a new plasma polymerization procedure that is fully compatible with the integrated optoelectronic technology. The dye

molecules in the films react to changes in the concentration of certain gases and/or in temperature or UV radiation by a change of their absorption/fluorescence properties.

Such devices could be used as stand alone disposable low cost sensors with multidetection capabilities. Devices based on photonic resonant structures can be easily integrated into measurement devices, communication networks etc. Their low cost and their compatibility to dangerous environments where electricity cannot be used make them a unique solution for a wide range of application areas (homes, hospitals, industry, explosives, traffic, etc.). PHODYE is intended by a consortium that integrates four research centres and three SME's companies that cover all the scientific-technological chain from the materials to the final devices. Manufacturing, packaging, testing and validation are also afforded by the partners.

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.

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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.

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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.

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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Propiedades foto-funcionales de capas delgadas de materiales óxido modificados mediante dopado y por infiltración de componentes ópticamente activos (PROMODO) Photo-functional PROperties of oxide thin films MOdified by DOping and by infiltration with optically active components (PROMODO)

Código/Code:	MAT2007-65764 (Plan Nacional)
Periodo/Period:	31-12-2007 / 31-12- 2010
Organismo Financiador/Financial source:	Ministerio de Educación y Ciencia
Importe total/Total amount:	242.000 €
Investigador responsable/Research head:	Cotrino Bautista, J.
Componentes/Research group:	González-Elipe, A.R., Espinós, J.P., Yubero, F., Barranco, A.

RESUMEN / ABSTRACT

Este proyecto persigue desarrollar una nueva familia de capas finas de óxido óptimamente activas capaces de desarrollar propiedades fotofuncionales útiles para una serie de aplicaciones en campos tales como óptica, aprovechamiento de la energía solar y sensores. Se prepararán capas finas de óxidos (TiO2, SiO2, ZnO) mediante diferentes métodos (PECVD, PVD, plasmas a presión atmosférica) con la característica de poseer una micro/nanostructure muy bien controladas. Estas capas se modificarán mediante la infiltración de componentes óptimamente activos (colorantes y partículas metálicas) o, en el caso del TiO2 y ZnO, mediante dopado con ciertos aniones (nitrógeno, fluor, carbono) que provocan que estos óxidos semiconductores puedan ser activos a la parte visible del espectro electromagnético. Las propiedades fotofuncionales de las capas finas preparadas se verificarán en relación con su aplicación como recubrimientos fotocrómicos, sensores de gases ópticos, elementos basados en la resonancia plasmón, capas con propiedades de mojado controlables mediante iluminación y celdas fotoelectroquímicas. El control de la micro/nanostructura de las láminas delgadas se conseguirá mediante la utilización de estrategias específicas para su crecimiento. Se realizará un estudio de los mecanismos de crecimiento conducentes a la obtención de una micro/nanoestructura dada mediante la utilización de los conceptos de la Teoría de Escalado Dinámico. Ello debe permitir el desarrollo de estrategias a medida para la síntesis de las capas que actúan como huésped. Igualmente, para los procesos PECVD, se estudiarán y modelizarán las condiciones del plasma con el objetivo de conseguir una descripción completa de los mecanismos de crecimiento para, llegado el caso, modificarlos si ello se precisa para las aplicaciones deseadas.

This project aims at the development of a new family of oxide thin films optically active that are able to develop a series of properties useful for several photo-functional applications in fields like optics, solar energy recovery or sensors. Oxide thin films (TiO2, SiO2, ZnO) with very well controlled microstructure will be prepared by different methods (PVD, PECVD and atmospheric pressure plasmas) and modified by infiltration with optically active components (dyes and metal particles) or, for TiO2 and ZnO, by doping with some anions (i.e., nitrogen, fluor or carbon)

suitable to make these oxide semiconductors active to the visible light of the electromagnetic spectrum. The photo-functional properties of the prepared thin film materials will be tested for their applications as photochromic coatings, optical gas sensors, plasmon resonant behavior, films with light-controlled wetting properties and photoelectrochemical cells. A strict control of the micro and nano-structure of the thin films will be achieved by using specific strategies for their growth. Analysis of the growing mechanisms leading to the different micro/nano-structures by means of the concepts of the Dynamic Scale Theory will permit a tailored synthesis of the host thin films. Similarly, the plasma conditions will be conveniently monitored and modeled to get a full description of the growing mechanisms and, in its case, be able to modify it if required for the desired applications.

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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:	Díaz Cuenca, A.
Componentes/Research group:	Ramiro Gutiérrez, M.L.

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 SiO2-CaO-P2O5 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 SiO2-CaO-P2O5 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

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

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:	Cotrino Bautista, J.
Componentes/Research group:	Gónzalez-Elipe, A.R., Yubero, F.

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 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.

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

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.

Nanotecnología de capas delgadas mixtas nanoestructuradas con funcionalidad óptica y fotónica Nanotechnology of nanostructured composite thin films with optical and photonic functionalities

Código/Code:	TEP2275 (Proyecto de Excelencia)
Periodo/Period:	01-06-2007 / 31-5- 2010
Organismo Financiador/Financial source:	Junta de Andalucía
Importe total/Total amount:	192.536,3 €
Investigador responsable/Research head:	Espinós Manzorro, J.P.
Componentes/Research group:	Cotrino, J., Caballero, A., González-Elipe, A.R., Holgado, J.P., Yubero, F., Barranco, A.

RESUMEN / ABSTRACT

Este proyecto persigue la obtención de capas nanoestructuradas (nanocomposites) con funcionalidad óptica, fotónica o mixta fotónica/magnética y fotónica/electrónica, de interés para el desarrollo de nuevos sistemas de comunicación fotónica, láseres, capas magnetoópticas, capas camaleónicas o recubrimientos autolimpiables. El armazón o base de las capas mixtas finales la constituirán materiales transparentes bien conocidos, de propiedades ópticas y fotoquímicas de interés, como el SiO_2 y el TiO_2, que actuarán como retículos huésped, y cuya estructura de poros (nano, micro o mesoporos) puede ser controlada a nivel nanométrico. En estos poros se incorporarán elementos activos (partículas metálicas con comportamiento plasmón (Ag, Au), puntos cuánticos semiconductores (CdS), moléculas fluorescentes (Rhodaminas,…), u óxidos magnéticos (CrO_2), que conferirán a los materiales finales su comportamiento multifuncional requerido. El control nanométrico de la microestructura es crítico, tanto en lo que respecta al retículo huesped: volumen y distribución de tamaño y conectividad de poros, tamaño, cristalinidad y orientación de los nanocristales …; como de la fase "alojada" en él: composición, tamaño y forma en el supuesto de nano-partículas, o estado de agregación (monómeros-dímeros) y naturaleza química del centro de adsorción, en el caso de moléculas fluorescentes. Para conseguir este elevado control microestructural, se ensayarán y en su caso desarrollarán nuevos métodos de depósito del retículo huesped y de infiltrado de la fase alojada en sus poros.

This project is focused to the syntesis of nano structured thin films (nanocomposites) with optical, photonic, electro-optical and magneto-optical capabilities. These new materials could be of great interest for the development of photonic communication devices, lasers, magneto-optical devices, self cleaning surfaces, etc. The frame and scaffold of these thin films will be made of transparent oxide thin films, with well defined optical and photochemical properties, such as columnar sculptured thin films of SiO_2 and TiO_2, whose porosity (nano, meso and microporous) can be tailored. Photoactive nano particles (Au and Ag particles with narrow distribution of sizes and shapes, semiconductor quantum dots of CdS), magnetic nanoparticles (CrO_2) and fluorescent dye organic molecules (Rhodamines,…) will fill up the porous or be adsorbed on the oxide surfaces, leading to a composite material with several capabilities. The fine control of the nanostructure of the films is essential to reach the pursued property. To this aim, host materials will be made of nanocrystals with well defined size, crystallinity, porous structure and porous volume. Also guest nanoparticles will have to be made with precise composition, particle size and shape… and, for the case that fluorescent dye molecules are used, the aggregation state (monomers, dimers, …) of the adsorbate, and the chemical nature of the adsorption site will have to be tailored. New methods for the syntesis and deposition of films and their subsequent infiltration with active nanoparticles and molecules will be tested and developed.

Avances en recubrimientos tecnológicos para aplicaciones decorativas Avances in technological coatings for decorative applications

Periodo/Period: 2007 / 2010
Organismo Financiador/Financial source: Centro para el Desarrollo Tecnológico Industrial (Programa CENIT) Ministerio de Industria (Contratos: INDO, S.A., TORRECID, DECOART)
Investigador responsable/Research head: González-Elipe, A.R.
Componentes/Research group: Cotrino, J. Espinós, J.P., Yubero, F., Gil-Rostra , L.

RESUMEN / ABSTRACT

El objetivo principal del proyecto ART-DECO es el desarrollo de nuevos procesos de recubrimiento decorativo, de cerámicas, vidrios, metales y polímeros, de aplicación en sectores de escala como construcción, automoción o electrodomésticos, mediante tecnologías avanzadas, que permitan una rápida implementación industrial. Estos procesos deben ser medio-ambientalmente limpios y deben sustituir, en los próximos años, a los tratamientos actuales con alto grado de contaminación (recubrimientos galvánicos, cromo hexavalente, etc.).

Los procesos puestos a punto en el proyecto ART-DECO, deben permitir el desarrollo de nuevos recubrimientos decorativos que, además, proporcionen nuevas funcionalidades específicas aportando soluciones y ventajas tecnológicas en distintas aplicaciones como:

- Recubrimientos óptico-decorativos para la industria del vidrio y óptica.
- Apantallamiento para aumento de la compatibilidad electromagnética.
- Recubrimientos biocidas y antialergénicos.
- Recubrimientos decorativos de alta resistencia al desgaste y a la erosión.

Como objetivo secundario, la ejecución del proyecto ART-DECO permitirá la creación de un polo de competencia en tratamientos y tecnologías avanzadas de superficies, donde los socios del proyecto, apoyados por los organismos de investigación, ejerzan un liderazgo a nivel mundial en el desarrollo y utilización de los nuevos procesos de recubrimiento.

The main objective of the ART-DECO Project is the development of new processes for the deposition of decorative processes on ceramics, glass, metals and polymers of application in large scale sectors such as building, automotive or household devices. The idea is to develop advanced technologies that enable a rapid transfer to the industry. The processes must environmentally clean and substitute during the next years the treatments used at present that imply a high degree of environmental aggression (galvanic coatings, hexavalent chromium, etc.).

The processes developed in the ART-DECO project must enable the development of decorative coatings that also act by supplying new specific functionalities to the materials that, in this way, will present new solutions and technological advantages in several applications such as:

- Opto-decorative coatings for the glass and optic industries
- Shielding for electromagnetic compatibility
- Biocide and anti-alergic coatings
- Decorative coatings with a high resistance against wear

Another objective of ART-DECO is to create a network of expertise in advanced treatment technologies of surfaces, where the partners of the project, supported by their research organisations, are able to create a world leadership in the development and use of these new processes of coating.

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.

OTROS PROYECTOS / OTHER PROJECTS

Nanomateriales ópticos: síntesis y propiedades de nanopartículas luminiscentes basadas en fluoruros de tierras raras con potenciales aplicaciones biomédicas

Código/Code:	Intramural
Oganismo Financiador/Financial source:	CSIC
Importe total/Total amount:	30.000 €
Investigador responsable/Research head:	Nuria O. Nuñez Álvarez

Procesos fundamentales en el crecimiento de películas delgadas nanoestructuradas crecidas mediante pulverización catódica reactiva

Código/Code:	Intramural
Oganismo Financiador/Financial source:	CSIC
Importe total/Total amount:	30.000 €
Investigador responsable/Research head:	Alberto Palmero Acebedo

Transferencia / Technological Transfer

Convenios y Contratos / Contracts and Agreements

CPV: Concentración fotovoltaica – Estudio sobre materiales y su aplicación en sistemas modulares de alta concentración fotovoltaica

Periodo/Period: 3-3-2008 / 3-3-2010
Organismo Financiador/Financial source: Abengoa Solar New Tecnologies, S.A.
Investigador responsable/Research head: Agustín R. González-Elipe
Componentes/Research group: José Cotrino Bautista, Juan Pedro Espinós Manzorro, Angel Barranco Quero

Acuerdo CSIC y Abengoa Solar New Technologies S.A., para el desarrollo de un estudio de la generación de hidrógeno en fluidos caloportadores

Periodo/Period: 18-01-2009 / 18-01-2010
Organismo Financiador/Financial source: Abengoa
Investigador responsable/Research head: Agustín R. González-Elipe
Componentes/Research group: Francisco Yubero, Juan Pedro Espinós, Angel Barranco, José Cotrino, Alberto Palmero , Enrique Jiménez, M. Carmen Jiménez de Haro

Integration of one-dimensional photonic crystals composed of nanoparticles into dye-sensitised solar cells

Periodo/Period: 30-06-2009 / 31-12-2010
Organismo Financiador/Financial source: Nanologica AB
Investigador responsable/Research head: Hernán Ruy Miguez
Componentes/Research group: Mauricio Calvo Roggiani, Silvia Colodrero

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: Manuel Ocaña Jurado
Componentes/Research group: Hernán R. Míguez García, Mauricio Calvo Roggiani, 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

Validación de la tecnología "Thin Film" fotovoltáica

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

Desarrollo de recubrimientos tecnológicos para aplicaciones decorativas

Periodo/Period: 29-3-2007 / 31-12-2010
Organismo Financiador/Financial source: Industrias de Óptica, S.A. (INDO), Decorados Artísticos Españoles, S.L. (DECOART, TORRECID)
Investigador responsable/Research head: Agustín R. González-Elipe
Componentes/Research group: Juan Pedro Espinós, Francisco Yubero, José Cotrino, Angel Barranco, Alberto Palmero

PATENTES / PATENTS

Procedimiento para obtener un espejo de Bragg flexible y espejo de Bragg obtenido por dicho procedimiento

Inventores: Hernán R. Míguez García, Mauricio E. Calvo Roggiani
Ámbito Geográfico: Internacional
PATENTE SOLICITADA. N. de solicitud: PCT/ES10/070044
Fecha Solicitud/Licencia: 26/enero/2010
Entidad Titular: CSIC

Procedimiento de marcaje, encriptación, etiquetado y codificación óptica

Inventores: Angel Barranco, Agustín R. González-Elipe, Juan R. Sánchez Valencia, Francisco J. Aparicio, Iwona K. Blaszczyk-Lezak, Miguel Holgado Bolaños, Rafael Casquel del Campo, José L. Ocaña Moreno, Carlos Molpeceres Alvarez, Juna J. García-Ballesteros, Miguel Morales Furió
Ámbito Geográfico: Internacional
PATENTE SOLICITADA. N. de solicitud: App.PCT/ES10/070054. Pub.WO2010089439
Fecha Solicitud/Licencia: 26/enero/2010
Entidad Titular: CSIC

PUBLICACIONES / PUBLICATIONS

ARTÍCULOS PUBLICADOS EN REVISTAS SCI / PAPERS IN SCI JOURNALS

Gallium Arsenide Infiltration of Nanoporous Multilayers: A Route to High-Dielectric-Contrast One-Dimensional Photonic Crystals
Sánchez-Sobrado, O., Thomas, K., Povey, I., Pemble, M.E., Míguez, H.
Small, **6** (2010) 1283–1287
DOI: 10.1002/smll.200902190

Periodic multilayers of wide photonic bandgap and high reflectance in the visible and near infrared regions are fabricated. Optical properties show that reflectance intensities close to 90% are reached for stacks of only six layers, as well as gap-to-midgap ratios of 50%. The optical response of the hybrid ensemble can be accurately tuned through the number of infiltration cycles performed.

Conformal growth of organic luminescent planar defects within artificial opals
Francisco J. Aparicio, Gabriel Lozano, Iwona Blaszczyk-Lezak, Angel Barranco and Hernán Míguez
Chem. Mater., **22** (2010) 379–385
DOI: 10.1021/cm902819x

Herein, we present the result of combining, for the first time, the techniques of colloidal self-assembly and plasma-enhanced chemical vapor deposition to create a novel, high-quality, purely organic active photonic crystal structure of controlled optical properties. We show a fast, reliable, and accurate procedure to introduce two-dimensional luminescent organic defect layers within artificial polystyrene opals via a versatile room-temperature remote plasma deposition process. This method is gentle enough to allow highly conformal growth on polystyrene microspheres without altering their morphology or the ordered arrangement that they form. The luminescent organic layer behaves both as an optical dopant, causing the opening of transmission windows within the forbidden frequency interval of the lattice, and as an optically active material, whose emission can be tailored by the photonic environment.

Flexible, Adhesive, and Biocompatible Bragg Mirrors Based on Polydimethylsiloxane Infiltrated Nanoparticle Multilayers
Mauricio E. Calvo and Hernán Míguez
Chem. Mater., **22** (2010) 3909–3915
DOI: 10.1021/cm1001016

Herein we present a series of self-standing, flexible, and biocompatible optical interference filters obtained through infiltration and polymerization of an elastomer (polydimethylsiloxane) in a porous Bragg mirror prepared by alternating deposition of layers of TiO_2 and SiO_2 nanoparticles. The method proposed yields the uniform filling of the nanopores of the multilayer by the polymer, which allows lifting off the hybrid structure as long as the ensemble is cooled to temperatures below the glass transition of the polymer. This multifunctional material combines the optical properties of the periodic nanoporous multilayer and the structural and physicochemical characteristics of polydimethylsiloxane. Experimental demonstrations of their potential use as flexible and adhesive UV-protecting filters, as well as of light, highly-efficient conformal back reflectors to enhance the efficiency of photovoltaic devices are provided.

Improved wear performance of ultra high molecular weight polyethylene coated with hydrogenated diamond like carbon

J.A. Puértolas, V. Martínez-Nogués, M.J. Martínez-Morlanes, M.D. Mariscal, F.J. Medel, C. López-Santos and F. Yubero
Wear, 269 (2010) 458-465
DOI: 10.1016/j.wear.2010.04.033

Hydrogenated diamond like carbon (DLCH) thin films were deposited on medical grade ultra high molecular weight polyethylene (UHMWPE) by radio frequency plasma enhanced chemical vapor deposition. The DLCH coating thicknesses ranged from 250 to 700 nm. The substrates were disks made of UHMWPEs typically used for soft components in artificial joints, namely virgin GUR 1050 and highly crosslinked (gamma irradiated in air to 100 kGy) UHMWPEs. Mechanical and tribological properties under bovine serum lubrication at body temperature were assessed on coated and uncoated polyethylenes by means of nano-hardness and ball-on-disk tests, respectively. Morphological features of the worn surfaces were obtained by confocal microscopy and scanning electron microscopy. This study confirms an increase in surface hardness and good wear resistance for coated materials after 24 h of sliding test compared to uncoated polyethylene. These results point out that to coat UHMWPE with DLCH films could be a potential method to reduce backside wear in total hip and knee arthroplasties.

Excitation transfer mechanism along the visible to the Near-IR in rhodamine J-heteroaggregates

Juan R. Sánchez-Valencia, Johann Toudert, Lola González-García, Agustín R. González-Elipe and Angel Barranco
Chem. Commun., **46** (2010) 4372–4374
DOI: 10.1002/smll.200902190

An enhanced fluorescent emission of the dye Rhodamine 800 in the Near-IR is observed in the presence of other xanthene dye molecules (RhX) when they are hosted in different matrices due to the formation of a new type of fluorescent J-heteroaggregates. This enhanced emission of the acceptor occurs despite the low spectral overlapping and the low quantum yield of Rh800.

TiO_2–SiO_2 one-dimensional photonic crystals of controlled porosity by glancing angle physical vapour deposition

Lola González-García, Gabriel Lozano, Angel Barranco, Hernán Míguez and Agustín R. González-Elipe
J. Mater. Chem., **20** (2010) 6408–3915
DOI: 10.1039/C0JM00680G

Herein we present a synthetic route to attain porous one-dimensional photonic crystals of high optical quality. The method employed, based on the alternate deposition of TiO2 and SiO2 porous layers by glancing angle physical vapour deposition, yields a highly accessible interconnected pore network throughout the entire multilayer structure. Furthermore, it allows a strict control over the average size and density of the interstitial sites, which results in the precise tuning of the refractive index of the individual layers and thus of the optical response of the ensemble. The controlled environmental response of the multilayer is confirmed by the optical monitoring of the infiltration of liquids of different refractive index.

Versatility and multifunctionality of highly reflecting Bragg mirrors based on nanoparticle multilayers
Olalla Sánchez-Sobrado, Mauricio E. Calvo and Hernán Míguez
J. Mater. Chem., **20** (2010) 8240–8240
DOI: 10.1039/C0JM01508C

The use of both supported and flexible self-standing nanoparticle-based one dimensional photonic crystal films as effective frequency selective filters in the UV-vis-NIR is herein evaluated. The requirements to achieve a flat spectral response at the desired frequency range are analyzed and a synthetic route to realize materials with such properties presented. Strict control over the structural parameters yields multilayers in which the opening or closing of higher order photonic band gaps can be devised, thus leading to films capable of blocking the UV and NIR ranges simultaneously. Furthermore, the physico-chemical properties of the mirror can be modified to yield either moisture-repelling or, on the contrary, environmentally responsive optical filters. These materials present a great potential to be used as versatile and multifunctional optical elements.

Effect of surface roughness and sterilization on bacterial adherence to ultra-high molecular weight polyethylene
Kinnari, T.J., Esteban, J., Zamora, N., Fernandez, R., López-Santos, C., Yubero, F., Mariscal, D., Puertolas, J.A., Gomez-Barrena, E.
Clinical Microbiology and Infection, **16** (2010) 1036–1041
DOI: 10.1111/j.1469-0691.2009.02995.x

Sterilization with ethylene oxide (EO) and gas plasma (GP) are well-known methods applied to ultra-high molecular weight polyethylene (UHMWPE) surfaces in the belief that they prevent major material changes caused by gamma irradiation. However, the influence of these surface sterilization methods on bacterial adherence to UHMWPE is unknown. UHMWPE samples with various degrees of roughness (0.3, 0.8 and 2.0 µm) were sterilized with either GP or EO. The variations in hydrophobicity, surface free energy and surface functional groups were investigated before and after sterilization. Sterilized samples were incubated with either Staphylococcus aureus or Staphylococcus epidermidis in order to study bacterial adherence to these materials. Fewer bacteria adhered to UHMWPE after sterilization with EO than after sterilization with GP, especially to the smoothest surfaces. No changes in chemical composition of the UHMWPE surface due to sterilization were observed using X-ray photoemission spectroscopy analysis. The decreased bacterial adherence to UHMWPE found at the smoothest surfaces after sterilization with EO was not directly related to changes in chemical composition. Increased bacterial adherence to rougher surfaces was associated with increased polar surface energy of EO-sterilized surfaces.

Band Gap Narrowing versus Formation of Electronic States in the Gap in N−TiO_2 Thin Films

P. Romero-Gómez, Said Hamad, J.C. González, A. Barranco, J. P. Espinós, J. Cotrino, and A.R. González-Elipe

J. Phys. Chem. C, **114** (2010) 22546–22557

DOI: 10.1021/jp104634j

N-containing TiO_2 thin films with different amounts of nitrogen have been prepared by plasma enhanced chemical vapor deposition (PECVD) by using different titanium precursors without (titanium isopropoxide, TTIP) and with (tetrakis diethylamino titanium, TDEAT and tetrakis dimethylamino titanium, TDMAT) nitrogen in their structures and different N_2/O_2 ratios as plasma gas. For low/high content of nitrogen, Ti−NO- and/or Ti−N-like species have been detected in the films by X-ray photoelectron spectroscopy (XPS). Their optical behavior is characterized by a red shift of their absorption edge when Ti−N species are a majority, and by an unmodified edge with localized absorption states in the gap when only Ti−NO-like species are present in the film. The experimental results have been interpreted by calculating the density of states of model systems consisting of a 2 × 2 × 3 repetition of the anatase unit cell. This basic structure incorporates nitrogen defects in either substitutional or interstitial lattice positions that are considered equivalent to the Ti−N- and Ti−NO-like species detected by XPS. To simulate the effect of, respectively, a low or a high concentration of nitrogen, calculations have been carried out by placing two nitrogen defects either in separated or in nearby positions of the anatase structure. The computational analysis reveals that the defects have different stabilization energies and confirm that an edge shift of the valence band is induced by the substitutional nitrogen centers, as observed when a high concentration of Ti−N species becomes incorporated into the films. In agreement with the experimental results, when only Ti-NO like species are detected by XPS, no band gap narrowing is obtained by the calculations that predict the appearance of localized electronic states in the gap. The fact that only these latter films present water wetting angle photoactivity when irradiated with visible light supports that the presence of Ti−NO-like species is a required condition for visible light photoactivity.

Theoretical Analysis of the Performance of One-Dimensional Photonic Crystal-Based Dye-Sensitized Solar Cells

Gabriel Lozano, Silvia Colodrero, Ophelie Caulier, Mauricio E. Calvo and Hernán Míguez

J. Phys. Chem. C, **114** (2010) 3681–3687

DOI: 10.1021/jp9096315

A simple analytical model that allows designing one-dimensional photonic crystal based dye sensitized solar cells of optimized performance, accounting for the actual optical features of the device, is herein presented. Based on the theoretical description of the effect of coupling such Bragg mirrors to the light harvesting electrode, recently reported experimental values of the spectral dependence of incident photon to current conversion efficiency attained for such structures are fairly reproduced and rationalized. A thorough analysis of them in terms of the interplay between the effect of the electrode thickness and the characteristics of the Bragg reflection, such as intensity, spectral position, and width, is provided. Predictions on the maximum enhancement factors expected for realistic structures are also presented.

Tunable Nanostructure and Photoluminescence of Columnar ZnO Films Grown by Plasma Deposition

Pablo Romero-Gómez, Johann Toudert, Juan R. Sánchez-Valencia, Ana Borrás, Angel Barranco, and Agustín R. González-Elipe
J. Phys. Chem. C, **114** (2010) 20932–20970
DOI: 10.1021/jp103902u

Nanoporous ZnO thin films presenting a tunable nanostructure and photoluminescence (PL) were grown by plasma enhanced vapor deposition on surface oxidized Si substrates. These films consist of c-axis oriented wurtzite ZnO nanocolumns whose topology, crystallinity, and PL can be tuned through the substrate temperature (varied in the 300−573 K range) and the nature of the plasma assistance (pure O_2, O_2/Ar, O_2/H_2, or O_2/N_2 mixture). In particular, these processing parameters influence the intensity of the UV and visible PL bands of the films, related to excitonic and defective radiative transitions, respectively. Increasing the substrate temperature enhances the UV PL and rubs out the visible PL due to the increase of grain size and the removal of interstitial defects. Additional tuning of the intensity ratio between the UV and visible bands can be done by controlling the film thickness. A decrease of the UV PL is observed when the films go thicker, an effect that is likely to be linked to the microstructure of the films rather than to their crystallinity that is improved upon increasing of the film thickness, as seen from PL spectroscopy and XRD measurements. Indeed, a gradient of stress, decreasing from the substrate to the surface, is evidenced and related to a concentration gradient of interstitial defects. The drawbacks of the thickness effect, which prohibits growing thick films with a high optical quality, can be bypassed by growing the films in a O_2/H_2 plasma.

Air- and Light-Stable Superhydrophobic Colored Surfaces Based on Supported Organic Nanowires

Borras, A., Gröning, P., Sanchez-Valencia, J.R., Barranco, A., Espinos, J.P., Gonzalez-Elipe, A.R.
Langmuir, **26** (2010) 1487–1492
DOI: 10.1021/la903701j

In this work, we report on a new type of superhydrophobic material consisting of supported organic nanowires prepared by vacuum deposition. Different intensely colored surfaces with water contact angles as high as 180° can be fabricated depending on the composition, morphology, and density of the nanowires. These surfaces are stable in air and under intense light irradiation. The wettability properties of coatings made of metalloporphyrins and metallophthalocyanines nanowires as well as other heterostructured binary and open core@shell nanowires are studied.

One-Step Dry Method for the Synthesis of Supported Single-Crystalline Organic Nanowires Formed by pi-Conjugated Molecules

Borras, A; Groning, O; Aguirre, M; Gramm, F; Groning, P
Langmuir, **26** (2010) 5763–5771
DOI: 10.1021/la1003758

We present for the first time a general vacuum process for the growth of supported organic nanowires formed by pi-conjugated molecules, including metalloporphyrins, metallophthalocyanines, and perylenes. This methodology consists on a one-step physical vapor deposition of the pi-conjugated molecules. The synthesis is carried out at controlled temperature on substrates with tailor morphology which allows the growth or organic nanowires in the form of squared nanofibers and nanobelts. The study of the nanowires by electron diffraction and HRTEM combining with the results of a theoretical analysis of the possible arrangement of the pi-conjugated molecules along the nanowires reveals that the nanowires show a columnar structure along the fiber axis consisting of pi-stacked molecules having a herringbone-like arrangement. The formation of these nanowires on different substrates demonstrates that the growth mechanism is independent of the substrate chemical composition. An in-depth phenomenological study of the Formation of the nanowires drives us to propose a growth mechanism based on a crystallization process. Furthermore, the growth method allows the fabrication of two particular ID heterostructures: binary and open core@shell organic nanofibers.

Wetting Properties of Polycrystalline TiO_2 Surfaces: A Scaling Approach to the Roughness Factors

Ana Borras, Agustín R. González-Elipe
Langmuir, **26** (2010) 15875–15882
DOI: 10.1021/la101975e

This work presents a thorough study on the wettability of polycrystalline anatase TiO_2 thin films prepared at 250 °C in a microwave plasma enhanced chemical vapor deposition (MW-PECVD) reactor with Ar/O_2 plasmas. Anatase polycrystalline thin films with different microstructures, textures, and surface roughness were obtained as a function of their thickness. The water contact angle of the samples was analyzed within the assumptions of the Wenzel, Cassie, and Miwa models to ascertain the effect of roughness and other surface heterogeneities on their characteristic parameters. The roughness factors defined in the different models were calculated from the atomic force microscopy (AFM) images of the films for two different observation scales within the premises of the dynamic scaling theories. The obtained results indicate that the wetting angle of an equivalent flat anatase surface with a value of 82° can only be properly estimated for observation scales of 5 × 5 μm^2 and using the Miwa model. The analysis of the UV induced hydrophilization of the surface state of the anatase films and the posterior recovery of the partially hydrophobic character of these surfaces in the absence of UV photons suggest a clear dependence of the light induced wettability on their texture and size of crystalline domains.

Environmentally responsive nanoparticle-based luminescent optical resonators

Sánchez-Sobrado, O., Calvo, M.E., Núñez, N., Ocaña, M., Lozano, G., Míguez, H.
Nanoscale, 2 (2010) 936-941
DOI: 10.1039/b9nr00338j

In this work, we demonstrate that optical resonators built using all-nanoparticle-based porous building blocks provide a responsive multifunctional matrix, totally different emission spectra being attained from the same embedded luminescent nanophosphors under varying environmental conditions. We show a clear correlation between modifications in the ambient surroundings, the induced changes of the resonant modes, and the resulting variations in the emission response. The method is versatile and allows nanophosphors of arbitrary shape to be integrated in the cavity. By precise control of the spectral features of the optical resonances, luminescence is strongly modulated in selected and tuneable wavelength ranges. Applications in the fields of sensing and detection are foreseen for these materials.

Tilt angle control of nanocolumns grown by glancing angle sputtering at variable argon pressures

J.M. García-Martín, R. Alvarez, P. Romero-Gómez, A. Cebollada and A. Palmero
Appl. Phys. Letters, **97** (2010) 173103 (3 pages)
DOI: 10.1063/1.3506502

We show that the tilt angle of nanostructures obtained by glancing angle sputtering is finely tuned by selecting the adequate argon pressure. At low pressures, a ballistic deposition regime dominates, yielding high directional atoms that form tilted nanocolumns. High pressures lead to a diffusive regime which gives rise to vertical columnar growth. Monte Carlo simulations reproduce the experimental results indicating that the loss of directionality of the sputtered particles in the gas phase, together with the self-shadowing mechanism at the surface, are the main processes responsible for the development of the columns.

Non-destructive depth compositional profiles by XPS peak-shape analysis

López-Santos, M.C., Yubero, F., Espinós, J.P., González-Elipe, A.R.
Analytical and Bioanalytical Chemistry, **396** (2010) 2757-2768
DOI: 10.1063/1.3506502

The measured peak shape and intensity of the photoemitted signal in X-ray photoelectron spectroscopy (XPS) experiments (elastic and inelastic parts included) are strongly correlated, through electron-transport theory, with the depth distribution of photoelectron emitters within the analyzed surface. This is the basis of so-called XPS peak-shape analysis (also known as the Tougaard method) for non-destructive determination of compositional in-depth (up to 6-8 nm) profiles. This review describes the theoretical basis and reliability of this procedure for quantifying amounts and distributions of material within a surface. The possibilities of this kind of analysis are illustrated with several case examples related to the study of the initial steps of thin-film growth and the modifications induced in polymer surfaces after plasma treatments.

Surface nanostructuring of TiO_2 thin films by high energy ion irradiation
P. Romero-Gomez, A. Palmero, T. Ben, J. G. Lozano, S. I. Molina, and A. R. González-Elipe
Phys. Rev. B, **82** (2010) 115420 (8 pages)
DOI: 10.1103/PhysRevB.82.115420

The effects of a high ion dose irradiation on TiO_2 thin films under different conditions of temperature and ion nature are discussed. We have shown that anatase TiO_2 thin films irradiated with N^+ ions at room temperature develop a typical microstructure with mounds and voids open to the surface whereas irradiations at 700 K generate a surface pattern of well-ordered nanorods aligned with the ion beam. The formation of these patterns is caused by the simultaneous effect of ion irradiation near the film surface and a film temperature favoring the structural mobilization of the defective network of the material. To explain these phenomena, a qualitative model has been proposed and further tested by irradiating the TiO_2 thin films with F^+ and S^+ ions under different conditions. The obtained results demonstrate that ion irradiation techniques enable the formation of tilted nanorod surface patterns with lengths of about 100 nm on anatase TiO_2 thin films.

Anomalous group velocity at the high energy range of a 3D photonic nanostructure
Muriel Botey, Jordi Martorell, Luis A. Dorado, Ricardo A. Depine, Gabriel Lozano, and Hernán Míguez
Optics Express, **18** (2010) 15682-15690
DOI: 10.1364/OE.18.015682

We report on a study of electromagnetic waves propagation in thin periodically ordered photonic nanostructures in the spectral range where the light wavelength is on the order of the lattice parameter. The vector KKR method we use allows us to determine the group index from finite photonic structures including extinction providing confirmation of recently emerged results. We show that for certain frequencies the group velocity of opal slabs can either be superluminal or approach zero depending on the crystal thickness and the unavoidable presence of losses. In some cases, group velocity can be negative. Such behavior can be clearly attributed to the finite character of the three-dimensional structure and reproduces previously reported experimental observations. Calculations show that contrary to the predictions of extraordinary group velocity reductions for infinite periodic structures, the group velocity of real opals may exhibit strong fluctuations at the high energy range. Hence, a direct identification between the calculated anomalous group velocities, for an actual opal film, and the predicted propagating low dispersion modes for an ideal infinite ordered structure seems difficult to establish.

Tunable In-Plane Optical Anisotropy of Ag Nanoparticles Deposited by DC Sputtering onto SiO_2 Nanocolumnar Films

Juan Ramon Sánchez-Valencia, Johann Toudert, Ana Borras, Carmen López-Santos, Angel Barranco, Inés Ortega Feliu and Agustin Rodriguez González-Elipe

Plasmonics, **5** (2010) 241–250

DOI: 10.1007/s11468-010-9139-6

This work reports an easy-to-handle method for growing two-dimensional assemblies of Ag nanostructures presenting a tunable in-plane optical anisotropy. Ag is deposited by DC sputtering in an Ar plasma at room temperature onto bundled nanocolumnar SiO_2 thin films grown by glancing angle physical vapor deposition. In contrast with previously reported processes involving the grazing angle deposition of the metal, DC sputtering is performed at normal incidence. By varying the deposition angle of SiO_2 and the Ar pressure, it was possible to tune the deposited amount of Ag and thus the topology of the Ag deposit from isolated spherical Ag nanoparticles with isotropic optical properties to strongly dichroic Ag nanostripes oriented along the bundling direction of the SiO_2 nanocolumns. Based on simple calculations taking into account the shadowing effects during metal deposition, it is proposed that the width and shape of the tip of the bundled SiO_2 nanocolumns influence significantly the metal local atom flux arriving to them and thus the final structure of the deposit.

A transparent TMPyP/TiO_2 composite thin film as an HCl sensitive optochemical gas sensor

Manuel Cano, Pedro Castillero, Javier Roales, José M. Pedrosa, Stuart Brittle, Tim Richardson, Agustín R. González-Elipe and Angel Barranco

Sensors and Actuators B: Chemical, **150** (2010) 764-769

DOI: 10.1016/j.snb.2010.07.059

Tetracationic porphyrin (TMPyP) molecules were incorporated into an optically transparent TiO2 thin film, prepared by Glancing Angle Physical Vapour Deposition (GAPVD), by simple infiltration (at pH 6.4). The preparation of optically transparent TMPyP/TiO_2 composite thin films provides a method for the integration of the porphyrin molecules into photonic devices for direct monitoring of gases. Previously, UV–visible and fluorescence spectral techniques have been used to study the reversible protonation of TMPyP in aqueous solution. The optical spectrum of TMPyP shows an intense Soret band at 423 nm with a 22 nm red shift upon protonation by HCl. The experimental conditions for monitoring the concentration of HCl gas by absorption spectroscopy have been optimized. The maximum absorbance change was observed at the Soret band wavelength. A selected temperature of 80 °C and a 300 s recovery period were found to be the optimum operating parameters (response time t50 = 16.8 ± 0.7 s). The composite with smaller surface concentration of TMPyP (Γ = 0.3 × 10−9 mol cm−2) presented the best detection limit (0.1 ppm). The response of the composite sensor was highly stable for several months.

Structure of Glancing Incidence Deposited TiO_2 Thin Films as Revealed by Grazing Incidence Small-Angle X-ray Scattering

González-García, L., Barranco, A., Páez, A.M., González-Elipe, A.R., García-Gutiérrez, M.C., Hernández, J.J., Rueda, D.R., Ezquerra, T.A., Babonneau, D.

ChemPhysChem., **11** (2010) 2205-2208

DOI: 10.1002/cphc.201000136

For the first time, grazing incidence small-angle X-ray scattering (GISAXS) analysis is used to characterize the morphology of TiO_2 thin films grown by glancing angle physical vapor deposition (GLAD). According to cross-section scanning electron microscopy (SEM) images, the films consist of near isotilted TiO_2 columns of different length and width depending on film thickness. The obtained GISAXS patterns show a characteristic asymmetry with respect to the incidence plane, which is associated with the tilted geometry of the TiO_2 columns. The patterns also show the existence of two populations of columns in these GLAD-TiO_2 films. The population of the thinnest columns appears related to the first grown layer and is common for all the films investigated, while the second population of columns grows with the thickness of the films and has been related to wider columns formed by shadowing at the expense of the initially formed columns.

Uniform YF3:Yb,Er up-conversion nanophosphors of various morphologies synthesized in polyol media through an ionic liquid

Nuria O. Nuñez, Marta Quintanilla, Eugenio Cantelar, Fernando Cussó and Manuel Ocaña

Journal of Nanoparticle Research, **12** (2010) 2553-2565

DOI: 10.1007/s11051-009-9824-6

We describe a facile procedure for the synthesis at low temperature (120°C) of waterdispersible uniform YF3:Yb,Er up-conversion nanophosphors of various morphologies (rhombic and spheroidal) by homogeneous precipitation in polyol solutions containing different lanthanide salts and an ionic liquid (1-butyl, 2-methylimidazolium tetrafluoroborate) as fluoride source. It is shown that the shape of the obtained nanoparticles is mainly determined by the nature of both, the polyol and the lanthanide precursors, which also affects to their colloidal stability in water suspensions. These morphological differences are explained on the basis of a different mechanism of particle formation. The efficiency of the up-conversion processes in the synthesized rhombic and spheroidal nanoparticles is also comparatively analyzed and the observed differences are justified on the basis of the different impurities incorporated to the nanophosphors during their synthesis process.

Citrate mediated synthesis of uniform monazite LnPO4 (Ln=La, Ce) and Ln:LaPO4 (Ln=Eu, Ce, Ce+Tb) spheres and their photoluminescence

Nuñez, N.O., Liviano, S.R., Ocaña, M.

Journal of Colloid and Interface Science, **349** (2010) 484-491

DOI: 10.1016/j.jcis.2010.05.079

A simple method for the synthesis of spherical $LaPO_4$ (monazite) particles with narrow size distribution and tailored size in the 150-500nm range is reported. The procedure is based on a homogeneous precipitation process at low temperature (120°C) from solutions containing La3+, citrate and phosphate ions under a very restrictive set of experimental conditions, which involves the use of La nitrate, citric acid and phosphoric acid as precursors and ethylene glycol as solvent. The growth mechanism of the spheres was investigated aiming at explaining the differences in particle size and shape observed when varying the experimental conditions. The applicability of this method for the synthesis of spherical particles of other lanthanide (Ce,Tb,Eu) phosphates is also analyzed. Finally, it is shown that the developed procedure can be used to dope the lanthanum phosphate particles with lanthanide cations, which resulted in spherical phosphors as illustrated for the Eu-doped, Ce-doped and Ce, Tb codoped systems, whose luminescent properties are also evaluated.

Active and Optically Transparent Tetracationic Porphyrin/TiO_2 Composite Thin Films
Castillero, P., Sánchez-Valencia, J.R., Cano, M., Pedrosa, J.M. , Roales, J., Barranco, A., González-Elipe, A.R.
ACS Applied Materials and Interfaces, 2 (2010) 712-721
DOI: 10.1021/am900746q

Fluorescent tetracationic porphyrin (TMPyP) molecules have been incorporated into optically transparent TiO_2 thin films acting as a host material. The films, with a columnar structure and open pores, were prepared by electron evaporation at glancing angles (GAPVD). The open porosity of the films has been estimated by measuring a water adsorption isotherm with a quartz crystal monitor. TMPyP molecules were infiltrated in the host thin films by their immersion into water solutions at controlled values of pH. The state of the adsorbed molecules, the infiltration efficiency, and the adsorption kinetics were assessed by analyzing the optical response of the films by UV?vis absorption and fluorescence techniques. The infiltration efficiency was directly correlated with the acidity of the medium, increasing at basic pHs as expected from simple considerations based on the concepts of the point of zero charge (PZC) developed for colloidal oxides. By a quantitative evaluation based on the analysis of the UV spectra, the infiltration process has been described by a Langmuir type adsorption isotherm and an Elovich-like kinetics. The accessibility of the infiltrated molecules in the TMPyP/TiO_2 composite films is assessed by following the changes of their optical properties when exposed to the acid vapors and their subsequent recovery with time.

Surface Functionalization, Oxygen Depth Profiles, and Wetting Behavior of PET Treated with Different Nitrogen Plasmas
Carmen López-Santos, Francisco Yubero, José Cotrino and Agustín R. González-Elipe
ACS Applied Materials and Interfaces, 2 (2010) 980-990
DOI: 10.1021/am900746q

Polyethylene terephthalate (PET) plates have been exposed to different nitrogen containing plasmas with the purpose of incorporating nitrogen functional groups on its surface. Results with a dielectric barrier discharge (DBD) at atmospheric pressure and a microwave discharge (MW) at reduced pressure and those using an atom source working under ultrahigh vacuum conditions have been compared for N_2 and mixtures Ar + NH_3 as plasma gases. The functional groups have been monitored by X-ray Photoemission Spectroscopy (XPS). Nondestructive oxygen and carbon depth profiles for the plasma treated and one month aged samples have been determined by means of the nondestructive Tougaard's method of XPS background analysis. The surface topography of the treated samples has been examined by Atomic Force Microscopy (AFM), while the surface tension has been determined by measuring the static contact angles of water and iodomethane. It has been found that the DBD with a mixture of Ar+NH_3 is the most efficient treatment for nitrogen and amine group functionalization as determined by derivatization by reaction with chlorobenzaldehyde. It is also realized that the nitrogen functional groups do not contribute significantly to the observed increase in surface tension of plasma treated PET.

Evaluation of Different Dielectric Barrier Discharge Plasma Configurations As an Alternative Technology for Green C-1 Chemistry in the Carbon Dioxide Reforming of Methane and the Direct Decomposition of Methanol

Victor J. Rico, José L. Hueso, José Cotrino and Agustín R. González-Elipe

J. Phys. Chem. A, **114** (2010) 4009-4016

DOI: 10.1021/jp100346q

Carbon dioxide reforming of methane and direct decomposition of methanol have been investigated using dielectric barrier discharges (DBD) at atmospheric pressure and reduced working temperatures. Two different plasma reactor configurations are compared and especial attention is paid to the influence of the surface roughness of the electrodes on the conversion yields in the first plasma device. The influence of different filling gap dielectric materials (i.e., Al_2O_3 or $BaTiO_3$) in the second packed configuration has been also evaluated. Depending on the experimental conditions of applied voltage, residence time of reactants, feed ratios, or reactor configuration, different conversion yields are achieved ranging from 20 to 80% in the case of methane and 7−45% for the carbon dioxide. The direct decomposition of methanol reaches 60−100% under similar experimental conditions. Interestingly, the selectivity toward the production of hydrogen and carbon monoxide is kept almost constant under all the experimental conditions, and the formation of longer hydrocarbon chains or coke as a byproduct is not detected. The maximum efficiency yields are observed for the packed-bed reactor configuration containing alumina for both reaction processes (1 mol H_2 per kilowatt hour for dry reforming of methane and 4.5 mol H_2 per kilowatt hour for direct decomposition of methanol).

Angular dependence of the intensity of light beams diffracted by colloidal crystals

Gabriel Lozano, Javier E. Mazzaferri, Luis A. Dorado, Silvia Ledesma, Ricardo A. Depine, and Hernán Míguez

Journal of the Optical Society of America B: Optical Physics, 27 (2010) 1394-1399

DOI: 10.1364/JOSAB.27.001394

An experimental and theoretical analysis of the angular dependence of the diffracted light beams emerging from three-dimensional colloidal photonic crystals is herein presented.

Diffracted beams are identified according to their associated reciprocal-lattice vectors, and their intensities are obtained as a function of the zenithal and azimuthal incidence angles. Significant changes in the beam intensities are observed for large zenithal incidence angles as the azimuthal angle is varied. This phenomenon is related to the excitation of new resonant modes inside the photonic crystal which cannot be observed under normal incidence conditions.

Morphological evolution of pulsed laser deposited ZrO2 thin films

R. Álvarez, A. Palmero, L. O. Prieto-López, F. Yubero, J. Cotrino, W. de la Cruz, H. Rudolph, F.H.P.M. Habraken, and A. R. Gonzalez-Elipe
J. Appl. Phys., 107 (2010) 054311 (10 pages)
DOI: 10.1063/1.3318604

Morphological evolution of ZrO_2 thin films deposited during pulsed laser deposition of Zr in O_2 atmosphere has been experimentally studied at two different film deposition temperatures, 300 and 873 K. The roughness exponent, α, the growth exponent, β, the coarsening exponent, $1/z$, and the exponent defining the evolution of the characteristic wavelength of the surface, p, for depositions at 300 K amounted to $\beta = 1.0\pm0.1$, $\alpha = 0.4\pm0.1$, $1/z = 0.34\pm0.03$, and $p = 0.49\pm0.03$, whereas for depositions carried out at 873 K amounted to $\beta = 0.3\pm0.3$, $\alpha = 0.4\pm0.2$, and $1/z = 0.0\pm0.2$. Experimental error becomes important due to the flat morphology of the films inherent to the deposition technique. The change in the surface topography with the film temperature has been studied with the help of a simple Monte Carlo model which indicates the existence of two different growth regimes: a shadowing dominated growth, occurring at low temperatures, characterized by calculated values $\beta = 1.00\pm0.04$, $\alpha = 0.50\pm0.04$, $p = 0.46\pm0.01$, and $1/z = 0.35\pm0.02$ and a diffusion dominated growth that takes place at high temperatures as well as at low deposition rates, characterized by calculated values $\beta = 0.15\pm0.08$, $\alpha = 0.33\pm0.04$, and $1/z = 0.33\pm0.07$. The good agreement obtained between the experimental and simulated parameters is discussed within the frame of the general characteristics of the deposition method.

On the microstructure of thin films grown by an isotropically directed deposition flux

R. Alvarez, P. Romero-Gomez, J. Gil-Rostra, J. Cotrino, F. Yubero, A. Palmero, and A. R. Gonzalez-Elipe
J. Appl. Phys., 108 (2010) 064316 (7 pages)
DOI: 10.1063/1.3483242

The influence of isotropically directed deposition flux on the formation of the thin film microstructure at low temperatures is studied. For this purpose we have deposited TiO_2 thin films by two different deposition techniques: reactive magnetron sputtering, in two different experimental configurations, and plasma enhanced chemical vapor deposition. The obtained results indicate that films grown under conditions where deposition particles do not possess a clear directionality, and in the absence of a relevant plasma/film interaction, present similar refractive indices no matter the deposition technique employed. The film morphology is also similar and consists of a granular surface topography and a columnarlike structure in the bulk whose diameter increases almost linearly with the film thickness. The deposition has been simulated by means of a Monte Carlo model, taking into account the main processes during growth. The agreement between simulations and experimental results indicates that the obtained microstructures are a consequence of the incorporation of low-energy, isotropically directed, deposition particles.

Preparation and structural properties of YBCO films grown on GaN/c-sapphire hexagonal substrate

Š. Chromika, P. Gierlowski, M. Španková, E. Dobročka, I. Vávra, V. Štrbík, T. Lalinský, M. Sojková, J. Liday, P. Vogrinčič and J.P. Espinos
Applied Surface Science, 256 (2010) 5618-5622
DOI: 10.1016/j.apsusc.2010.03.035

Epitaxial YBCO thin films have been grown on hexagonal GaN/c-sapphire substrates using DC magnetron sputtering and pulsed laser deposition. An MgO buffer layer has been inserted between the substrate and the YBCO film as a diffusion barrier. X-ray diffraction analysis indicates a c-axis oriented growth of the YBCO films. Φ-scan shows surprisingly twelve maxima. Transmission electron microscopy analyses confirm an epitaxial growth of the YBCO blocks with a superposition of three a–b YBCO planes rotated by 120° to each other. Auger electron spectroscopy and X-ray photoelectron spectroscopy reveal no surface contamination with Ga even if a maximum substrate temperature of 700 °C is applied.

Improved wear performance of ultra high molecular weight polyethylene coated with hydrogenated diamond like carbon

Puertolas, JA; Martinez-Nogues, V; Martinez-Morlanes, MJ; Mariscal, MD; Medel, FJ; Lopez-Santos, C; Yubero, F
Wear, 269 (2010) 458-465
DOI: 10.1016/j.wear.2010.04.033

Hydrogenated diamond like carbon (DLCH) thin films were deposited on medical grade ultra high molecular weight polyethylene (UHMWPE) by radio frequency plasma enhanced chemical vapor deposition. The DLCH coating thicknesses ranged from 250 to 700 nm The substrates were disks made of UHMWPEs typically used for soft components in artificial Joints, namely virgin GUR 1050 and highly crosslinked (gamma irradiated in air to 100 kGy) UHMWPEs Mechanical and tribological properties under bovine serum lubrication at body temperature were assessed on coated and uncoated polyethylenes by means of nano-hardness and ball-on-disk tests, respectively Morphological features of the worn surfaces were obtained by confocal microscopy and scanning electron microscopy This study confirms an increase in surface hardness and good wear resistance for coated materials after 24 h of sliding test compared to uncoated polyethylene. These results point out that to coat UHMWPE with DLCH films could be a potential method to reduce backside wear in total hip and knee arthroplasties.

Determination of the decay rate constant for hepatocytes immobilized in alginate microcapsules

Aldo Leal-Egaña, Aránzazu Díaz-Cuenca, Augustinus Bader
Journal of Microencapsulation, 27 (2010) 86-93
DOI: 10.3109/02652040903050550

Primary mouse hepatocytes (between 10–250 cells per capsule) were immobilized within 1.0% w/v alginate microbeads. The textural properties of the alginate matrix were characterized and a full protocol based upon the measurement of the initial rate of Resazurin reduction was studied and standardized. Using this method, the decay rate constant (Kd = 0.45 ± 0.01 days−1) and the time in which the cell viability decreases in half (VI50 = 37 ± 0.7 h) have been measured. The method was compared with the analysis of cell vitality using Calcein A/M and Ethidium Homodimer I. Differences between the two methods were found in the viability profile due to the significant presence of double stained cells along the culture time. According to the author's knowledge, this is the first report of a systematic study and determination of the Kd value for immobilized hepatocytes, incorporating a wide range of cell concentrations within the alginate matrix.

Porous one-dimensional photonic crystal coatings for gas detection

Hidalgo, N., Calvo, M.E., Colodrero, S., Míguez, H.
IEEE Sensors Journal, 10 (2010) 1206-1211
DOI: 10.1109/JSEN.2010.2043525

Herein, we present an overview of recent progress on the development of different types of porous 1-D photonic crystal coatings which are optically responsive to gas pressure changes in the environment. Modification of the surrounding vapor pressure gives rise to adsorption and condensation phenomena within the porous networks of the photonic crystal building blocks, varying their refractive index and hence their optical features. This effect can be put into practice to precisely detect and monitor changes in the ambient through the spectral shift of either the photonic bandgap of the structure or of some other optical features. Our results demonstrate the potential of these optical coatings as new materials for gas sensing devices.

Synthesis, characterization, and photoactivity of $InTaO_4$ and $In_{0.9}Ni_{0.1}TaO_4$ thin films prepared by electron evaporation

Rico, VJ; Frutos, F; Yubero, F; Espinos, JP; Gonzales-Elipe, AR
Journal of Vacuum Science & Technology A, 28 (2010) 127-134
DOI: 10.1116/1.3273597

$InTaO_4$ and $In_{0.9}Ni_{0.1}TaO_4$ thin films have been prepared by electron evaporation of successive layers of the single oxide components and posterior annealing at T > 800 degrees C. The annealed thin films presented the monoclinic crystallographic structure typical of these mixed oxides. The electrical and optical behaviors of the films, assessed by C-V measurements, surface conductivity as a function of temperature, and UV-vis absorption spectroscopy, indicate that these oxides are wide band gap semiconductors with a variable dielectric constant depending on the annealing conditions. By reflection electron energy loss spectroscopy some electronic states have been found in the gap at an energy that is compatible with the activation energy deduced from the conductivity versus 1/T plots for these oxides. The photoactivity of these materials has been assessed by looking to the evolution of the wetting contact angle as a function of the irradiation time. All the films became superhydrophilic when irradiated with UV light, while the $In_{0.9}Ni_{0.1}TaO_4$ thin films also presented a small partial decrease in wetting angle when irradiated with visible photons.

Study of the morphology of NiO nanostructures grown on highly ordered pyrolytic graphite, by the Tougaard method and atomic force microscopy: a comparative study

I. Preda, L. Soriano, L. Alvarez, J. Méndez, F. Yubero, A. Gutiérrez, J. M. Sanz

Surface and Interface Analysis, 42 (2010) 869-873

DOI: 10.1002/sia.3222

We studied the morphology of the deposits of NiO grown on highly ordered pyrolytic graphite (HOPG), by means of inelastic peak shape analysis and atomic force microscopy. The results obtained by both techniques show an excellent agreement. The results indicate that NiO grows on HOPG by following the Stransky–Krastanov type of growth.

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

Towards a full understanding of the growth dynamics, optical response and crystalline structure of self-assembled photonic colloidal crystal films

G. Lozano, L.A. Dorado, R.A. Depine and H.R. Míguez

SPIE 7713, 771303 (2010)

Mesostructured thin films as photonic crystal building blocks for sensing applications

N. Hidalgo, M.E. Calvo and H.R. Míguez

SPIE 7713, 77131I (2010)

LIBROS Y OTRAS PUBLICACIONES / BOOKS AND OTHER PUBLICATIONS

Plasma Deposition of N-TiO2 thin films

P. Romero-Gómez, A. Barranco, J. Cotrino, J.P. Espinós, F. Yubero, A.R. González-Elipe

En: Industrial Plasma Technology. Applications from Environmental to Energy Technologies, 2010, pp. 349-356
Editorial Wiley, Weinhaim (Alemania)
ISSN: 978-3-527-32544-3

Ingeniería Tisular y Medicina Regenerativa Esquelética
J.Becerra, J.A. Andrades, L. Santos-Ruiz, M. Cifuentes, P.M. Arrabal, R. Visser, S. Claros, A. Diaz-Cuenca, P.Zamora, E. Guerado
En: Perspectivas en la Investigación con células troncales; Aspectos Científicos, Éticos, Sociales y Legales 2010, pp. 29-42
Editorial Comares, S.L. (Ed. M. Moreno)
ISSN: 978-84-9836-680-8

CONGRESOS Y REUNIONES INTERNACIONALES / INTERNATIONAL CONGRESS AND MEETINGS

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

SPIE, The International Society for Optics and Photonics
10 abril [Bruselas, Bélgica]
Hernán Míguez [Miembro del Comité Organizador]

12th Internationational Ceramic Congress
16-18 junio [Montecatini, Italia]
Manuel Ocaña [Miembro del Comité Científico]

11th European Vacuum and 6th European Topical Conference on Hard Coatings
20-24 septiembre [Salamanca, España]
Agustín R. González-Elipe [Miembro del Comité Científico]

COMUNICACIONES EN CONGRESOS Y REUNIONES / COMMUNICATIONS IN CONGRESS AND MEETINGS

International Workshop on Nanomedicine
23-26 marzo [Málaga, España]

“Synthesis of HA-nano-Organised silica materials with potential for bone tissue engineering”, M.L. Ramiro-Gutiérrez, J. Becerra, A. Díaz-Cuenca. Poster

Nanospain 2010

23-26 marzo [Málaga, España]

“Control of the aggregation state of Rhodamine 6G Dye Molecules adsorbed in porous columnar GAPVD thin films”, Juan Ramón Sánchez Valencia, Iwona Blaszczyk Lezak, Juan Pedro Espinós Manzorro, Agustín R. González-Elipe, Angel Barranco Quero. Poster

“Growth of organic luminescent planar defects within artificial opals”, Francisco J. Aparicio Rebollo, Gabriel S. Lozano Barbero, Angel Barranco Quero, Hernán R. Míguez García. Poster

“Luminescent Nanocomposities for photonic sensing”, Francisco J. Aparicio Rebollo, Iwona K. Blaszczyk Lezak, Ana Isabel Borrás Martos, Miguel Holgado, Juan Ramón Sánchez Valencia, Amadeo Griol, Hans Sohlstrom, Antelius Mikael, Agustín R. González-Elipe, Angel Barranco Quero. Poster

“Tunable in plane optical anisotropy of Ag Nanostructures growth on columnar SiO2 template thin films”, Juan Ramón Sánchez Valencia, Johan Toudert, Ana Isabel Borrás Martos, María del Carmen López Santos, Angel Barranco Quero, Inés Ortega Feliu, Agustín R. González-Elipe. Poster

“Uniform YF3: Yb, Er up-conversion nanophosphors of various morphologies synthesised in polyol media through ionic liquids”, N.O.Nuñez, M. Quintanilla, E. Cantelar, F. Cussó, M. Ocaña. Poster

MRS (Material Research Society) Spring Meeting

5-10 abril [San Francisco, Estados Unidos de América]

“The dominant ionization processes in a RF reactive magnetron plasma”, M. Labora, Alberto Palmero Acebedo, F.H.P.M. Habraken, H. Rudolph. Poster

SPIE Photonics Europe 2010

12-14 abril [Bruselas, Bélgica]

“Incorporation of luminescent nanometric films in photonic crystals and devices for development of photonic sensors”, Francisco J. Aparicio, Miguel Holgado, Iwona K. Blaszczyk Lezak, Ana Isabel Borrás Martos, Amadeo Griol, Carlos Angulo Barrios, Hans Sohlstrom, Agustin R. González-Elipe, Angel Barranco Quero. Comunicación oral

Hybrid and organic photovoltaics conference HOPV 2010

23-27 mayo [Assisi, Italia]
“Improved photovoltaic Grätzel cells based on TiO2 porous layers prepared by physical vapor deposition at Glancing angles”, Lola González García, Irene González-Valls, Mónica Lira-Cantu, Angel Barranco Quero, Agustín R. González-Elipe. Comunicación oral

EMRS 2010 Spring Meeting

8-10 junio [Estraburgo, Bélgica]

“Photonic sensor on glass based on nanometric luminescent plasma polymers”, Francisco J. Aparicio Rebollo, Ana Isabel Borrás, Miguel Holgado, Carlos Angulo Barrios, Amadeo Griol, Hans Sohlstrom, Agustín R. González-Elipe, Angel Barranco Quero. Comunicación oral

“Visual gas sensor based on dye thin films and subwavelength structures”, Laurent Davoine, Marc Schnieper, Angel Barranco Quero, Francisco J. Aparicio Rebollo. Comunicación oral

Surface Modification and functionalization of materials for biomedical applications (BIOCOAT 2010)

24 junio [Zaragoza, España]

“Impact of DLC/DLC-F coatings in teh bacterial adhesion on polyethylene surfaces”, Antonia Terriza Fernández, Gema del Prado, M.J. Martínez-Morlanes, D. Molina-Manso, Agustín R. González-Elipe, Francisco Yubero Valencia, Enrique Gómez-Barrena, Jaime Esteban. Comunicación oral

“Improved wear performance of UHMWPE coated with hydrogenated DLC”, V. Martinez-Nogues, M.J. Martínez-Morlanes, Maria Dolores Mariscal, F.J. Medel, María del Carmen López Santos, Francisco Yubero Valencia, José Antonio Puértolas. Comunicación oral

“Tribological performance of DLC coatings deposited by physical and chemical techniques on UHMWPE”, F.J. Medel, V. Martínez-Nogues, María Dolores Mariscal, J.L. Endrino, Francisco Yubero Valencia, José Antonio Puértolas. Comunicación oral

Nanotechnology for sustainable energy

4-9 julio [Obergurgl, Austria]

“Vertically-aligned TiO2 nanocolumn layers prepared by physical vapor deposition at glacing angles (PVD-GLAD)”, Lola González García, Irene González-Valls, Mónica Lira-Cantu, Angel Barranco Quero, Agustín R. González-Elipe. Comunicación oral

Molecular materials (MOLMAT 2010)

5-8 julio [Montpellier, Francia]

"Infiltration of a tetracationic porphyrin into TiO2 transparent thin films", Pedro Castillero Durán, Manuel Cano Luna, Javier Roales Batanero, Juan Ramón Sánchez Valencia, Angel Barranco Quero, Agustín R. González-Elipe, José María Pedrosa Poyato. Poster

"Optochemical sensing of HCl gas based on a transparent TMPYP/TiO2 composite thin films", Manuel Cano Luna, Pedro Castillero Durán, Javier Roales Batanero, Palma Mendoza, Angel Barranco Quero, Agustín R. González-Elipe, Tim Richardson, José María Pedrosa Poyato. Poster

Synchrotron Radiation in Material Sciences

11-14 julio [Oxford, Gran Bretaña]

"Study of metallic pieces from the Andalusian Baroque period with µXRD µXRF", A. Muñoz-Páez, L.K. Herrera, A.Justo, J. Sans, G. Martínez-Criado. Comunicación oral

"Reflexafs study of the surface region of layered samples", A. Muñoz-Páez, V. López-Flores, S. Díaz-Moreno, D.T. Bowron, S. Ramos, S. Ansell. Comunicación oral

20th European Conference on the Atomic and Molecular Physics of Ionized Gases ESCAMPING

13-17 julio [NoviSad, Serbia]

"Plasma sheath effects for the formation of supported 1D nanostructures by plasma deposition", Ana Isabel Borrás Martos, Pablo Romero Gómez, Manuel Macías, Juan Ramón Sánchez Valencia, Rafael Alvarez Molina, José Cotrino Bautista, Agustín R. González-Elipe. Poster

240th American Chemical Society National Meeting and Exposition

22-26 agosto [Boston, Estados Unidos de América]

"Plasma assited catalysis applied to enviromental chemistry and energy conversion processes", José Luis Hueso; Victor Rico Gavira; José Cotrino; Agustín R. González-Elipe. Comunicación oral

18th International Vacuum Congress (IVC-18)

23-27 agosto [Beijing, China]

"Surface and thin film nanostructuring by plasma enhanced chemical vapour deposition", Agustín R. González-Elipe, Ana Isabel Borrás Martos, Angel Barranco Quero, José Cotrino Bautista, Angel Yanguas Gil. Conferencia Invitada

Ordered 1 dimensional Nanostructures for photovoltaics 2010
12-15 septiembre [Mallorca, España]

“Improving the performance of DSSCS by using aligned nanocolumnar crystalline TiO2 thin film electrodes deposited by GLAD-PVD”, Lola González García, Irene González-Valls, Mónica Lira-Cantu, Angel Barranco Quero, Agustín R. González-Elipe. Comunicación oral

13th International Conference on Plasma Surface Engineering
13-17 septiembre [Garmisch-Partenkirchen, Alemania]

“Dye luminescent thin films prepared by plasma deposition”, Agustín R. González-Elipe, Francisco J. Aparicio Rebollo, Iwona K. Blaszczyk Lezak, Ana Isabel Borrás Martos, Angel Barranco Quero. Conferencia Invitada

“Nanostructure of thin films grown by deposition of isotropically distributed gaseous particles”, Rafael Alvarez Molina, Pablo Romero Gómez, Jorge Gil Rostra, José Cotrino Bautista, Francisco Yubero Valencia, Alberto Palmero Acebedo, Agustín R. González-Elipe. Comunicación oral

“Plasma functionalization and bioactivity of polymers and DLC materials: the role of amine groups in the growth of cells”, María del Carmen López Santos, Francisco Yubero Valencia, José Cotrino Baustista, Agustín R. González-Elipe, Mar Fernández, Blanca Vázquez, J. San Román. Comunicación oral

11th European Vacuum Conference EVC-11
20-24 septiembre [Salamanca, España]

“Functionalization by plasma techniques: from chemical activation to surface nanostructuring”, Agustín R. González-Elipe, Angel Barranco Quero, Ana Isabel Borrás Martos, María del Carmen López Santos, Francisco Yubero Valencia, José Cotrino Bautista. Conferencia Invitada

“Fluorinated DLC thin films and related materials prepared by plasma deposition”, Antonia Terriza Fernández, Francisco Yubero Valencia, José Cotrino Bautista, Agustín R. González-Elipe. Comunicación oral

“Tunable nanostructure and photoluminescence of columnar LNO films grown by plasma deposition”, Pablo Romero Gómez, Johan Toudert, Angel Barranco Quero, Agustín R. González-Elipe. Comunicación oral

2010 International School on Organic Photovoltaics (ISOPHOS)
22-26 septiembre [Ventotene, Italia]

“Photonic Nanostructure for Enhanced Photovoltaic Performance”, Hernán Míguez. Conferencia Invitada

XXIX Congreso Latinoamericano de Química
27 septiembre-1 octubre [Cartagena de Indias, Colombia]

“Síntesis y Caracterización del cerámico superconductor (Y0.8Ca0.2)(Ba0.5SR0.5)2Cu3O7-D”, Ana María Osorio, I. de los Santos, A.O. Bustamante, Juan Carlos González González, D. Hilda, A. Castro. Comunicación oral

5th World Congress on Preventive and Regenerative Medicine
5-7 octubre [Hannover, Alemania]

“Biomaterials-Nano Organised silica material with improved bioactivity”, M.L. Ramiro-Gutiérrez, J. Becerra; A. Díaz-Cuenca. Comunicación oral

XII Latin American conference on the applications of the Mössbauer Spectroscopies (LACAME 2010)
7-12 noviembre [Lima, Perú]

“Kinetic analysis of the thermal transformation from limonite to hematite by X-Ray diffraction and Mössbauer Spectroscopies”, Juan Carlos González González. Comunicación oral

CONGRESOS Y REUNIONES NACIONALES / NATIONAL CONGRESS AND MEETINGS

COMUNICACIONES EN CONGRESOS Y REUNIONES / COMMUNICATIONS IN CONGRESS AND MEETINGS

VI Reunión del grupo especializado de física de estado sólido de la RSEF – GEFES 2010
3-5 febrero [Zaragoza, España]

“Luminescent plasma nanocomposites for the fabrication of photonic sensing devices”, Francisco J. Aparicio, Iwona K. Blaszczyk Lezak, Ana Isabel Borrás Martos, Miguel Holgado, Carlos Angulo Barrios, Amadeo Griol, Hans Sohlstrom, Angel Barranco Quero. Comunicación oral

XI Congreso Nacional de Materiales
23-25 junio [Zaragoza, España]

“Capas Mixtas SIMXOY para el desarrollo de Recubrimientos Oftálmicos Coloreados”, Francisco Yubero, Jorge Gil Rostra, Agustín R. González-Elipe. Comunicación oral

“Crecimiento mediante PVD de Nanocables orgánicos monocristalinos soportados”, Ana Iabel Borrás, Agustín R. González-Elipe. Comunicación oral

“Desarrollo de sensores fotónicos mediante la integración de capas luminiscentes nanométricas sobre cristales fotónicos”, Francisco J. Aparicio Rebollo, Ana Isabel Borrás, Iwona K. Blaszczyk Lezak, Miguel Holgado, Amadeo Griol, Hans Sohlstrom, Agustín R. González-Elipe, Angel Barranco Quero. Comunicación oral

“Superhidrofobicidad en nanoestructuras 1D soportadas”, Ana Isabel Borrás Martos; Agustín R. González-Elipe. Comunicación oral

“Nanoestructura y propiedades luminiscentes de capas columnares de ZNO preparadas mediante PECVD”, Pablo Romero Gómez, Johan Toudert, Angel Barranco Quero, Agustín R. González-Elipe. Comunicación oral

“Un procedimiento para la síntesis de nanopartículas esféricas luminiscentes de Ln3+:NaYF4 (Ln=Eu, Tb, Er+Yb)”, N.O. Núñez, M. Quintanilla, E. Cantelar, F. Cussó, M. Ocaña. Poster

50 Congreso SECV

27-29 octubre [Madrid, España]

“Deposición de capas metálicas conductoras sobre substratos de vidrio comercial mediante ablación láser”, Ruth Lahoz, Francisco Yubero Valencia, Germán de la Fuente. Comunicación oral

“Estudio de la transformación cromática y de fases de un pigmento de limonita procedente de Perú”, Romero P., González J.C., Bustamante A., Arjonilla M., Ruiz A. y Sánchez-Soto P.J. Poster

4th Spanish Workshop on Nanolithography

7-12 noviembre [Oviedo, España]

“Fabry-perot optical sensors developed by e-beam lithography process”, Amadeo Griol, Javier Mira Navarro, Juan Hurtado Montañés, Laurent Bellieres, José Ángel Ayúcar Ruiz, Francisco López Royo, Javier Marti Sendra, Miguel Holgado, Rafael Casquel del Campo, Francisco Javier Sanza Gutiérrez, Francisco J. Aparicio Rebollo, Angel Barranco Quero, Ana Isabel Borrás Martos, Agustín R. González-Elipe. Comunicación oral

FORMACION / TRAINING

TESIS DOCTORALES/ DOCTOR DEGREE THESIS

Título: **Pigmentos cerámicos de tonalidad roja: síntesis mediante pirólisis de aerosoles y estudio cristaloquímico**
Autor: Elena López Navarrete
Directores: Manuel Ocaña Jurado
Calificación: Sobresaliente “Cum Laude”
Centro: Universidad de Sevilla

Título: **Fabricación de Láminas Delgadas Mixtas Nanoestructuradas con Funcionalidad Óptica y Fotónica**
Autor: Juan Ramón Sánchez Valencia
Directores: Ángel Barranco Quero, Juan Pedro Espinós Manzorro
Calificación: Sobresaliente “Cum Laude”
Centro: Universidad de Sevilla

Título: **Láminas delgadas de óxidos fotoactivos para el aprovechamiento de la Energía Solar**
Autor: Victor J. Rico Gavira
Directores: Agustín R. González-Elipe, Juan Pedro Espinós Manzorro
Calificación: Sobresaliente “Cum Laude”
Centro: Universidad de Sevilla

Título: **Análisis del crecimiento y las propiedades ópticas en alta energía de cristales fotónicos coloidales**
Autor: Gabriel S. Lozano Barbero
Directores: Hernán R. Míguez García
Calificación: Sobresaliente “Cum Laude”
Centro: Universidad de Sevilla

EQUIPAMIENTO CIENTÍFICO AVAILABLE EQUIPMENT

- 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

PROYECTOS DE INVESTIGACIÓN / RESEARCH PROJECTS

Reacciones complejas en estado sólido para el almacenamiento eficiente de hidrógeno Complex solid state reactions for energy efficient hydrogen storage

Código/Code:	MRTN-CT-2006-035. Marie Curie Research Training Network
Periodo/Period:	01-11-2006 / 30-09-2010
Organismo Financiador/Financial source:	Unión Europea
Importe total/Total amount:	180.834 €
Investigador responsable/Research head:	Fernández, A.
Componentes/Research group:	Rojas, T.C., Sánchez López, J.C., Martínez, D.

RESUMEN / ABSTRACT

Los hidruros reactivos compuestos se presentan como materiales de gran potencial para el almacenamiento de hidrógeno, al mejorar las limitaciones termodinámicas que presenta el uso de hidruros complejos de elementos ligeros. Sin embargo, las cinéticas de ab- y de-sorción son todavía lentas debido al hecho de que los procesos de carga y descarga de hidrógeno ocurren a través de reacciones complejas en estado sólido. Es objetivo de este proyecto explorar los mecanismos fundamentales de estas reacciones. Para ello, los estudios experimenales de cinéticas de carga/descarga, medidas termodinámicas, de estructura cristalina y propiedades electrónicas; se combinarán con cálculos “ab-initio” y modelización teórica. Los resultados proporcionarán una base para mejorar las propiedades de los materiales y para desarrollar nuevos catalizadores para mejora de las cinéticas de ab- y de-sorción. Finalmente, la optimización de los métodos de síntesis y, en particular, el escalado de los procesos de preparación de materiales para almacenamiento de hidrógeno, serán explorados en colaboración con fabricantes interesados en el proyecto.

Reactive hydride composites reveal great potential as hydrogen storage/materials as they overcome the thermodynamic limitations hindering the use of light-weight complex hydrides. However, their sorption kinetics is still slow due to the fact that the hydrogen sorption process takes place within complex solid state reactions. Is is aim of this project to explore the fundamental mechanisms involved in these reactions. It is aim of this project to explore the fundamental mechanisms involved in these reactions. For this, experimental studies on sorption kinetics, thermodynamics, crystal structure and electronic properties of the nanostructured materials are cross-linked to ab-initio calculations and theoretical modelling. The results will provide a basis to improve materials properties and to develop new catalysts for hydrogen sorption. Finally, the optimization of synthesis methods and in particular the upscaling of hydrogen storage materials preparation will be explored in collaboration with manufacturers.

Red de Excelencia para superar la fragmentación de la investigación europea en películas delgadas multifuncionales Network of excellence: to overcome the fragmentation of European research in multifunctional thin films

Código/Code:	NMP3-CT-2005-515703
Periodo/Period:	01-04-2005 / 31-03-2010
Organismo Financiador/Financial source:	Unión Europea
Importe total/Total amount:	868.026,40 €
Investigador responsable/Research head:	Fernández, A.
Componentes/Research group:	Fernández-Ramos, C., Godinho, V., Sánchez López, J.C., Martínez. D., Loir, A.S., López Cartes, C., Rojas, T.C., Abad M.D, Muñoz, M.A.

RESUMEN / ABSTRACT

Los objetivos de EXCELL se basan en superar la fragmentación que existe en la investigación europea en el área de los recubrimientos multifuncionales. EXCELL refuerza la excelencia en Europa en esta área de gran potencial industrial en Europa y a nivel mundial. EXCELL se desarrolla bajo las premisas de durabilidad y pervivencia. EXCELL pretende contribuir no solo a mejorar el nivel científico y tecnológico sino también a mejorar la calidad de vida de los ciudadanos europeos. Contribuye a la seguridad de los lugares de trabajo y tiene un excelente potencial para mejorar las prospectivas de empleo en la industria de manufactura de herramientas y en otros sectores industriales. EXCELL mueve fronteras en la ciencia y la tecnología relacionadas con los recubrimientos multifuncionales y mejora la competitividad europea a través de la transferencia de tecnología. Los resultados de EXCELL encuentrarán un amplo rango de aplicaciones tales como recubrimientos de baja fricción de amplio uso en ingeniería mecánica, nuevas películas delgadas protectoras contra la corrosion de uso en construcción, navegación y transporte terrestre, moldes de mejores prestaciones de baja fricción, películas biocompatibles resistentes al desgaste, nuevos recubrimientos con "nano-clusters" embebidos para aplicaciones en microelectrónica, etc. EXCELL a través de sus participantes y colaboradores diseña un plan de investigación y un plan de negocios que planifica su pervivencia y expansión para los próximos años.

The EXCELL's objectives are aimed at overcoming the fragmentation of the European research landscape in the area of multifunctional films. EXCELL strengthens European excellence in this given area that has a great industrial potential in Europe and worldwide. EXCELL is built on premise of long term sustainability and durability. EXCELL does not only contribute to science and technology but also improves the quality of life of European citizen. It contributes to safety of working places and has an excellent potential for improving the employment prospects in tools manufacture and other industrial sectors. EXCELL moves frontiers of science and technology related to multifunctional films and improves European competitiveness by technology transfer. The EXCELL's results will find a wide range of applications such as low-friction coatings earmarked for a wide use in mechanical engineering, new protective anticorrosion nano-films to be used in construction, marine and land transportation, etc., novel superior moulds (CDs and DVDs) with reduced friction, high wear resistance biocompatible films, novel coatings with imbedded nano-clusters to be used in computer industry, etc... EXCELL, through its partners and

collaborators designed a research roadmap along with its business plan that shows its long-lasting existence and expansion in years to come.

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 nanoescala. 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.

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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.

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 / 30-09-2010
Organismo Financiador/Financial source:	Ministerio de Educación y Ciencia
Importe total/Total amount:	232.320 €
Investigador responsable/Research head:	Sánchez López, J.C.
Componentes/Research group:	Fernández, A., Fernández, C., Muñoz-Márquez, M.A., El Mrabet, S., Godinho, V., Abad, M.D.

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.

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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. MgH2) con un hidruro complejo (típicamente un compuesto borohidruro, i.e LiBH4) 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: MgH2+2LiBH4 ↔ MgB2+LiH+4H2 (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 (TiO4C12H28) , TiO2 y VCl3 . También se prepararan en nuestro laboratorio otros catalizadores como Co3B, Ni3B 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 siguientes 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. MgH2) with a complex hydride (typically a borohydride compound, i.e LiBH4) 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: MgH2+2LiBH4 ↔ MgB2+LiH+4H2 (11.4 wt% hydrogen storage capacity). The reaction is improving the heat transfer handling, as compared to pure MgH2, 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 (TiO4C12H28) , TiO2 and VCl3 have been selected as additives for this study. Also other catalysts like Co3B, Ni3B 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.

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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.

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

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 (USE), Arturo Domínguez Rodríguez (USE), Robert Luis González Romero (becario AECID)

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 impurezas. 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.

Biomimética de Materiales. Síntesis de Biopoliésteres Tipo Cutina y sus aplicaciones tecnológicas y farmacológicas Biomimetic materials. Synthesis cutin-like biopolyesters and their technological and pharmacological applications

Código/Code:	TEP-02550 (Proyecto de Excelencia)
Periodo/Period:	01-01-2008 / 31-12-2010
Organismo Financiador/Financial source:	Junta de Andalucía
Importe total/Total amount:	137.100 €
Investigador responsable/Research head:	Benítez Jiménez, J.J.
Componentes/Research group:	Sánchez-Soto, P.J., Ruiz-Conde, A., Raigón, M., Garzón, E., Heredia, A., San Miguel, M.A., Ginés Dorado, J.M., Moyano, J.R., Rabasco, A.M., R. Patino, J.M., Rodríguez Niño, M.R., Carrera, C.

RESUMEN / ABSTRACT

El proyecto de investigación consiste en el análisis de las interacciones a nivel molecular de los monómeros constituyentes del biopolímero natural cutina con vistas al diseño de rutas

de síntesis y reconstrucción "botton-up" de materiales biomiméticos artificiales no tóxicos y biodegradables con aplicaciones como material de envasado y de encapsulado y liberación controlada de fármacos.

Se parte de hipótesis novedosas tanto desde el punto de vista de la bioquímica molecular del producto natural como de la estrategia de reconstrucción del material biomimético.

This research project is focused in the study of the molecular interactions between monomer units of natural cutin polymer. Such analysis is the base to design synthetic routes of alike materials following a botton-up strategy. New biomimetic materials are potential candidates to be used as non-toxic and biodegradable raw material for food and drug encapsulation and/or storage. Scientific hypothesis used in this approach will also be adapted to explain the biochemical route of cutin formation in nature.

Ayuda complementaria al proyecto "Superar la fragmentación de la investigación europea en películas delgadas multifuncionales"
Complementary support to the Project "To overcome the fragmentation of European research in multifunctional thin films"

Periodo/Period:	01-04-2005 / 31-03-2010
Organismo Financiador/Financial source:	Junta de Andalucía (Proyecto Internacional)
Importe total/Total amount:	110.000 €
Investigador responsable/Research head:	Fernández, A.
Componentes/Research group:	Fernández-Ramos, C., Godinho, V., Sánchez López, J.C., Martínez. D., Loir, A.S., López Cartes, C., Rojas, T.C., Abad M.D, Muñoz, M.A.

RESUMEN / ABSTRACT

El proyecto está dedicado a promover la investigación europea en capas finas "nanoestructuradas" y "nºanocomposites" multifuncionales. En particular el laboratorio andaluz participa en el desarrollo de recubrimientos resistentes al desgaste, a la corrosión y a las altas temperaturas a la vez que presenten buenas propiedades de alta dureza y baja fricción. La consecución de todas estas propiedades mejoradas en un único recubrimiento (multifuncionalidad) es un objetivo prioritario de la investigación a desarrollar en la NOE. En el consorcio participan las siguientes Instituciones: ARCELOR-MITTAL (ARC, Bélgica, coordinador); Technical University Munich (TUM, Alemania); Universitá Politecnica delle Marche (UPM, Italia); University of Nottingham (UNIN, UK); Free University of Brussels (ULB, Bélgica); Technological University for Steel and Alloys (MSISA, Rusia); Institute for Spectroscopy RAN (ISP, Rusia); SH SISTEMI s.r.l. (SHS, Italia); Technion (TEC, Israel); Instituto de Ciencia de Materiales de Sevilla (ICMSE, España); Johann Wolfgang Goethe University (GU, Alemania); CRC HAS Chemical Research Center of the Hungarian Academy of Sciences (CRC, Hungría); Cambridge University (CU, UK); INNO Group (INNO, France); Eurogroup Consulting (EURG, Bélgica).

The Project is dedicated to promote the European Research in multifunctional nanostructured and nanocomposite coatings and thin Films. In particular the Andalucian laboratory participates in the development of wear and corrosion resistant coatings at high temperatures that combine high hardness and low friction. The consecution of all these improved properties in one coating (multifunctional) is a prioritary objective of the research carried out in the NoE. The following Institutions participate in the consortium: ARCELOR-MITTAL (ARC, Bélgica, coordinador); Technical University Munich (TUM, Alemania); Universitá Politecnica delle Marche (UPM, Italia); University of Nottingham (UNIN, UK); Free University of Brussels (ULB, Bélgica); Technological University for Steel and Alloys (MSISA, Rusia); Institute for Spectroscopy RAN (ISP, Rusia); SH SISTEMI s.r.l. (SHS, Italia); Technion (TEC, Israel); Instituto de Ciencia de Materiales de Sevilla (ICMSE, España); Johann Wolfgang Goethe University (GU, Alemania); CRC HAS Chemical Research Center of the Hungarian Academy of Sciences (CRC, Hungría); Cambridge University (CU, UK); INNO Group (INNO, France); Eurogroup Consulting (EURG, Bélgica).

Nanopartículas magnéticas de metales nobles con funcionalización controlada para tratamientos de hipertemia Noble metal magnetic nanoparticles of controlled functionalization for hyperthermia treatments

Código/Code:	P06-FQM-02254 (Proyecto de Excelencia)
Periodo/Period:	01-04-2007 / 31-03- 2010
Organismo Financiador/Financial source:	Junta de Andalucía
Importe total/Total amount:	225.999 €
Investigador responsable/Research head:	Fernández, A.
Componentes/Research group:	Sánchez-López, J.C., López-Cartes, C., Rojas, T.C., Muñoz-Márquez, M.A., Guerrero, E.

RESUMEN / ABSTRACT

En esta propuesta se establece una colaboración multidisciplinar para desarrollar investigación, nuevas técnicas experimentales y aplicaciones biomédicas sobre la base de las propiedades y procedimientos originales de fabricación de un nuevo tipo de nanopartículas magnéticas híbridas de núcleo metálico (Au y Pd) y funcionalización orgánica por enlace Au-S. Partiendo de la colaboración previa de los grupos TEP217 y FQM271 se pretende ahora abordar extensamente y en profundidad aspectos fundamentales y aplicaciones biomédicas de hipertermia. Por una parte se propone una investigación dirigida a comprender las causas del magnetismo permanente observado en estas nanopartículas y esclarecer los factores que gobiernan este comportamiento. Por otro se propone investigar la potencialidad de producción de calentamiento local por aplicación de un campo electromagnético (rango de microondas) utilizando las nanopartículas biofuncionales de metales nobles.

In this proposal we establish a multidisciplinar collaboration to develop research, new experimental methodologies and biomedical applications based on the new properties and new preparation procedures of hybrid nanoparticles constituted by a metallic core (Au and Pd) and

an organic functionalization as achieved through Au-S bonds. With the starting point of the previous collaboration of the TEP217 and FQM271 groups, we intend now to develop extensively the fundamental aspects and the biomedical applications of the hyperthermia treatments based on the developed nanoparticles. On one side the research will be devoted to understand the origin of the permanent magnetism observed in these nanoparticles and to clarify the parameters that control the magnetic behaviour. On the other side it is proposed to investigate the potentiality of producing local heating by application of an electromagnetic field (in the microwave range) using the noble metal nanoparticles functionalised with biomolecules.

PROYECTOS GESTIONADOS POR OTRAS INSTITUCIONES / PROJECT MANAGE BY OTHER INSTITUTIONS

Viscoelasticidad en aerogeles híbridos orgánicos-inorgánicos

Periodo/Period:	01-01-2010 / 31-12-2012
Código/Code:	P09-TEP-5463
Oganismo Financiador/Financial source:	Junta de Andalucía
Importe total/Total amount:	56.250 €
Investigador responsable/Research head:	Piñero de los Ríos, M. (Universidad de Cádiz)
Componentes/ Research Group:	Piñero de los Ríos, M., Esquivias Fedriani, L., De la Rosa Fox, Morales Flórez, Victor

OTROS PROYECTOS / OTHER PROJECTS

Procesado y caracterización eléctrica de nanocomposites de circonia estabilizada con itria/nanotubos de carbono

Código/Code:	Intramural
Oganismo Financiador/Financial source:	CSIC
Importe total/Total amount:	30.000 €
Investigador responsable/Research head:	Rosalía Poyato Galán

Transferencia / Technological Transfer

Convenios y Contratos / Contracts and Agreements

Caracterización microestructural y química de materiales para avisadores sonoros

Periodo/Period:	19-01-2010 / 19-01-2011
Organismo Financiador/Financial source:	Clarton Horn
Investigador responsable/Research head:	Asunción Fernández Camacho
Componentes/Research group:	Vanda C. Fortio Godinho, Inmaculada Rosa Cejudo

Patentes / Patents

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

Inventores: Luis Esquivias Fedriani, Alberto Santos Sánchez, Víctor Morales Flórez
Ámbito Geográfico: Nacional
PATENTE SOLICITADA. N. de solicitud: P201000062
Fecha Solicitud/Licencia: 19/enero/2010
Entidades Titulares: Universidad de Sevilla y Universidad de Cádiz

Procedimiento para la síntesis del poliéster de polialeurato

Inventores: José Jesús Benítez Jiménez, Antonio Heredia Bayona, Alejandro Heredia Guerrero
Ámbito Geográfico: Nacional
PATENTE SOLICITADA. N. de solicitud: P201030763
Fecha Solicitud/Licencia: 20/mayo/2010
Entidades Titulares: Universidad de Málaga y CSIC

Procedimiento de obtención de recubrimientos mediante pulverización catódica y recubrimiento obtenible mediante dicho procedimiento

Inventores: Asunción Fernández Camacho, Vanda Fortio
Ámbito Geográfico: Internacional
PATENTE SOLICITADA. N. de solicitud: P200930039 – PCT/ES/070245
Fecha Solicitud/Licencia: 21/abril/2010
Entidad Titular: CSIC

Proceso de producción de hidrógeno mediante hidrólisis catalizada de un hidruro complejo, e Instalación con reactor semicontinuo para llevar a cabo el procedimiento
Inventores: Maria de los Angeles Jiménez Domínguez, Maria del Mar Jiménez Vega, Belén Sarmiento Marrón, Asunción Fernández Camacho, Gisela Mariana Arzac, Enrique Jimenez Roca
Ámbito Geográfico: Internacional
PATENTE SOLICITADA. N. de solicitud: P2010031899
Fecha Solicitud/Licencia: 22/diciembre/2010
Entidad Titular: Hynergreen Technologies, S.A.

PUBLICACIONES / PUBLICATIONS

ARTÍCULOS PUBLICADOS EN REVISTAS SCI / PAPERS IN SCI JOURNALS

Oxidation state and local structure of Ti-based additives in the reactive hydride composite $2LiBH_4 + MgH_2$

E. Deprez, Miguel A. Muñoz-Márquez, Manuel A. Roldán, C. Prestipino, F. Javier Palomares, C. Bonatto Minella, U. Bsenberg, M. Dornheim, R. Bormann and A. Fernández
Journal of Physical Chemistry C, **114** (2010) 3309–3317
DOI: 10.1021/jp910955r

Nowadays, the technological utilization of reactive hydride composites (RHC) as hydrogen storage materials is limited by their reaction kinetics. However, addition of transition-metal-based additives, for instance titanium isopropoxide (Ti-iso), to the 2LiBH4+MgH2 system, results in a significant improvement of sorption kinetics. In this work, the evolution of chemical state and local structure of the Ti-based additive has been investigated by means of X-ray absorption (XAS) and photoemission (XPS) spectroscopy. X-ray absorption near-edge structure (XANES) as well as extended X-ray absorption fine structure (EXAFS) analysis have been undertaken at the Ti K-edge. The measurements reveal the formation of a highly dispersed and disordered TiO2-like phase during ball milling. During first desorption reduced titanium oxide and titanium boride are formed and remain stable upon cycling. The surface analysis performed by XPS shows that the reduction processes of the Ti-based additive during first desorption is coupled to the migration of the Ti species from the surface to the bulk of the material. Several factors, related to favoring heterogeneous nucleation of MgB2 and the increase of interfacial area through grain refinement are proposed as potential driving force, among other effects, for the observed kinetic improvement.

Steering the Self-Assembly of Octadecylamine Monolayers on Mica by Controlled Mechanical Energy Transfer from the AFM Tip

J.J. Benítez, J.A. Heredia-Guerrero and M. Salmerón
Journal of Physical Chemistry C, **114** (2010) 12630–12634

DOI: 10.1021/jp102813s

We have studied the effect of mechanical energy transfer from the tip of an atomic force microscope on the dynamics of self-assembly of monolayer films of octadecylamine on mica. The formation of the self-assembled film proceeds in two successive stages, the first being a fast adsorption from solution that follows a Langmuir isotherm. The second is a slower process of island growth by aggregation of the molecules dispersed on the surface. We found that the dynamics of aggregation can be altered substantially by the addition of mechanical energy into the system through controlled tip–surface interactions. This leads to both the creation of pinholes in existing islands as a consequence of vacancy concentration and to the assembly of residual molecules into more compact islands.

Self-assembly of supramolecular lipidnanoparticles in the formation of plant biopolyester cutin

Eva Domínguez, José Alejandro Heredia-Guerrero, José Jesús Benítez and Antonio Heredia
Mol. BioSyst., **6** (2010) 948–950
DOI: 10.1039/B927186D

The implication of a self-assembly process in the early stages of cutin biosynthesis has been shown by means of antibodies raised against polyhydroxy fatty acid nanoparticles (cutinsomes).

Microstructural study of the $LiBH_4$-MgH_2 reactive hydride composite with and without Ti-isopropoxide additive

E. Deprez, A. Justo, T.C. Rojas, C. López-Cartés, C. Bonatto Minella, U. Bösenberg, M. Dornheim, R. Bormann and A. Fernández
Acta Materialia, **58** (2010) 5683–5694
DOI: 10.1039/B927186D

An exhaustive microstructural characterization is reported for the $LiBH_4$–MgH_2 reactive hydride composite (RHC) system with and without titanium isopropoxide additive. X-ray diffraction with Rietveld analysis, transmission electron microscopy coupled to energy dispersive X-ray analysis, selected-area electron diffraction and electron energy loss spectroscopy are presented in this paper for the first time for this system for all sorption steps. New data are reported regarding average crystallite and grain size, microstrain, phase formation and morphology; these results contribute to the understanding of the reaction mechanism and the influence of the additives on the kinetics. Microstructural effects, related to the high dispersion of titanium-based additives, result in a distinct grain refinement of MgB_2 and an increase in the number of reaction sites, causing acceleration of desorption and absorption reactions. Considerations on the stability of phases under electron beam irradiation have also been reported.

Segregation-induced grain boundary electrical potential in ionic oxide materials: A first principles model

D. Gómez-García, Juan J. Meléndez, Robert L. González-Romero, A. Domínguez Rodríguez
Acta Materialia, **58** (2010) 6404-6410
DOI: 10.1016/j.actamat.2010.08.002

A first principles continuum analytical model for cationic segregation to the grain boundaries in complex ceramic oxides is presented. The model permits one to determine the electric charge density and the segregation-induced electric potential profiles through the grain and can be extrapolated to the range of nanostructured grain sizes. The theoretical predictions are compared with existing data for yttria-stabilized tetragonal zirconia polycrystals. The implications for physical properties (mainly high temperature plasticity and hardening behaviour) are then discussed.

Aleuritic (9,10,16-trihydroxypalmitic) acid self-assembly on mica

José Alejandro Heredia-Guerrero, Miguel Angel San-Miguel, Mark S. P. Sansom, Antonio Heredia and José Jesús Benítez
Phys. Chem. Chem. Phys., **12** (2010) 10423–10428
DOI: 10.1039/C0CP00163E

Aleuritic (9,10,16-trihydroxypalmitic) acid self-assembly on mica from solution has been studied using AFM, ATR-FTIR and MD simulations. The goal of this study is to define the role of hydroxyl groups in the interaction between molecules as reference data to understand the mechanism of formation of synthetic and natural biopolyesters from polyhydroxylated long chain carboxylic acids. In a confined structure, such as the one imposed by a vertically self-assembled layer on mica, aleuritic acid has a tendency to adopt a monolayer configuration ruled by the lateral interactions between molecules via the two secondary hydroxyl groups. This (2D) growth competes with the multilayer formation (3D), which is conditioned by the terminal primary hydroxyl group. As the self-assembly spatial constraint is relaxed, MD has shown that the structure tends to become an amorphous and crosslinked phase that can be characterized by topographic and friction force AFM data.

Permanent magnetism in phosphine- and chlorine-capped gold: from clusters to nanoparticles

Miguel A. Muñoz-Márquez, Estefanía Guerrero, Asunción Fernández, Patricia Crespo, Antonio Hernando, Raquel Lucena and José C. Conesa
Journal of Nanoparticle Research, **12** (2010) 1307–1318
DOI: 10.1007/s11051-010-9862-0

Magnetometry results have shown that gold NPs (similar to 2 nm in size) protected with phosphine and chlorine ligands exhibit permanent magnetism. When the NPs size decreases down to the subnanometric size range, e.g. undecagold atom clusters, the permanent magnetism disappears. The near edge structure of the X-ray absorption spectroscopy data points out that charge transfer between gold and the capping system occurs in both cases. These results strongly suggest that nearly metallic Au bonds are also required for the induction of a magnetic response. Electron paramagnetic resonance observations indicate that the contribution to magnetism from eventual iron impurities can be disregarded.

Structural characterization of polyhydroxy fatty acid nanoparticles related to plant lipid biopolyesters

José A. Heredia-Guerrero, Eva Domínguez, Mónica Luna, José J. Benítez and Antonio Heredia
Chemistry and Physics of Lipids, **163** (2010) 329–333
DOI: 10.1016/j.chemphyslip.2010.01.006

In the present work, we report the physico-chemical properties and structural characteristics of special polyhydroxy fatty acid nanoparticles after their fusion by means of attenuated total reflection-Fourier transform infrared spectroscopy (ATR-FTIR), X-ray diffraction (XRD), differential scanning calorimetry (DSC), scanning electronic microscopy (SEM), atomic force microscopy (AFM), and light microscopy. All the characteristics and properties investigated have an important degree of similarity to the native plant cutin, the main biopolymer present in the plant cuticles. The supramolecular organization of these polymerized prime nanoparticles after their interaction on cellulose substrate and isolated cuticle samples, simulating the in vivo conditions in epidermal plant cells, strongly suggests a growth of these nanoparticles after a self-assembly process.

A first study of the high-temperature plasticity of ceria-doped zirconia polycrystals

Santiago de Bernardi-Martín, Diego Gómez-García, Arturo Domínguez-Rodríguez and Goffredo de Portu
Journal of the European Ceramic Society, **30** (2010) 3357–3362
DOI: 10.1016/j.jeurceramsoc.2010.07.043

Ceria–zirconia ceramic alloys were sintered by high-temperature annealing, considering several synthesis temperatures to obtain a full-dense ceria–zirconia ceramic material using a temperature as low as possible. It was found that fully density is achieved at temperatures of 1450 °C. Monolithic specimens were crept under compression at high temperatures. The creep results fitted an empirical constitutive equation consistent with a classical Ratchinger mechanism for grain switching. This result was confirmed through microstructural characterization of as-received and post-mortem specimens. Since the conventional Ashby–Verrall model is contrary to the mechanism controlling creep in other zirconia alloys, the results are considered in the framework of a new grain boundary sliding model, with particular discussion of the validity of that model for the ceria–zirconia case.

Characterization of $Ti_{1-x}Al_xN$ coatings with selective IR reflectivity

V. Godinho, D. Philippon, T.C. Rojas, N.N. Novikova, V.A. Yakovlev, E.A. Vinogradov, A. Fernández
Solar Energy, **84** (2010) 1397–1401
DOI: 10.1016/j.solener.2010.04.021

Ti1−xAlxN thin films were deposited by reactive magnetron sputtering. The obtained different stoichiometries give rise to different optical properties as the films change from metallic to dielectric. In this work the IR reflectivity of these coatings is investigated taking into account different application fields for IR selective Ti1−xAlxN thin films.
Low Al content coatings present high reflectivity, high absorptance and low thermal emittance. High Al compositions give raise to coatings with high absorptance and high thermal emittance.
The composition of the coatings was evaluated combining electron energy loss spectroscopy (EELS) and energy dispersive spectroscopy. Scanning electron microscopy (SEM) revealed a columnar structure. Reflectance spectra for the visible and infrared spectral ranges were used to obtain the solar absorptance and thermal emittance values, used to calculate the equilibrium temperature of the coatings.
The thermal stability in air from 300 to 600 °C was also evaluated., with particular discussion of the validity of that model for the ceria–zirconia case.

Microstructural Effects on the Creep Deformation of Alumina/Single-Wall Carbon Nanotubes Composites

Zapata-Solvas, E., Gómez-García, D., Poyato, R., Lee, Z., Castillo-Rodríguez, M., Domínguez-Rodríguez, A., Radmilovic, V., Padture, N.P.
Journal of the American Ceramic Society, **93** (2010) 2042-2047
DOI: 10.1111/j.1551-2916.2010.03681.x

The enhanced high-temperature creep resistance in aluminasingle-wall carbon nanotubes (SWNTs) composites has been attributed to the unprecedented grain-boundary structure of these composites, where the SWNTs bundles segregated at the alumina grain boundaries partially impede grain-boundary sliding. In this study, the effect of SWNTs distributions at alumina grain boundaries on the creep behavior of aluminaSWNTs composites has been investigated. Microstructures of two different alumina10 vol% SWNTs composites, one with heterogeneous and the other with homogenous distributions of SWNTs at grain boundaries, have been characterized quantitatively. The steady-state creep rate (uniaxial compression) in the heterogeneous composite has been found to be over three times higher than that in the homogeneous composite at 1300° and 1350°C (argon atmosphere). It is argued that the less uniform distribution of SWNTs at the alumina grain boundaries in the heterogeneous composite results in less effective obstruction of grain-boundary sliding, and attendant higher creep rate. This also results in more efficient recovery in that composite.

Effect of process parameters on mechanical and tribological performance of pulsed-DC sputtered TiC/a-C:H nanocomposite films

K.P. Shaha, Y.T. Pei, D. Martinez-Martinez, J.C. Sanchez-Lopez and J.Th.M. De Hosson

Surface and Coatings Technology, **205** (2010) 2633-2642
DOI: 10.1016/j.surfcoat.2010.10.020

Mechanical, structural, chemical bonding (sp3/sp2), and tribological properties of films deposited by pulsed-DC sputtering of Ti targets in Ar/C2H2 plasma were studied as a function of the substrate bias voltage, Ti-target current, C2H2 flow rate and pulse frequency by nanoindentation, Raman spectroscopy and ball-on-disc tribometry. The new findings in this study comprise: dense, column-free, smooth, and ultra-low friction TiC/a-C:H films are obtained at a lower substrate bias voltage by pulsed-DC sputtering at 200 and 350 kHz frequency. The change in chemical and phase composition influences the tribological performance where the TiC/a-C:H films perform better than the pure a-C:H films. In the case of TiC/a-C:H nanocomposite films, a higher sp2 content and the presence of TiC nanocrystallites at the sliding surface promote formation of a transfer layer and yield lower friction. In the case of a-C:H films, a higher sp3 content and higher stress promote formation of hard wear debris during sliding, which cause abrasive wear of the ball counterpart and yield higher friction.

Si-doped multifunctional bioactive nanostructured films

D.V. Shtansky, N.A. Gloushankova, A.N. Sheveiko, Ph.V. Kiryukhantsev-Korneev, I.A. Bashkova, B.N. Mavrin, S.G. Ignatov, S.Yu. Filippovich and C. Rojas

Surface and Coatings Technology, **205** (2010) 728-739
DOI: 10.1016/j.surfcoat.2010.07.063

Si-doped multifunctional bioactive nanostructured films (MuBiNaFs) were deposited by DC magnetron sputtering of composite TiC0.5 + CaO + Si (A) and TiC0.5 + CaO + Si3N4 (B) targets produced by self-propagating high-temperature synthesis method. The films were characterized in terms of their structure, elemental and phase composition using X-ray diffraction, scanning and transmission electron microscopy, electron energy loss spectroscopy, glow discharge optical emission spectroscopy, Raman, and IR spectroscopy. The Ti–Si–Ca–P–C–O–(N) films consisted of TiC(N) as a main phase with a minor amount of TiOx, SiNx, SiOx, SiC, and CaO phases probably mainly in amorphous state at the grain boundaries and COO– groups on the film surface. The excess of carbon atoms in the Ti–Si–Ca–P–C–O–N film (target A) precipitated in a DLC form. The films showed hardness in the range of 26–31 GPa, reduced Young's modulus of 200–270 GPa, and high percentage of elastic recovery of 60–71%. The best Ti–Si–Ca–C–O–N films exhibited low friction coefficient both in physiological solution and Dulbecko modified Eagle medium with fetal calf serum, hydrophilic properties, improved electrochemical characteristics, and excellent impact resistance. Nevertheless, the wear resistance of the Ti–Si–Ca–C–O–N films against Al2O3 ball was lower compared with the best Si-free MuBiNaFs. In vitro studies showed that the Si-doped Ti–Ca–C–O–N films possess improved osteoconductive characteristics during early stage of cell/material interaction. The film surface was highly adhesive for IAR-2 epithelial and MC3T3-E1 osteoblastic cells. The films revealed a high level of biocompatibility and biostability in experiments in vivo. The Ti–Si–Ca–C–O–N film (target A) did not show any bactericidal activity during cultivation of bacterial strains both on solid and in liquid Luria Bertani mediums. The film did not reveal any bactericidal and toxic activity against macrophages and therefore did not change bacterial status and defence system of macro-organisms.

Tailored synthesis of nanostructured WC/a-C coatings by dual magnetron sputtering
M.D. Abad, M.A. Muñoz-Márquez, S. El Mrabet, A. Justo and J.C. Sánchez-López
Society and Coatings Technology, **204** (2010) 3490-3500
DOI: 10.1016/j.surfcoat.2010.04.019
Nanostructured coatings with variable contents of tungsten carbide (WC) and amorphous carbon (a-C) are prepared by controlling the sputtering power ratio using WC and graphite targets. XRD and TEM/ED analysis shows that increasing the C incorporation, the WC nanocrystalline phases evolve from γ-W2C to β-WC1 − x. Further C enrichment leads to a nanocomposite structure of small WC1 − x crystals dispersed in a-C matrix. The a-C at.% is estimated by XPS analysis and correlated with the observed tribo-mechanical properties. The hardness and friction properties vary from hard/high friction (36–40 GPa; μ = 0.6–0.8) to moderate-hard/low friction (16–20 GPa; μ not, vert, similar 0.2) coatings depending on the film composition. The transition point is found for a-C content of 10 at.%. This correlates with a change from nanocrystalline WC to nanocomposite WC1 − x/a-C coatings. The overall study will help to understand the previous literature data and will serve as guide for a tailored synthesis of these WC/a-C nanocomposites.

Magnetometry and electron paramagnetic resonance studies of phosphine- and thiol-capped gold nanoparticles
E. Guerrero, M.A. Muñoz-Márquez, A. Fernández, P. Crespo, A. Hernando, R. Lucena, and J.C. Conesa
J. Appl. Phys., **107** (2010) 064303 (7 pages)
DOI: 10.1063/1.3327414

In the last years, the number of studies performed by wholly independent research groups that confirm the permanent magnetism, first observed in our research lab, for thiol-capped Au nanoparticles (NPs) has rapidly increased. Throughout the years, the initial magnetometry studies have been completed with element-specific magnetization measurements based on, for example, the x-ray magnetic circular dichroism technique that have allowed the identification of gold as the magnetic moment carrier. In the research work here presented, we have focused our efforts in the evaluation of the magnetic behavior and iron impurities content in the synthesized samples by means of superconducting quantum interference device magnetometry and electron paramagnetic resonance spectrometry, respectively. As a result, hysteresis cycles typical of a ferromagnetic material have been measured from nominally iron-free gold NPs protected with thiol, phosphine, and chlorine ligands. It is also observed that for samples containing both, capped gold NPs and highly diluted iron concentrations, the magnetic behavior of the NPs is not affected by the presence of paramagnetic iron impurities. The hysteresis cycles reported for phosphine-chlorine-capped gold NPs confirm that the magnetic behavior is not exclusively for the metal-thiol system.

Structure of diamondlike carbon films deposited by femtosecond and nanosecond pulsed laser ablation
A. Sikora, F. Garrelie, C. Donnet, A.S. Loir, J. Fontaine, J.C. Sánchez-López, T.C. Rojas

J. Appl. Phys., **108** (2010) 113516 (9 pages)
DOI: 10.1063/1.3510483

The characterization of diamondlike carbon (DLC) films is a challenging subject, considering the diversity of carbon-based nanostructures depending on the deposition process. We propose to combine multiwavelength (MW) Raman spectroscopy and electron energy-loss spectroscopy (EELS) to probe the structural disorder and the carbon hybridizations of DLC films deposited by pulsed laser ablation performed either with a nanosecond laser (film labeled ns-DLC), either with a femtosecond laser (film labeled fs-DLC). Such deposition methods allow to reach a rather high carbon sp3 hybridization but with some significant differences in terms of structural disorder and carbonaceous chain configurations. MW Raman investigations, both in the UV and visible range, is a popular and nondestructive way to probe the structural disorder and the carbon hybridizations. EELS allows the determination of the carbon plasmon energy in the low-loss energy region of the spectra, as well as the fine structure of the ionization threshold in the high-loss energy region. The paper shows that the combination of MW Raman and EELS is a powerful way to elucidate the nanostructure of DLC films. Complementary nanoindentation investigations allow to correlate the analytical results with the mechanical properties of the films. The ns-DLC film presents a stronger sp3-bonded C character (74%–85%) with a significant content of sp2 chains, whereas the fs-DLC contains less sp3 bonds (35%–50%) with a significant content of sp2-bonded C rings. The ns-DLC film exhibits a higher proportion of disordered sp2 C mainly in the form of chains. Comparatively, the fs-DLC exhibits a predominance of more ordered sp2 C structures in the form of graphitic aggregates whose size has been estimated near three aromatic rings. The film characteristics are in agreement with their mechanical properties. We also propose a correlation between the nanostructure and composition of the films with the deposition mechanisms. The difference in kinetic energy distribution in the plasma plume, together with an absence of interaction between the plasma plume and the femtosecond laser, are responsible for the observed differences in sp3 C content and sp2 C configuration ranging between a predominance of more ordered sp2 rings in the fs-DLC film and a predominance of sp2 chains in the ns-DLC film. These results are consistent with the mechanisms of subplantation occurring during DLC deposition.

Influence of carbon chemical bonding on the tribological behavior of sputtered nanocomposite TiBC/a-C coatings

Abad, M.D., Sánchez-López, J.C., Brizuela, M., García-Luis, A., Shtansky, D.V.

Thin Solid Films, **205** (2010) 5546-5552
DOI: 10.1016/j.tsf.2010.04.038

The tribological performance of nanocomposite coatings containing Ti–B–C phases and amorphous carbon (a-C) are studied. The coatings are deposited by a sputtering process from a sintered TiB2:TiC target and graphite, using pulsed direct current and radio frequency sources. By varying the sputtering power ratio, the amorphous carbon content of the coatings can be tuned, as observed by X-ray photoelectron spectroscopy (XPS) and Raman spectroscopy. The crystalline component consists of very disordered crystals with a mixture of TiB2/TiC or TiBxCy phases. A slight increase in crystalline order is detected with the incorporation of carbon in the coatings that is attributed to the formation of a ternary TiBxCy phase. An estimation of the carbon present in the form of carbide (TiBxCy or TiC) and amorphous (a-C) is performed using fitting analysis of the C 1s XPS peak. The film hardness (22 to 31 GPa) correlates with the fraction of the TiBxCy phase that exists in the coatings. The tribological properties were measured by a pin-on-disk tribometer in ambient conditions, using 6 mm tungsten carbide balls at 1 N. The friction coefficients and the wear rates show similar behavior, exhibiting an optimum when the fraction of C atoms in the amorphous phase is near 50%. This composition enables significant improvement of the friction coefficients and wear rates (μ not, vert, similar 0.1; k < 1 × 10−6 mm3/Nm), while maintaining a good value of hardness (24.6 GPa). Establishing the correlation between the lubricant properties and the fraction of a-C is very useful for purposes of tailoring the protective character of these nanocomposite coatings to engineering applications.

On the microstructure of single wall carbon nanotubes reinforced ceramic matrix composites

Zapata-Solvas, E., Gómez-García, D., Domínguez-Rodríguez, A.
Journal of Materials Science, **45** (2010) 2258-2263
DOI: 10.1007/s10853-009-4126-z

A microstructural modelling of the microstructure in single wall carbon nanotubes reinforced alumina ceramics has been developed. The model accounts for the main microstructural features, being quite useful to describe the carbon nanotube distribution along the ceramic matrix. The microstructural analysis derived from this model is found to give a deeper insight into the high-temperature creep of these composites.

SiOxNy thin films with variable refraction index: Microstructural, chemical and mechanical properties

Godinho, Jiménez de Haro, M.C., García-López, J., Goosens, V., Terryn, H., Delplancke-Ogletree, M.P., Fernández, A.
Applied Surface Science, **256** (2010) 4548-4553
DOI: 10.1016/j.apsusc.2010.02.045

In this work amorphous silicon oxynitride films with similar composition (ca. Si0.40N0.45O0.10) were deposited by reactive magnetron sputtering from a pure Si target under different N2–Ar mixtures. Rutherford backscattering (RBS) studies revealed that the coatings presented similar composition but different density. The mechanical properties evaluated by nanoindentation show also a dependence on the deposition conditions that does not correlate with a change in composition. An increase in nitrogen content in the gas phase results in a decrease of hardness and Young's modulus.

The microstructural study by high resolution scanning electron microscopy (SEM-FEG) on non-metalized samples allowed the detection of a close porosity in the form of nano-voids (3–15 nm in size), particularly in the coatings prepared under pure N2 gas. It has been shown how the presence of the close porosity allows tuning the refraction index of the films in a wide range of values without modifying significantly the chemical, thermal and mechanical stability of the film.

Behaviour of sonogels under isotropic pressure
Luis Esquivias
Comptes Rendus Chimie, **13** (2010) 282-289
DOI: 10.1016/j.crci.2009.09.011

The aim of this article is to present a method that simplifies the standard procedure to determine the yield point providing complementary information about changes in the behaviour of the materials under study. It is generally accepted that the yield point is determined by the inflection point of the curve of pressure versus apparent volume of the sample, P(V), from Hg porosimetry runs. Although compressible materials present an easily identifiable neat inflection point, in resilient materials, the inflection point is not easy to identify by simple visual inspection of the curve. A physical magnitude (K’) is introduced to characterise the evolution of the material's compliance under isotropic pressure. The physical meaning of K’ is the variation in the resistance to uniform compression with the pressure applied, helping to identify the yield point and the plastic mechanism beyond the yield point in a single run.

Superplasticity in nanocrystalline ceramics: pure grain boundary phenomena or not?
Arturo Domínguez-Rodríguez, Diego Gómez-García, Miguel Castillo-Rodríguez, Eugenio Zapata-Solvas, Rachman Chaim
International Journal of Materials Research, **45** (2010) 2258-2263
DOI: 10.1007/s10853-009-4126-z

Superplasticity in ceramics has been the subject of intense research activity for the last two decades. Quite recently, the fabrication of fully dense nanocrystalline oxides with grain size below 100 nm enabled examination of their superplastic behaviour. This work presents a critical analysis of the plasticity of two important nanostructured oxide systems: MgO and yttria tetragonal zirconia polycrystals. A thorough comparison of their plastic deformation reveals that nano-structuring may be a necessary, but not a sufficient condition for superplasticity in ceramics as commonly assumed. Instead, the changes in the chemical composition and the transport properties, through the bulk and at grain boundaries, versus temperature and grain size can induce a rich variety of mechanical responses.

Structural models of randomly packed Tobermorite-like spherical particles: A simple computational approach
González-Teresa, R., Morales-Florez, V., Manzano, H., Dolado, J.S.
Materiales de Construccion, **298** (2010) 7-15
DOI: 10.3989/mc.2010.57010

In this work, and in order to bring together the atomistic and colloidal viewpoints, we will present a Monte Carlo computational scheme which reproduces the colloidal packing of nano-spherical crystalline tobermorite-like particles. Different Low Density (LD) CS- H and High Density (HD) C-S-H structures will be developed just by varying the computational packing parameters. Finally, the structures resulting from our computational experiments will be analyzed in terms of their densities, surface areas and their mechanical properties.

Advances in Aerogels made by Sonocatalysis
L. Esquivias, V. Moralez-Florez, N. de la Rosa-Fox
Transactions of the Indian Ceramic Society, **69** (2010) 125-130

High power ultrasound applied to liquids produces cavities. When an alkoxide/water mixture is sonicated, the cavities, which attain very high temperatures and pressures, act as nanoreactors, where the hydrolysis reaction starts. When the resultant sonosol gels to produce a sonogel, it is denser, with finer and more homogeneous porosity than that of a classic counterpart. Thus, acoustic cavitation permits to obtain nanostructured materials. Sono-aerogels have a high surface/volume ratio and are built by small particles (similar to 1 nm radius) and a high cross-linked network with low -OH surface coverage radicals. Structural models based on randomly-packed spheres in several hierarchical levels that represent the real sono-aerogel are shown. Finally, these materials find application, between others, for CO2 sequestration, since the small size of the pore permits hosting silicate nanocrystals that carbonate easily in the presence of CO_2 in aqueous solution.

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

Superplasticity in ceramics: applications and new trends
Dorninguez-Rodriguez, A; Gomez-Garcia, D; DelaRosa Fox, N
Key Engineering Materials, 423 (2010) 3-13

Mechanical properties of bioactive hybrid organic/inorganic
V. Morales-Flórez, J. A. Toledo-Fernández, R.Mendoza, A. Santos, N. de la Rosa-Fox, M. Piñero, L.Esquivias
Key Engineering Materials, 423 (2010) pp 155-160

Creep and stress relaxation of hybrid organic-inorganic
V. Morales-Flórez, J. A. Toledo-Fernández, R. Mendoza, A. Santos, N. de la Rosa-Fox, M. Piñero, L.Esquivias
Key Engineering Materials, 423 (2010) pp 167-172

Extended X-ray absorption fine structure (EXAFS) investigations of Ti bonding environment in sputter-deposited nanocomposite TiBC/a-C thin films
J.L. Endrino, M.D. Abad, R. Gago , D. Horwat, I. Jiménez, J.C. Sánchez-López
IOP Conf. Ser.: Mater. Sci. Eng., 12 (2010) 012012

Diseño de un reactor isotérmico para producción de H2 por hidrólisis de borohidruro sódico en condiciones de alimentar una pila de combustible tipo PEM de 60W
G.M. Arzac, A. Fernández, B. Sarmiento, M.M. Jiménez, N. Ibáñez, M.A Jiménez
IV Congreso Nacional de Pilas de Combustible, ISBN.: 978-84-693-2330-4, Sevilla 2010, p. 325-328.

Hidruros sólidos como acumuladores de hidrógeno
A.Fernández, C. Sánchez, O. Friedrichs, J.R. Ares, F. Leardini, J. Bodega, J.F. Fernández
Revista Española de Física, Vol. 24, Nr. 1, Enero-Marzo 2010, 63-68

Beneficial silver: antibacterial nanocomposite Ag-DLC coating to reduce osteolysis of orthopaedic implants
J. L. Endrino, J.C. Sánchez-López, R. Escobar Galindo, D. Horwat, A. Anders
Journal of Physics: Conference Series,. 252, 2010, 012005-1/012005-7

LIBROS Y OTRAS PUBLICACIONES / BOOKS AND OTHER PUBLICATIONS

Aerogels synthesis by sonocatalysis – sonogels
L. Esquivias, M Piñero, V. Morales-Flórez and N. de la Rosa-Fox
En: Aerogels Handbook, 2010
Editorial Springer (Eds. Michel A. Aegerter, Nicholas Leventis, Matthias M. Koebel)
ISSN: 1132-0346

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)

CONGRESOS Y REUNIONES INTERNACIONALES / INTERNATIONAL CONGRESS AND MEETINGS

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

Advanced Nanocoatings for Mechanical & Tribological Applications. European Conference on Nanofilms ECNF
1 marzo [Liége, Bélgica]
Asunción Fernández Camacho [Presidencia de Sesión]

37th International Conference on Metallurgical Coatings and Thin Films ICMCTF 2010
26-30 abril [San Diego, Estados Unidos de América]
Asunción Fernández Camacho [Chairmain of Session]
Juan Carlos Sánchez López [Chairmain of Session]

3rd International Congress on Ceramics
10 noviembre [Osaka, Japón]
Diego Gómez García [Chairman of Session]

COMUNICACIONES EN CONGRESOS Y REUNIONES / COMMUNICATIONS IN CONGRESS AND MEETINGS

VI Reunión del grupo especializado de física de estado sólido de la RSEF – GEFES 2010
3-5 Febrero [Zaragoza, España]

"The role of additives in nanocrystalline hydride materials for hydrogen storage: A microstructural and chemical characterization", A. Fernández Camacho, E. Deprez, M.A. Muñoz Márquez, M.A. Roldán Gutierrez, F.J. Palomares Simón, C. Prestipino, O. Friedrichs. Poster

European Conference on Nanofilms 2010

22-25 Marzo [Liege, Bélgica]

"Endurance of Ti-Al-Si-N thin films under tribological sollicitations", D.Philippon, V.Godinho,P.M.Nagy, M.P.Delplancke-Ogletree, A.Fernández. Comunicación oral

"Structure and properties of TiAlC(N), TiCrAlC(N), and CrAlC(N) coatings deposited by sputtering of Max-phase $Ti_{2-x}Cr_xAlC$ targets", D.V.Shtansky, Ph.V.Kiryukhantsev-Korneev, A.N.Sheveyko, B.N.Marvin, C.Rojas, A.Fernández, E.A.Levashov. Comunicación oral

"Characterization of TiAlN coatings", V.N.Denisov, B.N.Marvin, V.D.Blank, E.A.Vinogradov, A.N.Kirichenko, S.N.Polyakov, K.V.Gogolinsky, A.S. Useinov, V.Godinho,J.C.Sánchez-López, D.Philippon, A. Fernández-Camacho. Comunicación oral

"SiOxNy thin films with tailored refraction index: Microstructure, mechanical properties and thermal stability", V.Godinho, V.Goossens, H.Terryn, M.P.Delplancke-Ogletree, A.Fernández. Comunicación oral

"Preparation and characterization of thiol- and phosphine-functionalized gold-clusters and nanoparticles: An X-ray absorption spectroscopy study", E.Guerrero, C.López-Cartés, T.C.Rojas, G.-L.Ciatto, M.A.Muñoz-Márquez, A.Fernández. Poster

37th International Conference on Metallurgical Coatings and Thin Films ICMCTF 2010

26-30 Abril [San Diego, Estados Unidos de América]

"Application of Electron Microscopy and Spectroscopy Techniques to the Characterization of Nanostructured TiAlSiN Coatings", V.Godinho, D.Philippon, T.C.Rojas, M.P. Delplanck-Ogletree, A.Fernández. Comunicación oral

"Comparative analysis on structure and tribo-mechanical properties of Ti-B-C nanocomposite coatings prepared by magnetron sputtering", J.C. Sánchez-López, M.D. Abad, A. Justo, M. Brizuela, A. Garcia-Luis. Comunicación oral

"Ag-Ti(C,N)-based coatings for biomedical applications: influence of composition and structure in the mechanical/tribological and biological behaviour", S. Ribeiro, J.C. Sánchez-López, M.D. Abad, R. Escobar-Galindo, M. Henriques, S. Carvalho. Comunicación oral

2nd International EJC-PISE Workshop

16-17 Junio [Kiev, Ucrania]

“Hard Nanocomposite Ti-(Al,Cr,Y)-Si-C-N Coatings with Improved Wear- and Oxidation Resistance Produced by Ion Implantation Assisted Magnetron Sputtering”, Ph.V.Kiryukhantsev-Korneev, A.N. Sheveyko, E.A. Levashov, K.A. Kuptsov, R. Cecchini, A. Fabrizi, A. Fernández, D.V. Shtansky. Comunicación oral

IV Congreso Nacional de Pilas de Combustible CONAPPICE 2010

16-18 Junio [Zaragoza, España]

“Diseño de un reactor isotérmico para producción de H2 por hidrólisis de borohidruro sódico en condiciones de alimentar una pila de combustible tipo PEM de 60W”, G.M.Arzac, A.Fernández, B.Sarmiento, M.M.Jimenez, N.Ibáñez, M.A.Jimenez. Comunicación oral

Surface modification and funcionalisation of materials for biomedical application

24 Junio [Zaragoza, España]

“Tribological properties of silver containing amorphous carbon films”, J. L. Endrino, R. Escobar Galindo, J.C. Sanchez-Lopez. Comunicación oral

12th International Ceramic Congress CIMTEC 2010

16-18 Junio [Sevilla, España]

“Nanocomposite Metal Carbide/amorphous carbon coatings for tribological applications”, J.C. Sánchez-López, M.D. Abad, D. Martínez-Martínez, A. Fernández. Conferencia Invitada

International Workshop and Exhibition. Solid State Hydrogen Storage: From Fundamental to Industrial Application

5-6 octubre [Turin, Italia]

“Electronic and microstructural characterization of the 2LiBH4/MgH2 system and its Ti-isopropoxide additive”, E. Deprez, A.Fernández. Poster

Materials Research Society Fall Meeting 2010

29 Noviembre – 3 Diciembre [Boston, Massachusetts, Estados Unidos de América]

“Nano-scale Creep Compliance of Hybrid Aerogels”, N. De la Rosa,-Fox, V. Morales Flórez, M. Piñero, L. Esquivias

FORMACION / TRAINING

TESIS DOCTORALES/ DOCTOR DEGREE THESIS

Título:	**Nanostructured lubricant systems for tribological applications**
Autor:	Manuel David Abad Roldán
Directores:	Juan Carlos Sánchez López
Calificación:	Sobresaliente “Cum Laude”
Centro:	Universidad de Sevilla

EQUIPAMIENTO CIENTÍFICO AVAILABLE EQUIPMENT

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

PROYECTOS DE INVESTIGACIÓN / RESEARCH PROJECTS

Microestructura y propiedades magnéticas de aleaciones amorfas y nanocristalinas y nanopolvos Microstructure and magnetic properties of amorphous and nanocrystalline alloys and nanopowders

Código/Code:	MAT2007-65227
Periodo/Period:	01-10-2007 / 30-09-2010
Organismo Financiador/Financial source:	Ministerio de Ciencia e Innovación
Importe total/Total amount:	72.600 €
Investigador responsable/Research head:	Alejandro Conde Amiano
Componentes/Research group:	Clara F. Conde Amiano, María Millán Muñoz, Josefa María Borrego Moro, Victorino Franco García, Javier S. Blázquez Gámez, Rafael Caballero Flores

RESUMEN / ABSTRACT

Se propone estudiar materiales magnéticos blandos (aleaciones amorfas y nanocristalinas y nanopolvos) obtenidos por solidificación rápida y por molienda/aleado mecánico. En la técnica de molienda, trataremos de profundizar en el conocimiento de la influencia de diversos parámetros experimentales (en la preparación y posterior procesado del polvo) en la microestructura y propiedades magnéticas del material. En las aleaciones nanocristalinas se plantea analizar la influencia de diferentes cambios de composición de la aleación en la microestructura del sistema nanocristales-fase intergranular y su correlación con las propiedades magnéticas del material, como vía para su optimización. Las interacciones responsables del acoplamiento de los granos y su modelización, para explicar la dependencia con la temperatura del comportamiento magnético de estos materiales, serán también objeto de estudio. En las aleaciones amorfas multicomponentes los objetivos se concretan en la optimización de sus propiedades magnéticas y en la viabilidad de desarrollar nanoestructuras que permitan mejorar sus propiedades magnéticas. Dado su interés actual, debido a su potencialidad tecnológica, estudiaremos la respuesta magnetocalórica de los diferentes materiales, tratando de optimizar su capacidad de refrigeración y temperatura óptima de operación, y analizaremos los cambios en la respuesta magnetocalórica debido a la presencia de nanocristales.

The study of soft magnetic materials obtained by rapid quenching and milling/mechanical alloying (amorphous and nanocrystalline alloys and nanopowders) is proposed. Concerning the milling technique, we will try to improve the knowledge of the influence of different experimental parameters (involved in the preparation and processing of the powder) on the microstructure and magnetic properties of the material. In the nanocrystalline alloys it is proposed to analyse the influence of different composition changes of the alloys on the microstructure of the nanocrystal-intergranular phase system and its correlation with the magnetic properties of the material, as a way to optimize them. The interactions responsible for the grain coupling and

their modelisation, to explain the temperature dependence of the magnetic behaviour of these materials, will be also a subject of our study. In the multicomponent amorphous alloys, the objetives are focused on the optimization of their magnetic properties and the viability to develop nanostructures improving their magnetic properties. In view of its current interest, due to their potential technological applications, we will study the magnetocaloric response of the different materials, trying to optimize its refrigeration capacity and the optimal operational temperature, and we will analyse changes in the magnetocaloric response in the presence of nanocrystals

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Propiedades termomagnéticas de materiales y optimización de su eficiencia energética Thermomagnetic properties of materials and optimization of energy efficiency

Código/Code:	MAT2010-20537
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Organismo Financiador/Financial source:	Ministerio de Ciencia e Innovación
Importe total/Total amount:	100.000 €
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.

Microestructura, propiedades magnéticas y aplicaciones de aleaciones amorfas y nanocristalinas Microstructure, magnetic properties and applications of amorphous and nanocrystalline alloys

Código/Code:	P06-FQM01823 (Proyecto de Excelencia)
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RESUMEN / ABSTRACT

Se propone un estudio de materiales amorfos y nanocristalinos magnéticamente blandos, preparados por técnicas de solidificación rápida y, como vía alternativa, por molienda/aleado mecánico. En las aleaciones nanocristalinas se plantea analizar la influencia de cambios de composición de la aleación en la arquitectura microestructural del sistema nanocristales-fase intergranular y su correlación con las propiedades magnéticas del material, como vía para su optimización. Las interacciones responsables del acoplamiento de los granos nanocristalinos y su modelización, para explicar la dependencia con la temperatura del comportamiento magnético de estos materiales, serán también objeto de estudio. En las aleaciones amorfas multicomponentes los objetivos planteados se concretan en la optimización de sus propiedades magnéticas manteniendo una alta amorfizabilidad y en la viabilidad de desarrollar nanoestructuras que pudieran mejorar el carácter magnéticamente blando del material. Prestaremos atención, dado el interés que concita el tema en la actualidad por su potencialidad tecnológica, al estudio de la respuesta magnetocalórica de las aleaciones amorfas, tratando de optimizar por ajustes composicionales su capacidad de refrigeración y temperatura óptima de operación, y analizaremos también los cambios en la respuesta magnetocalórica debidos a la presencia de nanocristales.

Cooperación Internacional y Otros International Cooperation and Others

Estudio y Optimización de Nanocomposites para Refrigeración Magnética

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Entidad Financiadora/Financial source:	Ministerio de Ciencia e Innovación (Proyecto FR2009-0101)
Importe total/Total amount:	12000 €
Investigador responsable/Research head:	Victorino Franco García

PUBLICACIONES / PUBLICATIONS

ARTÍCULOS PUBLICADOS EN REVISTAS SCI / PAPERS IN SCI JOURNALS

Scaling analysis of the magnetocaloric effect in $Gd_5Si_2Ge_{1.9}X_{0.1}$ (X=Al, Cu, Ga, Mn, Fe, Co)
V. Franco, A. Conde, V. Provenzano, R.D. Shull
Journal of Magnetism and Magnetic Materials, **322** (2) (2010) 218–223
DOI: 10.1016/j.jmmm.2009.08.039 Copyright

The field dependence of the magnetic entropy change has been studied for a series of doped $Gd_5Si_2Ge_2$ alloys, which possess a magnetic phase transition that is either entirely second order or a combination of primarily second-order mixed to a very minor degree with a first-order transition arising from a magneto-structural phase change. By analyzing the field scaling of the refrigerant capacity as well as of the reference temperatures used for constructing a universal scaling curve, a procedure for estimating the values of the critical exponents for the alloys was developed. For the cases where the transition is entirely second order, the results obtained from this procedure are comparable to the values obtained from the Kouvel–Fisher method. For the case of Fe-doped alloys which partially possess a first-order phase change, the Kouvel–Fisher method is inapplicable. However, their critical exponents determined by our developed procedure can be used to estimate the Curie temperature of the orthorhombic majority phase.

Influence of Co and Ni addition on the magnetocaloric effect in $Fe_{88-2x}Co_xNi_xZr_7B_4Cu_1$ soft magnetic amorphous alloys
R. Caballero-Flores, V. Franco, A. Conde, K. E. Knipling, and M. A. Willard
Appl. Phys. Lett, **96** (2010) 182506
DOI: 10.1063/1.3427439

We have studied the magnetocaloric effect in a series of Fe88−2xCoxNixZr7B4Cu1 alloys. The partial substitution of Fe by Co and Ni leads to a monotonic increase in the Curie temperature (TC) of the alloys from 287 K for x = 0 to 626 K for x = 11. The maximum magnetic entropy change (ΔSMpk) at an applied field of 1.5 T, shows a value of 1.98 J K−1 kg−1 for x = 8.25. The refrigerant capacity (RC) has maximum values near 166 J kg−1 (for x = 0 and 2.75). These values place the present series of alloys among the best magnetic refrigerant materials, with an RC - 40% larger than Gd5Si2Ge1.9Fe0.1 and - 15% larger than Fe-based amorphous alloys.

Scaling laws for the magnetocaloric effect in second order phase transitions: From physics to applications for the characterization of materials
V. Franco, A. Conde
International Journal of Refrigeration, **33** (2010) 465-473
DOI: 10.1016/j.ijrefrig.2009.12.019

The detailed procedure for constructing the recently proposed phenomenological universal curve for the magnetic entropy change is presented, together with the exponents which control the field dependence of the different magnetocaloric-related magnitudes. Practical applications of the universal curve are also outlined: as a simple screening procedure of the performance of materials, as a method for making extrapolations to temperatures or fields not available in the laboratory, for the reduction of the experimental noise, for correcting the influence of non-saturating conditions, or as a way to eliminate the contribution of minority magnetic phases, among others.

Mechanical amorphization of $Fe_{75}Nb_{10}B_{15}$ powder: microstructural and magnetic characterization
J.J. Ipus, J.S. Blázquez, V. Franco, A. Conde, L.F. Kiss
Intermetallics, **18** (2010) 565-568
DOI: 10.1016/j.intermet.2009.10.007

The evolution of the amorphous fraction developed during the mechanical alloying of a mixture of pure 75 at.% Fe, 10 at.% Nb and 15 at.% B, XAm, has been followed by different techniques: X-ray diffraction, Mössbauer spectroscopy and magnetic permeability measurements; in order to compare their sensitivity in the detection of small fractions. The values obtained for the amorphous fraction from the three techniques show a roughly linear correlation above ∼20%. The most sensitive technique was Mössbauer spectroscopy (XAm obtained from the low hyperfine field contributions) and the less sensitive technique was X-ray diffraction. The Curie temperature of the amorphous phase increases with the milling time due to a slow and progressive incorporation of boron into this phase and the nanocrystals from the boron inclusions.

Influence of Co addition on the magnetic properties and magnetocaloric effect of Nanoperm $(Fe_{1-X}Co_X)_{75}Nb_{10}B_{15}$ type alloys prepared by mechanical alloying
J.J. Ipus, J.S. Blázquez, V. Franco, A. Conde
Journal of Alloys and Compounds, **496** (2010) 7-12
DOI: 10.1016/j.jallcom.2009.12.029

Magnetic properties and magnetocaloric response of mechanically alloyed $(Fe_{1-X}Co_X)_{75}Nb_{10}B_{15}$ (X = 0.15 and 0.30) powders have been studied as a function of crystalline fraction. From X-ray diffraction, it was observed that the amorphization process is delayed with the Co addition in the alloy. Crystallization temperature of the amorphous phase developed during milling decreases as Co content increases. Temperature dependence of magnetization curves shows that the Curie temperature of the amorphous phase increases as the Co content increases. The peak magnetic entropy change slowly increases with Co addition for low crystalline fractions and the refrigerant capacity decreases as Co increases in the alloy.

Structure and magnetic properties of Fe-Nb-B amorphous/nanocrystalline alloys produced by compaction of mechanically alloyed powders

J.J. Ipus, J.S. Blázquez, V. Franco, A. Conde, M. Krasnowski, T. Kulik, S. Lozano-Prez

Journal of Applied Physics, **107** (2010) 073901

DOI: 10.1063/1.3319669

Mechanical alloying of Fe_{75} $Nb_{10}B_{15}$ and $Fe_{85}Nb_5B_{10}$ systems has been performed from an initial mixture of elemental powders. A bcc supersaturated solid solution is developed during milling for both alloys. However, $Fe_{75}Nb_{10}B_{15}$ alloy also develops an amorphous phase, which amount increases with milling time. Milled powder samples were compacted at 7.7 GPa at different temperatures. Scanning electron microscopy images show that the presence of amorphous phase enhances the quality of compaction. Compaction at 823 K preserves both microstructure and magnetic properties of as-milled powders in both alloys. Compaction at 973 K affects mainly the crystalline fraction of the alloy with 10 at. % Nb. Compaction at 1273 K yields the formation of bcc Nb and fcc Fe23 B6 phases, which magnetically harden the material.

Field dependence of the magnetocaloric effect in core-shell nanoparticles

V. Franco, A. Conde, D. Sidhaye, B.L.V. Prasad, P. Poddar, S. Srinath, M.H. Phan, H. Srikanth

Journal of Applied Physics, **107** (2010) 09A902

DOI: 10.1063/1.3335514

The field dependence of the magnetic entropy change peak at the low temperature surface spin freezing transition in chemically synthesized, monodispersed Co, Co-Ag, and Ni-Ag core-shell nanoparticles is studied, with the aim of gaining insight into the critical exponents of this transition. It is evidenced that although the magnitude of the peak entropy change and position of the peak can be tuned by changing the composition and nature (metallic or organic) of the shell and surfactant layers, the characteristics of the spin freezing transition are not altered. The field dependence of the refrigerant capacity also confirms this finding.

Study of the field dependence of the magnetocaloric effect in $Nd_{1.25}Fe_{11}Ti$: a multiphase magnetic system

R. Caballero-Flores, V. Franco, A. Conde, Q. Y. Dong and H. W. Zhang

Journal of Magnetism and Magnetic Materials, **322** (2010) 804-807

DOI: 10.1016/j.jmmm.2009.11.007

The field dependence of magnetic entropy change ΔSM(T,H) has been studied in the crystalline sample Nd1.25Fe11Ti, a multiphase system constituted by three phases: Fe17Nd2, Fe7Nd and Fe11TiNd. The magnetic entropy change has been calculated from the numerical derivative of magnetization curves M(T,H) with respect to temperature and subsequent integration in field. To determine the field dependence of the experimental ΔSM, a local exponent n(T,H) can be calculated from the logarithmic derivative of the magnetic entropy change vs. field. In contrast with the results for single phase materials, where n at the Curie temperature TC is field independent, it is shown that for a multiphase system n evolves with field both at the Curie temperature of the system and the Curie temperatures of the constituent phases. This is in agreement with numerical simulations using the Arrott–Noakes equation of state.

Nanocrystallization kinetics under instantaneous growth approximation: experiments and celcellular automata simulations

J. S. Blázquez, M. Millán, C. F. Conde, A. Conde
Physica Status Solidi (A) Applications and Materials, **207** (2010) 1148-1153
DOI: 10.1002/pssa.200983359

Nanocrystallization kinetics is analyzed in the frame of instantaneous growth approximation, which implies that the time required for a crystallite to reach its final size is negligible with respect to the time required for the nanocrystallization process. This approach strongly simplifies the kinetic analysis and allows us to obtain the nucleation rate from both isothermal and non-isothermal nanocrystallization processes. Moreover, as no constraining mechanism is considered but the absence of growth, the results could be discussed in the frame of Johnson-Mehl-Avrami-Kolmogorov theory with a growth index equal to zero. Cellular automata simulations are in agreement with the observed kinetics and microstructure.

Nucleation rate and nanocrystallization of Co60-(Fe, Mn) 18-Nb6-B16 amorphous alloys in the frame of instantaneous growth approximation

J.S. Blázquez, M. Millán, C.F. Conde, A. Conde
Journal of Alloys and Compounds, **505** (2010) 91-95
DOI: 10.1016/j.jallcom.2010.06.034

Instantaneous growth approximation is based on the fact that the time required by a new nucleus to reach its saturation size is negligible in comparison with the time required for the whole crystallization process. This approximation has been applied to analyze the kinetics of the nanocrystallization process of $Co_{60}Fe_{18-x}Mn\ xNb_6B_{16}$ (x = 0 and 4) alloys. Direct application of JMAK theory leads to divergences at very high transformed fractions. Although this divergence could be due to some artifacts, it can also be solved after a reinterpretation of the geometrical impingement effect on nanocrystalline systems. A modified Arrhenius relationship can be used for a general description of the double dependency of nucleation rate on the transformed fraction (only through the local activation energy) and the temperature.

Influence of Mn on the magnetocaloric effect of nanoperm-type alloys

R. Caballero-Flores, V. Franco, A. Conde, L.F. Kiss
Journal of Applied Physics, **108** (2010) 073921
DOI: 10.1063/1.3489990

In this paper, the influence of the Mn content on the magnetocaloric response of ribbon-shaped amorphous samples of Fe80-xMn xB20 (x=10, 15, 18, 20, and 24), has been studied. For this purpose, the temperature and field dependence of the magnetic entropy change (Δ SM) have been obtained from magnetization curves. The partial substitution of Fe by Mn leads to a monotonous change in the Curie temperature (TC) of the alloys from 438 K for x=10 to 162 K for x=24, in agreement with the coherent-potential approximation. These Curie temperatures could make them good candidates to be used for magnetic refrigeration at room temperature. For an applied field of 1.5 T, the maximum entropy change (Δ SMpk) passes from 1 J K -1 kg-1 (x=10) to 0.5 J K-1 kg-1 (x=24), and the refrigerant capacity varies between 117 J kg-1 (x=10) and 68 J kg-1 (x=24). A linear relationship between Δ S Mpk and the average magnetic moment per transition metal atom (〈μ〉 Fe,Mn) has been presented.

A new criterion to distinguish the order of magnetic transitions by means of magnetic measurements

C.M. Bonilla, F. Bartolom, L.M. García, M. Parra-Borderías, J. Herrero-Albillos, V. Franco
Journal of Applied Physics, **107** (2010) 09E131
DOI: 10.1063/1.3366614

A universal curve for the magnetic entropy change has been found to exist for a variety of materials with second order phase transitions. We have studied whether this universal behavior of the magnetocaloric effect is maintained in materials with first order phase transition, including R Co2 Laves phases and mixed La2/3 (Cax Sr1-x) 1/3 MnO3 manganites, which present both second order and first order magnetic ordering phase transitions. The rescaled magnetic entropy change curves for different applied fields collapse onto a single curve only for materials with second order phase transition. This universal curve may be used as a criterion for determining the order of magnetic phase transitions from purely magnetic measurements.

Magnetocaloric effect and refrigerant capacity in Sr-doped Eu8 Ga16 Ge30 type-I clathrates

M.H. Phan, V. Franco, A. Chaturvedi, S. Stefanoski, H. Kirby, G.S. Nolas, H. Srikanth
Journal of Applied Physics, **107** (2010) 09A910
DOI: 10.1063/1.3349409

Magnetic properties, the magnetocaloric effect (MCE) and refrigerant capacity (RC) were investigated in Eu8 Sr8-xGa16 Ge30 (x=0,4) type-I clathrates. The substitution of Sr for Eu decreases the Curie temperature (TC) and saturation magnetization (MS) from 35 K and 65 emu/g for the x=0 composition to 15 K and 35 emu/g for the x=4 composition. This is attributed to the increase in the Eu-Eu distance with Sr substitution. The large MCE and RC are achieved in both specimens. For a field change of 3 T, the MCE and RC reach the largest values of 5.8 J/kg K and 127.6 J/kg for x=0 composition and 4.3 J/kg K and 72.1 J/kg for x=4 composition. The broadening of the MCE curves is likely associated with the ordering of the magnetic moments of Eu that occurs below 10 K. The large values of MCE and RC, in addition to the absence of thermal and field hysteresis indicate that these clathrate materials are very interesting for cryogenic magnetic refrigeration applications.

Nanocrystalline Nd2Fe17 synthesized by high-energy ball milling: Crystal structure, microstructure and magnetic properties

P. Alvarez, P. Gorria, V. Franco, J.S. Marcos, M.J. Pérez, J.L. Sánchez Llamazares, I.P. Orench, J.A. Blanco

Journal of Physics Condensed Matter, **22** (2010) 216005

DOI: 10.1088/0953-8984/22/21/216005

Nanocrystalline Nd2Fe17 powders have been obtained by means of high-energy ball milling from nearly single-phase bulk alloys produced by arc melting and high temperature homogenization annealing. The rhombohedral Th2Zn17-type crystal structure of the bulk alloy remains unaltered after the milling process, with almost unchanged values for the cell parameters. However, the severe mechanical processing induces drastic microstructural changes. A decrease of the mean crystalline size down to around 10nm is observed, giving rise to a considerable augmentation of the disordered inter-grain boundaries. This modification of the microstructure affects the magnetic behaviour of the milled powders, although the magnetic structure remains collinear ferromagnetic. While a unique ferro-to-paramagnetic transition temperature, TC = 339 2K, is observed in the bulk alloy, the nanocrystalline samples exhibit a more likely distribution of TC values. The latter seems to be responsible for the significant broadening of the temperature range in which magneto-caloric effect is observed, and the lowering of the maximum value of the magnetic entropy change.

Tricritical point and critical exponents of La0.7Ca0.3−xSrxMnO3 (x = 0, 0.05, 0.1, 0.2, 0.25) single crystals

M.H. Phan, V. Franco, N.S. Bingham, H. Srikanth, N.H. Hur, S.C. Yu

Journal of Alloys and Compounds, **508** (2010) 238-244

DOI: 10.1016/j.jallcom.2010.07.223

The nature of ferromagnetic phase transition and its critical properties in La0.7Ca0.3−xSrxMnO3 (x = 0, 0.05, 0.1, 0.2 and 0.25) single crystals have been studied systematically. Based on magnetic measurements and critical behavior analysis using Banerjee criterion and Kouvel–Fisher method, we demonstrate the existence of a tri-critical point, with critical exponents (β = 0.26 ± 0.01, γ = 1.06 ± 0.02) at $x \sim 0.1$, that separates “discontinuous” first-order magnetic transition (FOMT) for $x < 0.1$ compositions from “continuous” second-order magnetic transition

(SOMT) for x > 0.1 compositions. Above the tricritical point, the system (e.g. x = 0.2) shows a SOMT with the critical exponents ($\beta = 0.36 \pm 0.01$, $\gamma = 1.22 \pm 0.01$) belonging to the Heisenberg universality class ($\beta = 0.365 \pm 0.003$, $\gamma = 1.336 \pm 0.004$). This suggests that the magnetic interaction in these manganites is of short-range type. Our systematic studies show that chemical (internal) pressure induced by substituting larger Sr ions for smaller Ca ions, cooperative Jahn–Teller distortions, antiferromagnetic coupling, and formation of ferromagnetic clusters all have significant impact on the nature of the ferromagnetic phase transition, the conduction mechanism and colossal magnetoresistance (CMR) in the doped manganites.

Tunable Curie temperatures in Gd alloyed Fe-B-Cr magnetocaloric materials
J.Y. Law, R.V. Ramanujan, V. Franco
Journal of Alloys and Compounds, **508** (2010) 14-19
DOI: 10.1016/j.jallcom.2010.08.049

The magnetocaloric effect of Fe80-xB12Cr 8Gdx (x = 1, 2, 3, 5, 8, 10, 11) amorphous alloys was studied. Gd addition increases the thermal stability of the alloy and allows tuning the Curie temperature (TC). A linear relationship between the magnetic entropy change and the magnetic moment of the alloy was observed. The experimental values of magnetic field dependence of the magnetic entropy change were consistent with a phenomenological universal curve. The maximum magnetic entropy change, for x = 1, was ∼33% larger than Fe80B 12Cr8, the refrigerant capacity (RC) is ∼29% larger than Gd5Si2Ge1.9Fe0.1 and within 10% of Fe82.5Zr7B4Co2.75Ni 2.75Cu1 which is the best Fe-based amorphous MCM to date. The tunable TC can be used to increase RC and the temperature span of layered multi-composition magnetocaloric regenerators.

Universal behavior for magnetic entropy change in magnetocaloric materials: An analysis on the nature of phase transitions
C.M. Bonilla, J. Herrero-Albillos, F. Bartolomé, L.M. García, M. Parra-Borderías, V. Franco
Physical Review B - Condensed Matter and Materials Physics, **81** (2010) 224424
DOI: 10.1103/PhysRevB.81.224424

A universal curve for the change in the magnetic entropy has been recently proposed for materials with second-order phase transitions. In this work we have studied the universal behavior of the magnetocaloric effect in the family of cobalt Laves phases, R Co2, and mixed manganites, La2/3 (Cax Sr (1-x)) 1/3 MnO3, which exhibit first- and second-order phase transitions. The rescaled magnetic entropy change curves for different applied fields collapse onto a single curve for materials with second-order phase transition as opposed to the first-order phase transition compounds, for which this collapse does not hold. This result suggests that the universal curve may be used as a further criterion to distinguish the order of the phase transition.

Magnetocaloric effect in nanostructured Pr_2Fe_{17} and Nd_2Fe_{17} synthesized by high-energy ball-milling

P. Alvarez, J. Sánchez-Marcos, J.L. Sánchez Llamazares, V. Franco, M. Reiffers, J.A. Blanco, P. Gorria

Acta Physica Polonica A, **118** (2010) 867-869

Nanocrystalline Pr2Fe17 and Nd2Fe 17 powders with rhombohedral Th2Zn17-type crystal structure and average particle sizes around 20 nm have been obtained by high-energy ball milling. While the bulk alloys show a well-defined and sharp drop in the low-field magnetization curve at the Curie temperature, T C = 285 K (Pr) and 335 K (Nd), the ball-milled samples exhibit a substantial broadening of the ferro-to-paramagnetic transition due to a considerable augmentation of the disordered inter-grain boundaries. The latter results in an increase of more than 25% in the values of the full width at half maximum of the temperature dependence of the magnetic entropy change maintaining almost unchanged the relative cooling power.

Avalanche criticality in the martensitic transition of $Cu_{67.64}$ $Zn_{16.71}$ $Al_{15.65}$ shape-memory alloy: A calorimetric and acoustic emission study

M.C. Gallardo, J. Manchado, F.J. Romero, J. Del Cerro, E.K.H. Salje, A. Planes, E. Vives, R. Romero, M. Stipcich

Physical Review B - Condensed Matter and Materials Physics, **81** (2010) 174102

The first-order diffusionless structural transition in Cu67.64 Zn16.71 Al15.65 is characterized by jerky propagation of phase fronts related to the appearance of avalanches. In this paper, we describe a full analysis of this avalanche behavior using calorimetric heat-flux measurements and acoustic emission measurements. Two different propagation modes, namely, smooth front propagation and jerky avalanches, were observed in extremely slow measurements with heating and cooling rates as low as a few 10-3 K/h. Avalanches show criticality where each avalanche leads to a spike in the heat flux. Their statistical analysis leads to a power law [P (E) ~ E-ε, where P (E) dE is the probability to observe an avalanche with energy E in an interval between E and E+dE] with an energy exponent of ε=2.15±0.15 in excellent agreement with the results of acoustic emission measurements. Avalanches appear to be more common for heating rates faster than 5× 10-3 K/h whereas smooth front propagation occurs in all calorimetric measurements and (almost) exclusively for slower heating rates. Repeated cooling runs were taken after a waiting time of 1 month (and an intermediate heating run). Correlations between the avalanche sequences of the two cooling runs were found for the strongest avalanche peaks but not for the full sequence of avalanches. The memory effect is hence limited to strong avalanches.

Deuteration effect on tricritical phase transition of triglycine selenate: Calorimetric and dielectric measurements analyzed in the framework of Landau theory

F.J. Romero, M.C. Gallardo, J.M. Martín-Olalla, J. Del Cerro

Journal of Applied Physics, **107** (2010) 124110

The ferroelectric phase transition of three single crystals of (TGSe) 1-x(DTGSe)x has been described by using specific heat, latent heat, and dielectric permittivity measurements. Pure, half-deuterated, and highly-deuterated TGSe single crystals were analyzed. Transition temperature and latent heat increase with increasing deuteration. Irrespective of the degree of deuteration, a 2-4-6 Landau model is suitable to describe the phase transition. The fourth-rank prefactor in Landau potential is found to be very sensitive to deuteration while the second-rank and the sixth-rank prefactors smoothly change with composition. The pyroelectric figure of merit for these materials has also been derived from the theoretical model.

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

Thermal stability of a supersaturated Fe-Ge-Nb solid solution produced by ball milling
J.J. Ipus, J. S. Blázquez, A. Conde
Journal of Physics: Conference Series, 217 (2010) 012083:1-5

CONGRESOS Y REUNIONES / CONGRESS AND MEETINGS

COMUNICACIONES EN CONGRESOS Y REUNIONES / COMMUNICATIONS IN CONGRESS AND MEETINGS

11th Joint MMM/Intermag Conference

17-21 Enero [Washington, Estados Unidos de América]

"Field dependence of the magnetocaloric effect in core-shell nanoparticles", V. Franco, A. Conde, P. Poddar, S. Srinath, M.H. Phan, H. Srikanth.

"Magnetocaloric effect and critical exponents in Sr doped Eu8Ga16Ge30 type I clathrates", A. Chaturvedi, M. H. Phan, H. Kirby, H. Srikanth, V. Franco, S. Stefanovski, G. S. Nolas.

"A new criterion to distinguish the order of magnetic transition by means of magnetic measurements", C. M. Bonilla, L. M. García-Vinuesa, J. Herrero, F. Bartolomé, M. Parra, V. Franco.

Tenth International Workshop on Non-crystalline Solids

21-23 Abril [Barcelona, España]

"Nanocrystalline nucleation rate for Co60-(Fe,Mn)18-Nb6-B16 amorphous alloys in the frame of instantaneous growth approximation", J.S. Blázquez, M. Millán, C. F. Conde, A. Conde

“Transmission electron microscopy and microanalytical studies of mechanically alloyed Fe-Ge-Nb powders”, J. J. Ipus, J. S. Blázquez, S. Lozano-Perez, A. Conde

XVII International Symposium on Metastable and Nano Materials (ISMANAM 2010)

4-9 Julio [Zurich, Suiza]

“Cellular automata simulations on nanocrystallization processes: From instantaneous growth approximation to limited growth”, J. S. Blázquez, C. F. Conde, A. Conde.

“The evolution of the structure, nanostructure and magnetic properties in Nd2Fe17 upon long-time high-energy ball milling”, P. Alvarez, J. Sánchez-Marcos, V. Franco, J.L. Sánchez Llamazares, J.A.Blanco, P. Gorria

“Factors affecting coercivity in soft magnetic Fe-Nb-B nanocrystalline alloys obtained by mechanical alloying”, J.J. Ipus, J. S. Blázquez, V. Franco, A. Conde

“Nucleation rates in nanocrystallization process of FeCrMoCuGaPCB amorphous alloys”, J.S. Blázquez, J. M. Borrego, C. F. Conde, A. Conde

14th Czech and Slovak Conference on Magnetism

6-9 Julio [Kosice, Slovakia]

“Magnetocaloric effect in the nanostructured R2Fe17 (R = Pr and Nd) synthesized by high-energy ball milling”, P. Alvarez, J. Sánchez-Marcos, V. Franco, J.L. Sánchez Llamazares, M. Reiffers, I. Puente Orench, J.A.Blanco, P. Gorria.

IV Baikal International Conference ”Magnetic Materials. New Technologies"

21-25 Septiembre [Irkutsk, Rusia]

“The magnetocaloric effect in soft magnetic amorphous alloys”, V. Franco, A. Conde.

55th MMM Conference

14-18 Noviembre [Atlanta, Estados Unidos de América]

“Magnetocaloric effect and critical exponents of Fe77Co5.5Ni5.5Zr7B4Cu1: a detailed study”, V. Franco, R. Caballero-Flores, A. Conde, K.E. Knipling, M. A. Willard.

IV Euro-Asian Symposium "Trends in Magnetism": Nanospintronics. EASTMAG – 2010
28 Junio – 2 Julio [Ekaterinburg, Rusia]

"Scaling laws for the magnetocaloric effect: their applications to the optimization of materials", V. Franco, R. Caballero-Flores, A. Conde.

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 (Fritszch 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 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 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 éste. Para que un modo vibracional sea activo en espectroscopia Raman es necesario que se produzcan cambios en la polarizabilidad del enlace o la molécula considerada, lo que conlleva la producción de momento dipolares inducidos. Su campo de aplicación es muy extenso: semiconductores, compuestos del carbono (grafito, diamante, nanotubos, fibras…), catálisis, 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 bonds or the considered molecule, which in turn results in the generation of induced dipolar momentum. 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 n´´umero de ondeas que va desde 5000 y 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 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 diferencia 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.

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 / FISI-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.

El servicio dispone de un analizador de adsorción de gases (Micromeritics, ASAP 2020) obtener 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 fisisorption 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.

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 y Ldo. Patrick Tuite Briales

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 color 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 Calorimétrica Diferencia de Barrido (CDB).

Thermal analysis techniques allows studying physical or chemical changes in samples as a function of the temperature. Those changes should involve either a mass change or a heat flow.
In the service 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 Differentical 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 y Ldo. Patrick Tuite Briales

TAMAÑO DE PARTÍCULAS Y POTENCIAL Z / PARTICLE SIZE AND Z POTENTIAL ANALYSIS

Se dispone de las técnicas de "Dynamic light scattering" y Difracción láser (LD) para determinar la distribución de tamaños de partícula de sistemas coloidales en suspensión (disolvente acuoso u orgánico) en los rangos 3-3000 nanómetros (DLS) y 0.05-900 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 distribution of colloidal systems (aqueous or organic dispersions) 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 modelo Zetamaster (DLS) y 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 carried 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 at ~ 5 nm). It can be applied to all type of materials including ceramics, polymers, metals, minerals, catalysts, samples from cultural heritage, thin films, coatings, interphases, 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 y Ldo. Patrick Tuite Briales

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

SERVICIO DE DIFRACCIÓN DE RAYOS X / DIFFRACTION 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 (⍰-2⍰), 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 transparente 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 (⍰-2⍰), 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 y Ldo. Patrick Tuite Briales

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 la 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

Típicamente 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 superficie de los sólidos (20-30 Å), lo que permite 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 de vídrios, fenómenos de flotación y adherencia, y los de segregación en metalúrgica, etc. Siendo el XPS/ESCA una técnica insustituible para abordar multitud de problemas que surgen en dichos campos tecnológicos.
La característica más importante de la Espectroscopía de Fotoelectrones (XPS/ESCA) es el permitir diferenciar distintos estados de oxidación y/o situaciones del entorno (coordinación) de los átomos en las muestras sólidas analizadas así como el estudio de perfiles de composición combinando la técnica con el desbastado iónico empleando iones Ar+ acelerados. 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 of glasses, floating and adhesion phenomena, or segregation processes in metallurgy, among others. All that makes confers XPS a unique technique to deal with multiple problems that arise in those technological fields.
The most remarkable characteristic of X-Ray Photoelectron Spectroscopy (XPS/ESCA) is that allows to discriminate, for a given element, between different oxidation states and/or chemical surroundings (coordination), and in combination with an sputtering process (using accelerated Ar+ ions) to obtain a compositional depth profile.

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, Alka y MgKa, 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 prechambers subjected submitted 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 treatment 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, Alka y MgKa).
  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, Inga. Patricia del Arco González

SERVICIO DE ESPECTROMETRÍA DE EMISIÓN ÓPTICA POR DESCARGA LUMINISCENTE/ GLOW DISCHARGE OPTICAL EMISSION SPECTROMETRY SERVICE (GD-OES)

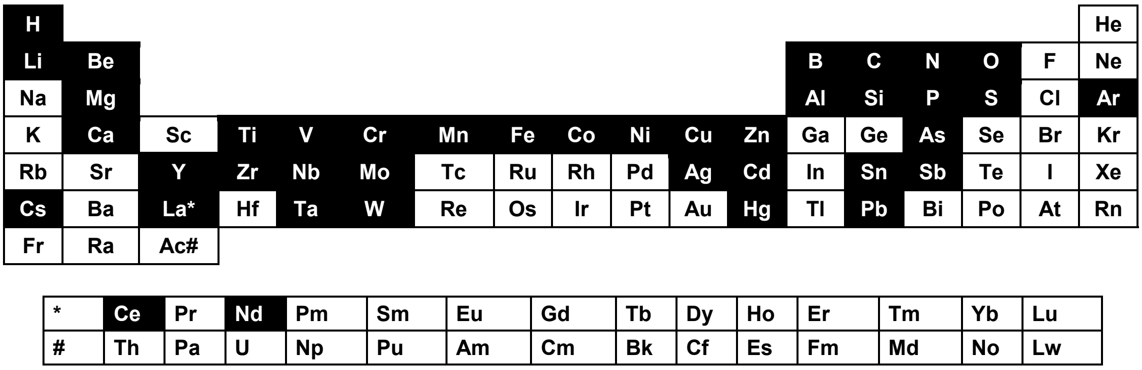
Las técnicas de espectrometría por descarga luminiscente constituyen una potente herramienta para el análisis rápido de sólidos tanto en masa como en superficie. Además se pueden determinar concentraciones elementales en función de la profundidad lo que permite realizar perfiles de concentración sobre materiales avanzados: metales tratados, metales y otros materiales recubiertos, multicapas, superficies pintadas, muestras duras recubiertas con polímeros, capas finas, procesos de corrosión y oxidación y muchos otros. 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 encuentran 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 an autosustained 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 offer 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/ MACHINING 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,…, 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: 28 junio al 2 de julio de 2010
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**:**
Interacción de Fotones, Electrones e Iones con la Materia. Métodos Experimentales de Análisis de Sólidos | Dr. Agustín R. González-Elipe
Espectroscopía de Fotoemisión de Rayos X: Composición Superficial | Dr. Juan Pedro Espinós
Espectroscopía de Fotoemisión de Rayos X: Estado Químico en la Superficie de Sólidos | Dr. Agustín R. González-Elipe
Microscopías Efecto Túnel y de Fuerzas Atómicas | Dr. José Jesús Benítez Jiménez
Determinación de Perfiles de Composición a partir del Análisis de Forma de Pico en XPS: Método de Tougaard | Dr. Francisco Yubero Valencia
Microscopía Electrónica de Transmisión y Barrido: Fundamentos y Aplicaciones Generales | Dra. Asunción Fernández Camacho
Microscopía Electrónica de Alta Resolución: Simulación | Dra. María Jesús Sayagués

Aplicaciones Avanzadas de las Capas Finas | Dr. Juan Pedro Espinós
Deposición de Láminas Delgadas mediante Métodos Basados en la Utilización de Plasmas| Dr. José Cotrino Bautista
Métodos de Determinación de Espesores de Capas Finas | Dr. Juan Pedro Espinós Manzorro
Microscopía Electrónica: Análisis PEELS y EFTEM| Dra. Cristina Rojas Ruiz
La Difracción y la Fluorescencia de Rayos X en el Análisis de Capas Delgadas| Dr. Angel Justo Erbez
Absorción de R-X: Orden a Corto Alcance en Superficie y Láminas Delgadas| Dra. Adela Muñoz Páez
Retrodispersión Rutherford: Perfiles de Composición | Dr. Miguel Angel Respaldiza (CNA)

Prácticas:
Microscopías Electrónicas de Transmisión y Barrido | Dra. Cristina Rojas | Lda. Carmen Jiménez de Haro | Lda. Olga Montes
XPS/ISS/AES/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: 27 al 29 de octubre de 2010
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
Difracción de Rayos X con Radiación Sincrotrón | Dr. Carlos Frontera, ICMB, Barcelona
Espectroscopía de Absorción de Rayos X | Dra. Adela Muñoz Páez
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
Macromolecular crystallography for industry at the advanced photon source of Argonne National Laboratory | Dr. Stephen R. Wasserman, Eli Lilly and Company
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 de Baja Energía | Dr. Agustín R. González-Elipe
Experimentos con Resolución Temporal | Dr. Victor López Flores, Universidad de Estraburgo, Bélgica
Microscopía de Rayos X: Principios y Aplicaciones | Dra. Gema Martínez Criado, ESRF, Grenoble, Francia
Combining synchrotron radiation techniques to the study disordered materials | Dr. Neville Greaves, Aberystwyth University, Gales, Gran Bretaña
La Fuente de Luz Sincrotrón "ALBA". Estado de la Fuente y Líneas en Construcción | Dr. Igor Sics, ALBA, Barcelona

DETERMINACIÓN DE ESTRUCTURAS EN SÓLIDOS REALES: TÉCNICA DE RESONANCIA MAGNÉTICA NUCLEAR

Curso de Postgrado del CSIC
Programa 2007-08

rmn SÓLIDOS

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: 13 al 17 de septiembre de 2010
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. Ana Isabel Becerro Nieto
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 y Lda. Esperanza Pavón
RMN de Sólido de Núcleos con Espín ½ Abundantes | Dr. Miguel Angel Castro Arroyo y Dra. María Dolores Alba
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
RMN de Sólido de Núcleos con Espín ½ y bajo gamma | Dra. María Dolores Alba Carranza
RMN de No-Sólido No-Líquido | Dr. Pedro Nieto
Profesores de Seminarios: Dra. María Dolores Alba, Dr. Pablo Chain, Ldo. Juan Isidro Corredor, Dr. Alberto Escudero, Ldo. Marco Mantovani, Lda. María del Mar Orta, Lda. Esperanza Pavón
Profesor de Prácticas: Dr. Miguel Angel Avilés Escaño

MÁSTER / MASTER

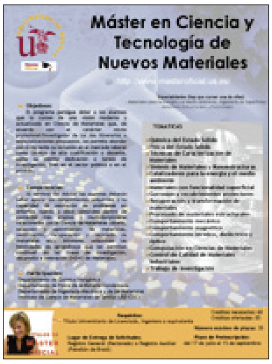
MÁSTER EN ESTUDIOS AVANZADOS EN QUÍMICA

Organizado por la Universidad de Sevilla
Coordinadora: Dra. Mª Angeles Alvarez Rodríguez
Fecha de Celebración: Curso Académico 2009-10
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 (USE) | Dra. Maria Angeles Pradera (USE) | Dr. José M. Fernández-Bolaños (USE)
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: 4) | Dr. Guillermo Munuera | Dr. Juan Cámpora (IIQ) | Dr. Antonio Pizzano (IIQ)

MÁSTER EN CIENCIA Y TECNOLOGÍA DE NUEVOS MATERIALES



Máster en Ciencia y Tecnología de Nuevos Materiales

Organizado por la Universidad de Sevilla
Coordinador: Dr. Antonio Córdoba Zurita
Fecha de Celebración: Curso Académico 2009-10
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) | Dr. Guillermo Munuera | Dr. Miguel Angel Castro | Dra. Pilar Malet
Fisica del Estado Sólido (Créditos Europeos: 5) | Dr. Alfonso Bravo | Dra. Josefa Borrego | Dr. Manuel Jiménez Melendo
Técnicas de Caracterización de Materiales (Créditos Europeos: 8) | Dra. Adela Muñoz Páez | Dr. Antonio Ramírez de Arellano | Dr. Julián Martínez Fernández | Dr. Juan M. Montes (USE) | Dr. Juan Pedro Holgado
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 Escolano (USE) | Dr. Juan Carlos Sánchez López | Dr. L. Soria Conde (USE) | Dr. Enrique Herrera (USE)
Recuperación y Transformación de Materiales (Créditos Europeos: 5) | Dr. Gerardo Colón | Dr. José Antonio Odriozola | Dr. Luis Pérez Maqueda
Procesado de Materiales Estructurales (Créditos Europeos: 5) | Dr. Alfonso Bravo León | Dr. Julián Martínez Fernández | Dr. José A. Rodríguez Ortiz (USE)
Comportamiento Mecánico (Créditos Europeos: 5) | Dr. Arturo Domínguez Rodríguez | Dra. Angela Gallardo López | Dr. Diego Gómez
Comportamiento Magnético (Créditos Europeos: 5) | Dr. Alejandro Conde Amiano | Dra. Clara F. Conde Amiano | Dr. Victorino Franco
Comportamiento Térmico, Dieléctrico y Óptico (Créditos Europeos: 5) | Dra. M. Carmen Gallardo Cruz | Dr. Hernán Míguez García | Dr. Jaime del Cerro

Computación en Ciencia de Materiales (Créditos Europeos: 5) | Dr. Antonio Córdoba (USE) | Dr. Agustín Galindo del Pozo (USE) | Dr. Felipe Gutiérrez Mora

Máster en Ciencia, Tecnología y Uso Racional del Medicamento.
Análisis y Control de Materias Primas
Dr. Miguel Angel Castro Arroyo
Organizado por la Universidad de Sevilla

Máster “Biotecnología Avanzada”
Módulo Biotecnología
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

OTROS / OTHER

Jornadas sobre “Soluciones catalíticas y de adsorción para la contaminación atmosférica”
Dr. José Antonio Odriozola
Curso Internacional de Postgrado. Programa Iberoamericano de Ciencia y Tecnología para el Desarrollo (CYTED) y la Agencia Española de Cooperación Internacional para el desarrollo (AECID)
Fecha de Celebración: 9 al 13 de diciembre de 2008
Organizado el Centro de Formación de la Cooperación Española en Antigua (Guatemala)

Arcilla y Salud
Dra. María Dolores Alba Carranza
Organizado por la Universidad de Sevilla

Training pre-program in European Conference
Dra. María Dolores Alba Carranza
Organizado por 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

Tratamiento de minerales de la arcilla por ultrasonido
José Luis Pérez Rodríguez
Lugar: Universidad de La Plata, Argentina

Daños en el Patrimonio Histórico Artístico
José Luis Pérez Rodríguez
Lugar: Universidad de Buenos Aires, Argentina

Superplasticity: current status and perspectives
Diego Gómez
Lugar: Japón

CONFERENCIAS Y SEMINARIOS IMPARTIDOS EN EL ICMS CONFERENCES AND SEMINAR IN THE ICMS

CICLO DE CONFERENCIAS / CONFERENCES

13 de abril |**Micro-Raman spectroscopy: a powerful tool to analyze textured thin films**
Juan Carlos González González
Instituto de Ciencia de Materiales de Sevilla

16 de marzo |**XPS imaging of nano-structures**
Sven Tougaard
University of Southern Denmark

8 de abril |**Self-Assembly of Functional Composites for Storing, Generating and Harvesting Photons and Electrons**
Paul V. Braun
Department of Materials Science and Engineering University of Illinois at Urbana-Champaign

13 de abril | **Mechanochemistry of Solids**
Peter Balaz
Departament of Mechanochemistry. Institute of Geotechnics (Academia Eslovaca de Ciencias), Kosice (Eslovaquia)

20 de mayo |**Self Assembly of Multicomponent Nanoparticles for Diverse Technological Application**
Beri N. Mbenkum
Max Planck Institute for Metals Research, Heisenbergstr. Stuttgart, Germany

28 de mayo | **Heterogeneous Photocatalysis at Liquid-Solid Interfaces. Some recent mechanistic developments**
Roger I. Bickley
University of Bradford, UK

7 de octubre | **Materials for Carbon Based Electronics**
Pierangelo Groening
Head of the Advanced Materials and Surfaces Dept. Swiss Federal Laboratories for Materials Testing and Research EMPA-ETH

14 de octubre | **Mejoramiento de las propiedades mecánicas en aleaciones base cobre mediante ordenamiento, precipitación y/o segregación de soluto**
Eduardo Donoso Catalán
Director del Departamento de Ciencia de Materiales. Facultad de Ciencias Físicas y Matemáticas. Universidad de Chile, Santiago (Chile)

19 de octubre | **Microscopía Electrónica de Ultra-alta resolución**
Tetsuo Oikawa
Director del grupo de especialistas de aplicaciones de JEOL Europa "Advanced Analytical TEM for material science"
Werfen Group. Izasa

4 de noviembre | **Catalytic chemistry and self-assembly on metal surfaces**
Richard M. Lambert
Cambridge University / Instituto de Ciencias de Materiales de Sevilla

ESTANCIAS Y VISITAS DE PERSONAL DEL ICMS EN OTROS CENTROS
PERSONNEL OF THE ICMS IN OTHER LABORATORIES

Université Louis Pasteur		
Estrasburgo, Francia	**Francisca Romero Sarria**	[3 dias]
	Miguel Angel Centeno Gallego	[3 dias]
	José Antonio Odriozola Gordón	[3 dias]
Instituto de Nanociencia de Aragón		
Zaragoza, España	**Nuria Ofelia Núñez Alvarez**	[3 días]

Universidad Autónoma de Nuevo León		
Monterrey, México	**Nuria Ofelia Núñez Alvarez**	[1 semana]
Universidad de Oriente		
Santiago de Cuba, Cuba	**Nuria Ofelia Núñez Alvarez**	[1 semana]
Departamento de Química Aplicada. Facultad de Ciencias Químicas de San Sebastián. Universidad del Pais Vasco		
San Sebastián, España	**María Isabel Domínguez Leal**	[8 dias]
Instituto de Geotécnica, Academia Eslovaca de Ciencias		
Kosice, Eslovaquia	**María Jesús Sayagués de Vega**	[10 dias]
	María Dolores Alcalá González	[10 dias]
	Francisco José Gotor Martínez	[10 dias]
Instituto de Química Inorgánica. Academia de Ciencia Checa		
República Checa	**José Manuel Criado Luque**	[10 dias]
	María Jesús Diánez Millán	[10 dias]
	Luis Pérez Maqueda	[10 dias]
	José Luis Pérez Rodríguez	[10 dias]
	Antonio Perejón Pazo	[1mes]
Departamento de Ciencia de Materiales, Universidad de Chile		
Santiago, Chile	**José Manuel Criado Luque**	[15 dias]
	María Jesús Diánez Millán	[15 dias]
Centro CIDIA de la Universidad de Las Palmas de Gran Canaria		
Las Palmas de Gran Canaria, España	**José Antonio Navío Santos**	[15 dias]
Universidad de Buenos Aires		
Buenos Aires, Argentina	**José Luis Pérez Rodríguez**	[15 dias]
Walther-Meißner-Institute		
Munich, Alemania	**Juan Poyato Ferrera**	[1 mes]
Universidad Pública de Navarra		
Pamplona, España	**Oscar H. Laguna Espitia**	[3 meses]
Department of Materials. Universidad de Oxford		
Oxford, Gran Bretaña	**Ernesto Chicardi Augusto**	[3 meses]
Universidad de Toronto		
Toronto, Ontario, Canadá	**Gabriel Lozano Barbero**	[3 meses]

Estancias y Visitas de Investigadores en el ICMS Personnel of the Other Laboratories in the ICMS

Université Louis Pasteur		
Estrasburgo, Francia	**Anne Cecile Roger**	[3 dias]
Kungliga Tekniskahögskolan (KTH) Chemical Science and Engineering Teknikringe		
Estocolmo, Suecia	**Magaly Boutonnet**	[3 dias]
	Sven Järas	[3 dias]
Université Louis Pasteur		
Estrasburgo, Francia	**Marcia Areque**	[1 semana]
Instituto de Geotécnica. Academia Eslovaca de Ciencias		
Kosice, Eslovaquia	**Peter Balaz**	[10 dias]
	Marcela Achimovicoca	[10 dias]
	Martin Fabian	[10 dias]
Institute of General and Inorganic Chemistry. Bulgarian Academy of Sciences		
Sofia, Bulgaria	**Mihail Mihaylov**	[2 semanas]
	Nikola Drenchev	[2 semanas]
Universidad de Pardubice		
Pardubic, República Checa	**Jiri Malek**	[15 dias]
Departamento de Ciencia de Materiales. Universidad de Chile		
Santiago, Chile	**Eduardo Donoso Catalán**	[15 dias]
Walther-Meißner-Institute		
Munich, Alemania	**Anton Lerf**	[15 dias]
Universidad de Antioquia		
Medellin, Colombia	**Juan Miguel Marín Sepúlveda**	[2 semanas]
	Laila Galeano Botero	[3 meses]
Universidad Pública de Navarra		
Pamplona, España	**Alberto Navajas León**	[1 mes]
Universidad de Concepción		
Concepción, Chile	**Claudia Margarita Campos Urrutia**	[2 meses]
L'Ecole Nationale Supérieure d'Ingenieurs de Caen et Centre de Recherche, ENSICAEN		
Caen, Francia	**Claudia Margarita Campos Urrutia**	[3 meses]

OTRAS ACTIVIDADES / OTHER ACTIVITIES

FERIA DE LA CIENCIA / FAIR OF SCIENCE

La VIII Feria de la Ciencia (6, 7 y 8 de mayo de 2010, 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: "Materiales, Nanomateriales y Color"

The VII Fair of Science (14, 15, and 16 May 2010, 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: "Materials, Nanomaterials and Colour"

SEMANA DE LA CIENCIA Y LA TECNOLOGÍA / SCIENCE AND TECHNOLOGY WEEK

Jornadas de puertas abiertas (Semana del 15 al 18 de Noviembre de 2010, 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.

"Open-door" week (15-18 November 2010). The Science and Technology week is open to every body. The event has an European character and is designer to demonstration in Science and Technology.

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