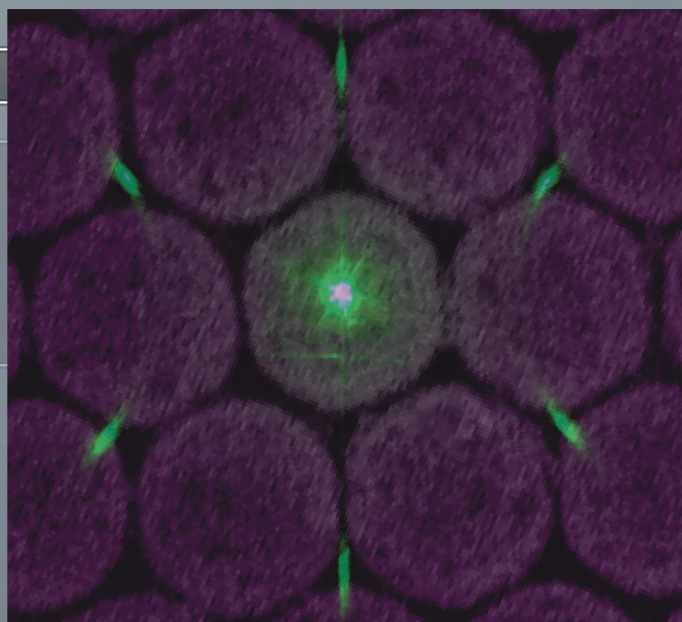


Instituto de Ciencia de Materiales de Sevilla

2009

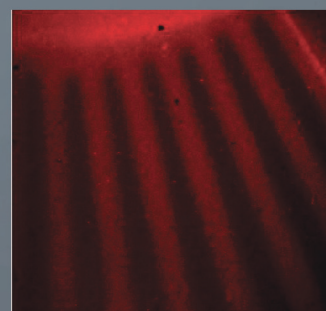
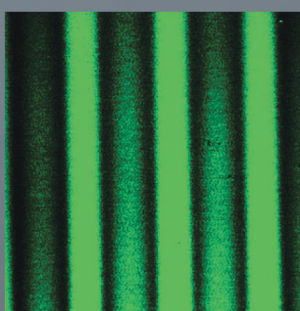
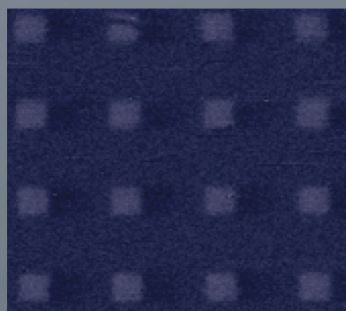
Memoria de Actividades Annual Report



Consejo
Superior de
Investigaciones
Científicas

Universidad
de Sevilla

Junta de
Andalucía



Consejo Superior de Investigaciones Científicas
Universidad de Sevilla
Junta de Andalucía

INSTITUTO DE CIENCIA DE MATERIALES DE SEVILLA

Memoria de Actividades
Annual Report
2009

Centro de Investigaciones Científicas “Isla de la Cartuja”
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EDITA**Instituto de Ciencia de Materiales de Sevilla (ICMS)**

Centro Mixto entre el Consejo Superior de Investigaciones Científicas y la Universidad de Sevilla

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<http://www.icmse.csic.es>

DISEÑO

José Carlos Rivero Cabello

COMISIÓN MEMORIA-ICMS

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

IMPRIME

Publidisa

DEPÓSITO LEGAL

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EI ICMS en 2009
ICMS in 2009

Presentación Presentation

A través de esta Memoria 2009, 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), pertenece al 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 más de 120 personas, 50 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 2009, 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), 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.

Datos Estadísticos del ICMS
Statistical Data of ICMS

■ PERSONAL / PERSONNEL

Distribución del personal por Categorías (Sede-CicCartuja)
Personnel distribution by categories Sede-CicCartuja

PERSONAL FUNCIONARIO **50**

CSIC

Profesores de Investigación	4
Investigadores Científicos	8
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Titulados Superiores Especializados	1
Titulados Técnicos Especializados	4
Ayudantes de Investigación y Laboratorio	3
Auxiliares de Investigación y Laboratorio	1

UNIVERSIDAD DE SEVILLA

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Profesores Titulares	9

PERSONAL LABORAL **4**

CSIC

Nivel I	1
Nivel III	1
Nivel V	1

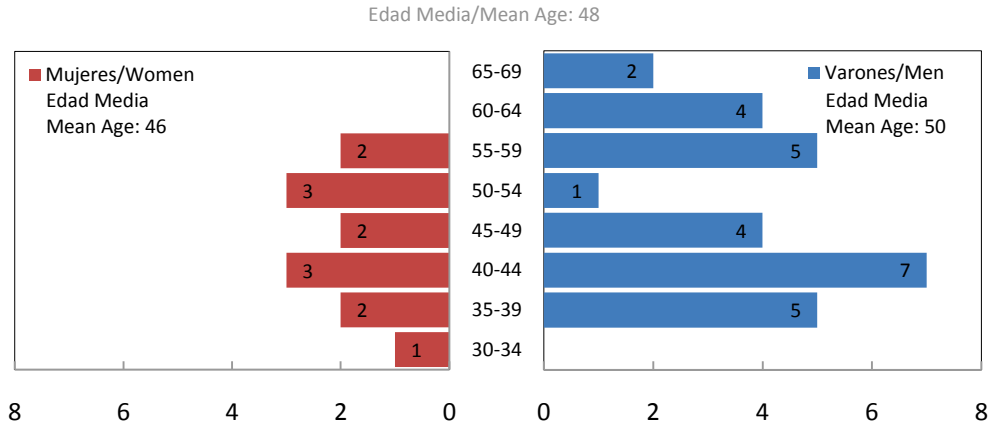
UNIVERSIDAD DE SEVILLA

Nivel III	1
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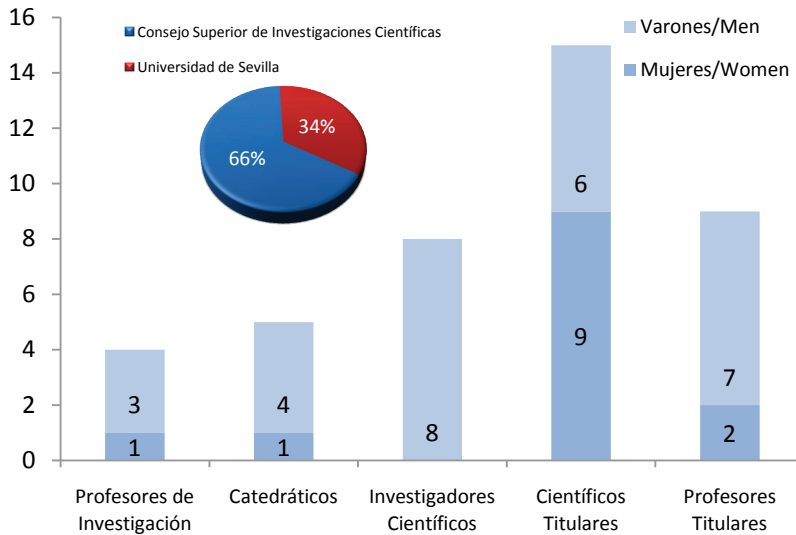
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Distribución del personal investigador por edad (Sede-CicCartuja) Histogram of the scientific Personnel's Age

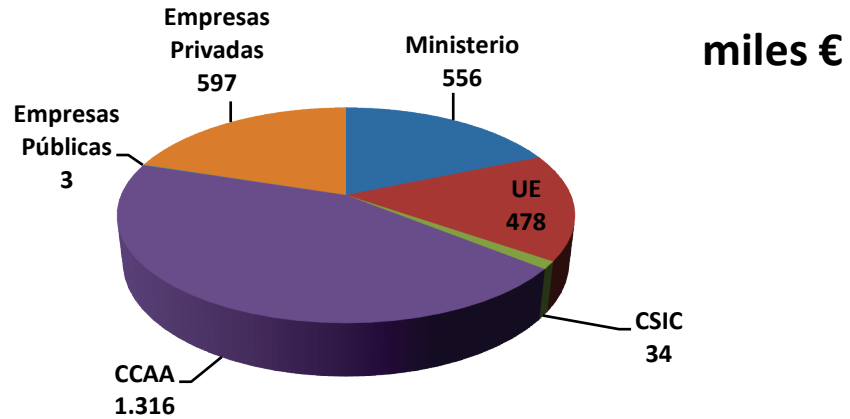


Distribución del Personal Investigador por Categoría y Sexo (Sede-CicCartuja) Histogram of the Scientific Personnel by Professional Category and Sex

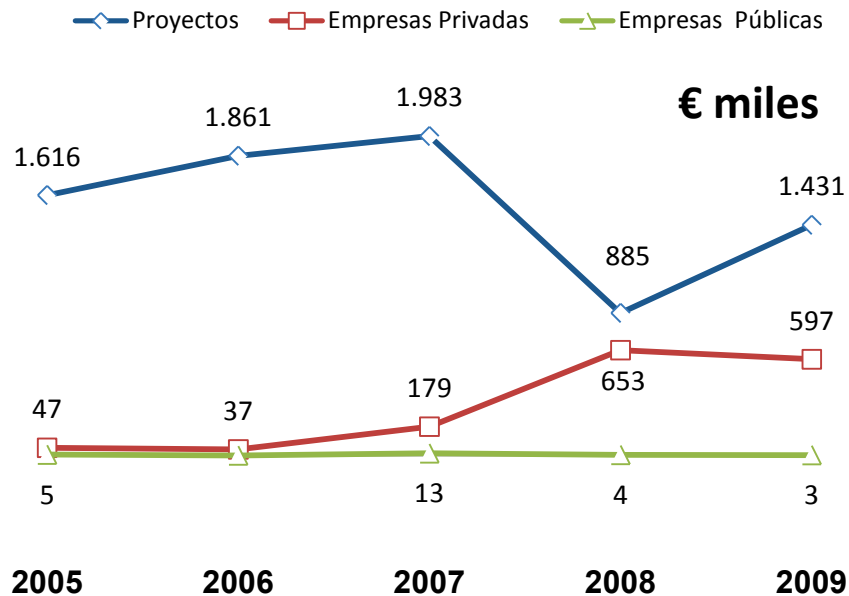


FINANCIACIÓN / FUNDING

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



Evolución 2005-2009 de la Financiación del ICMS (PCO)
Evolution of the funding of the ICMS in the period 2005-2009



■ 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(*)
NANO TODAY	1	8.795
ADVANCED MATERIALS	1	8.191
PHYSICAL REVIEW LETTERS	1	7.18
SMALL	1	6.525
CHEMISTRY-A EUROPEAN JOURNAL	1	5.454
CHEMICAL COMMUNICATIONS	1	5.34
JOURNAL OF CATALYSIS	1	5.167
APPLIED CATALYSIS B-ENVIRONMENTAL	5	4.853
JOURNAL OF MATERIALS CHEMISTRY	2	4.646
ENVIRONMENTAL SCIENCE & TECHNOLOGY	1	4.458
CRYSTAL GROWTH & DESIGN	1	4.215
JOURNAL OF PHYSICAL CHEMISTRY B	1	4.189
LANGMUIR	4	4.097
OPTICS EXPRESS	1	3.88
APPLIED PHYSICS LETTERS	1	3.726
NANOTECHNOLOGY	1	3.446
JOURNAL OF PHYSICAL CHEMISTRY C	8	3.396
POLYMER	1	3.331
ANALYTICAL AND BIOANALYTICAL CHEMISTRY	3	3.328
PHYSICAL REVIEW B	2	3.322
TALANTA	1	3.206
APPLIED CATALYSIS A-GENERAL	3	3.19
CATALYSIS TODAY	3	3.004
JOURNAL OF HAZARDOUS MATERIALS	2	2.975
PLASMA PROCESSES AND POLYMERS	5	2.921
SCRIPTA MATERIALIA	1	2.887
CHEMICAL ENGINEERING JOURNAL	3	2.813
ULTRASONICS SONOCHEMISTRY	1	2.796
CATALYSIS COMMUNICATIONS	2	2.791
SOLAR ENERGY MATERIALS AND SOLAR CELLS	1	2.788
JOURNAL OF BIOMEDICAL MATERIALS RESEARCH PART A	1	2.706
MICROPOROUS AND MESOPOROUS MATERIALS	4	2.555

REVISTA JOURNAL	ARTÍCULOS PAPERS	FACTOR DE IMPACTO IMPACT FACTOR(*)
BIOINTERPHASES	1	2.347
POLYMER DEGRADATION AND STABILITY	1	2.32
JOURNAL OF APPLIED PHYSICS	6	2.201
JOURNAL OF PHYSICS D-APPLIED PHYSICS	1	2.104
JOURNAL OF THE AMERICAN CERAMIC SOCIETY	3	2.101
APPLIED CLAY SCIENCE	4	2.005
JOURNAL OF THE EUROPEAN CERAMIC SOCIETY	2	1.999
AMERICAN MINERALOGIST	2	1.962
JOURNAL OF NANOSCIENCE AND NANOTECHNOLOGY	1	1.929
JOURNAL OF PHYSICS-CONDENSED MATTER	3	1.9
THIN SOLID FILMS	2	1.884
CATALYSIS LETTERS	2	1.867
SURFACE & COATINGS TECHNOLOGY	4	1.86
APPLIED GEOCHEMISTRY	1	1.857
SOLID STATE SCIENCES	1	1.742
SURFACE SCIENCE	1	1.731
THERMOCHIMICA ACTA	1	1.659
JOURNAL OF THERMAL ANALYSIS AND CALORIMETRY	1	1.63
JOURNAL OF MOLECULAR STRUCTURE	1	1.594
APPLIED SURFACE SCIENCE	2	1.576
JOURNAL OF ALLOYS AND COMPOUNDS	3	1.51
WEAR	1	1.509
CHEMICAL VAPOR DEPOSITION	1	1.483
JOURNAL OF NON-CRYSTALLINE SOLIDS	2	1.449
JOURNAL OF SOL-GEL SCIENCE AND TECHNOLOGY	1	1.433
X-RAY SPECTROMETRY	1	1.39
INTERNATIONAL BIODETERIORATION & BIODEGRADATION	3	1.375
CERAMICS INTERNATIONAL	1	1.369
MOLECULAR SIMULATION	2	1.325
JOURNAL OF MAGNETISM AND MAGNETIC MATERIALS	2	1.283
CLAYS AND CLAY MINERALS	1	1.171
NUCLEAR INSTRUMENTS & METHODS IN PHYSICS RESEARCH SECTION B-BEAM INTERACTIONS WITH MATERIALS AND ATOMS	1	0.999
CENTRAL EUROPEAN JOURNAL OF CHEMISTRY	1	0.741
EUROPEAN PHYSICAL JOURNAL-SPECIAL TOPICS	1	0.689
BOLETIN DE LA SOCIEDAD ESPANOLA DE CERAMICA Y VIDRIO	2	0.531

REVISTA JOURNAL	ARTÍCULOS PAPERS	FACTOR DE IMPACTO IMPACT FACTOR(*)
JOURNAL OF ADVANCED OXIDATION TECHNOLOGIES	1	0.495
REVISTA DE METALURGIA	1	0.47
INTERNATIONAL JOURNAL OF ARCHITECTURAL HERITAGE	-	-

(*) Factor de Impacto correspondiente al año 2008
Journal Citation Reports of 2008

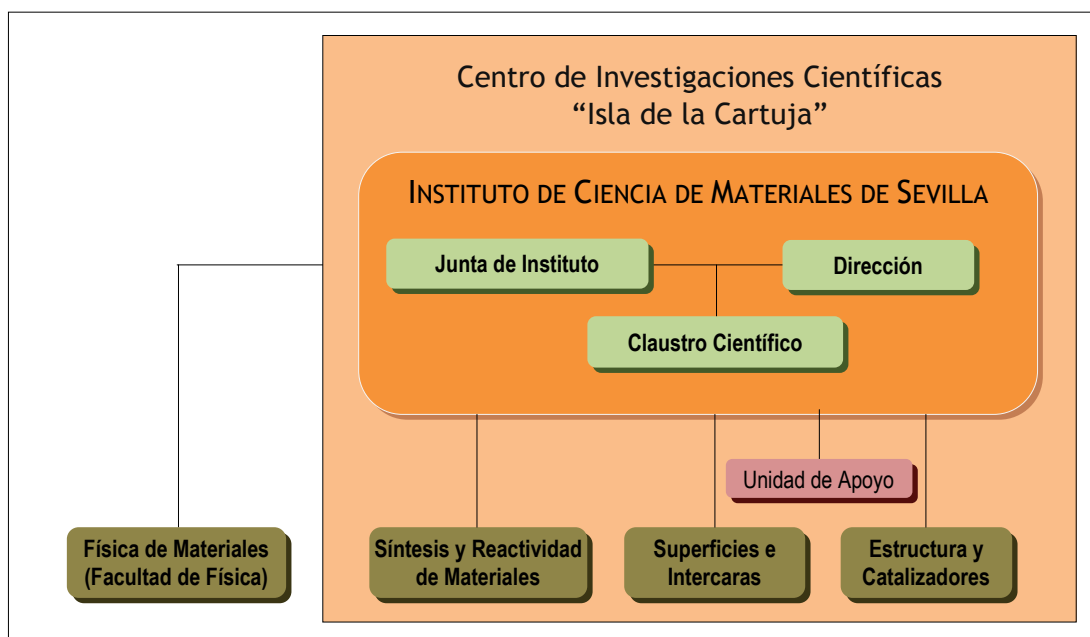
COMPOSICIÓN Y ESTRUCTURA

STRUCTURE AND ORGANISATION

- 1.1.** Organigrama
Organization chart
- 1.2.** Dirección
Directorate
- 1.3.** Junta de Instituto
Institute Board
- 1.4.** Claustro Científico
Scientific Board
- 1.5.** Unidades de Investigación
Research units



1.1. ORGANIGRAMA / ORGANIZATION CHART



1.2. DIRECCIÓN / DIRECTION

Director / **Director**: Alfonso Caballero Martínez
 Vicedirector / **Vicedirector**: Juan Pedro Espinós Manzorro

1.3. JUNTA DE INSTITUTO / INSTITUTE BOARD

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 Vicedirector / **Vicedirector**: D. Juan Pedro Espinós Manzorro

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D. Juan Pedro Holgado Vázquez. **Representante UI "Superficies e Intercaras"**

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D. José Antonio Odriozola Gordón. **Representante del Profesorado de plantilla de la Universidad de Sevilla**

D. Francisco Yubero Valencia. **Representante del Personal Científico de plantilla del CSIC**

D. Miguel Angel Avilés Escaño. **Representante del Personal No Científico y No Profesorado de Plantilla**

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Alvero Reina, Rafael	Fernández Camacho, Asunción	Ocaña Jurado, Manuel
Avilés Escaño, Miguel Angel	Franco García, Victorino	Odriozola Gordón, J. Antonio
Ayala Espinar, María Regla	Gallardo Cruz, Carmen	Ortega Romero, Andrés
Barranco Quero, Angel	Gómez García, Diego	Palmero Acebedo, Alberto
Becerro Nieto, Ana Isabel	González González, Juan Carlos	Penkova, Anna Dimitrova
Benítez Jiménez, José Jesús	Gotor Martínez, Francisco José	Pérez Maqueda, Luis Allan
Borrás Martos, Ana Isabel	Hidalgo López, M. Carmen	Pérez Rodríguez, José Luis
Borrego Moro, Josefa	Holgado Vázquez, Juan Pedro	Philippon, David
Bravo León, Alfonso	Ivanova, Svetlana	Poyato Ferrera, Juan
Calvo Roggiani, Mauricio	Jiménez Melendo, Manuel	Poyato Galán, Rosalía
Castro Arroyo, Miguel Angel	Jiménez de Haro, M. Carmen	Real Pérez, Concepción
Centeno Gallego, Miguel Angel	Justo Erbez, Angel	R. González-Elipe, Agustín
Cerro González, Jaime del	López Cartes, Carlos	Rojas Ruiz, Cristina
Colón Ibáñez, Gerardo	López Santos, M. Carmen	Romero Sarria, Francisca
Conde Amiano, Clara F.	Macías Azaña, Manuel	Ruiz Conde, Antonio
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Criado Luque, José Manuel	Martínez Fernández, Julián	Sánchez López, Juan Carlos
Diánez Millán, María Jesús	Míguez García, Hernán	Sánchez Soto, Pedro José
Díaz Cuenca, María Aranzazu	Morales Florez, Victor Manuel	Sayagués De Vega, M. Jesús
Domínguez Leal, María Isabel	Munuera Contreras, Guillermo	Yubero Valencia, Francisco
Domínguez Rodríguez, Arturo	Muñoz Bernabé, Antonio	
Durán Benito, Adrián	Muñoz Márquez, Miguel Angel	

1.5. UNIDADES DE INVESTIGACIÓN / RESEARCH UNITS

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Investigador Científico

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Dr. Manuel Ocaña Jurado

Dr. Pedro José Sánchez Soto

Dr. Hernán R. Míguez García

Dr. Luis Allan Pérez Maqueda

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Dra. Nuria Núñez Álvarez

Dra. Concepción Real Pérez

Dr. Francisco José Gotor Martínez

Dra. Rosalía Poyato Galán

Dra. María Jesús Sayagués de Vega

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Dr. Andrés Ortega Romero

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Lda. Stella Despina Kocanis

D^a. Cristina Gallardo López

Lda. Belinda Sigüenza Carballo

Doctor Vinculado "Ad Honorem"

Dr. José Luis Pérez Rodríguez

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Dr. Agustín Rguez. González-Elipe

Dra. Asunción Fernández Camacho

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Dr. José Antonio Odriozola Gordón

Investigador Científico

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Dr. Francisco Yubero Valencia

Dr. Juan Carlos Sánchez López

Científico Titular

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Dra. María Aránzazu Díaz Cuenca
Dr. Alberto Palmero Acebedo

Dr. José Jesús Benítez Jiménez
Dr. Juan Pedro Holgado Vázquez

Profesor Titular

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Dr. Carlos López Cartes

Investigador Contratado

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Dr. Juan Carlos González-González
Dr. Miguel Angel Muñoz Márquez
Dra. Anna Dimitrova Penkova
Dra. M. Carmen Ruiz Herrero

Dra. Ana Isabel Borrás Martos
Dr. Said El Mrabet
Dra. Svetlana Ivanova
Dr. David Philippon
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Becario Predoctoral

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Ldo. Luis F. Bobadilla Baladrón
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Ldo. Willinton Y. Hernández Enciso
Ldo. Oscar H. Laguna Espitia
Ldo. Youssef Oulad Zian
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Lda. Sylvia Andrea Cruz Torres
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Ldo. Pablo Romero Gómez
Ldo. Juan Ramón Sánchez Valencia
Lda. Antonia Terriza Fernández

Contratado con Cargo a Proyectos

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 Ldo. Jorge Gil Rostra
 Dra. Carmen López Santos
 D^a Inmaculada Rosa Cejudo

Lda. Gisela M. Arzac de Calvo
 Ldo. Dirk Huschmidt
 Ldo. Victor Joaquín Rico Gavira

ESTRUCTURA Y CATALIZADORES / STRUCTURE AND CATALYSTS

Personal / [Personnel](#):

Catedrático

Dr. Miguel Angel Castro Arroyo
 Dr. Guillermo Munuera Contreras

Dra. Pilar Malet Maenner
 Dr. José Antonio Navío Santos

Científico Titular

Dra. María Dolores Alba Carranza
 Dr. Gerardo Colón Ibáñez ´

Dra. Ana Isabel Becerro Nieto
 Dra. M^a Carmen Hidalgo López

Profesor Titular

Dr. Rafael Alvero Reina
 Dra. Adela Muñoz Páez

Dr. Manuel Macías Azaña

Investigador Contratado

Dra. Regla Ayala Espinar

Becario Predoctoral

Lda. Marina Maicu
 Ldo. Sebastián Murcia López
 Lda. Esperanza Pavón González

Ldo. Marco Mantovani
 Lda. Julie Joseane Murcia Mesa

UNIDAD DE APOYO / SUPPORT UNIT

Administración

D^ª Margarita Adorna Muñoz
D^ª Ana García Martín
D^ª Nieves Rivero Rodríguez

**Visitas Institucionales y Apoyo a la
Prevención de Riesgos Laborales**
Dr. Antonio Ruiz Conde

Informática – Apoyo Dirección

D. José Carlos Rivero Cabello

I3P – Apoyo Investigación

D. Justo Díaz-Alejo
D. Santiago Domínguez Meister
D. Julián Parra Barranco

Espectroscopía de Fotoelectrones

D. Antonio Macías Pérez
Ldo. David Benítez Sánchez
Ing. Patricia del Arco González

Difracción y Fluorescencia de Rayos X

Ldo. José María Martínez Blanes

Espectroscopías IR, Raman y UV-visible

Dr. Miguel Angel Avilés Escaño

Fisi-quimisorción y GDL

D. Juan Carlos Millán Renquel
D^ª. Paula Sánchez Labrador

Taller de Mecanizado

D. Enrique Jiménez Roca
D. Juan Carlos Martín Sánchez

Microscopía Electrónica de Barrido

Dra. M. Carmen Jiménez de Haro
D^ª. María José Durán Galván

Microscopía Electrónica de Transmisión

Dra. Cristina T. Rojas Ruiz
Lda. Olga Montes Amorín (CICIC)

FÍSICA DE MATERIALES (UNIDAD EXTERNA DE INVESTIGACIÓN) PHYSICS OF MATERIALS (EXTERNAL UNIT)

Personal / [Personnel](#):

Catedrático

Dr. Alejandro Conde Amiano	Dra. Clara F. Conde Amiano
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Profesor Titular

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Dr. José María Martín Olalla	Dra. María Millán Muñoz
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Dra. Ana Morales Rodríguez	Dr. Joaquin Ramírez Rico

Profesor Contratado Doctor

Dr. José Javier Quispe Camcapa

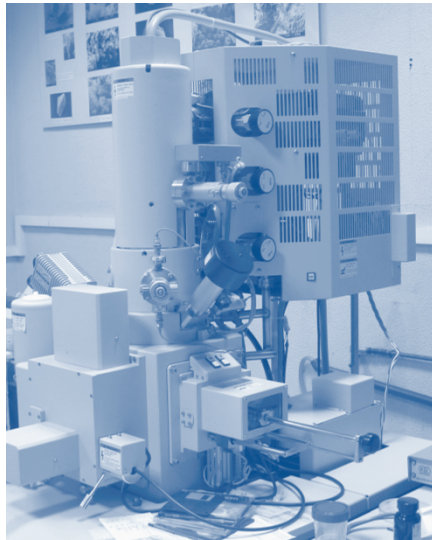
Profesor Emérito

Dr. Manuel Zamora Carranza

ACTIVIDADES DE INVESTIGACIÓN

RESEARCH ACTIVITIES

- 2.1.** Proyectos de Investigación
Research Projects
- 2.2.** Convenios y Contratos
Contracts and Agreements
- 2.3.** Técnicas y equipos instrumentales
Techniques and equipment



2.1. 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 experimentales 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. It 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 Car-tes, 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 perspectivas 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 encontrarán un amplio rango de aplicaciones tales como recubrimientos de baja fricción de amplio uso en ingeniería mecánica, nuevas películas delgadas protectoras contra la corrosión 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.



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.



Desarrollo y diseminación de nuevas técnicas de caracterización nanomecánica y standards

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

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

RESUMEN / ABSTRACT

El proyecto se dedica al desarrollo, mejora, y standarización de las técnicas de caracterización, los métodos y los equipos en los ensayos nano-mecánicos. Las actividades a nivel Europeo, coordinadas por un centro virtual, mejorarán la metrología de nanoindentación actual y permitirán un conocimiento más profundo de la relación estructura-propiedades en la nano-escala. Estos métodos son una herramienta única para caracterizar el comportamiento mecánico en la nanoescala de nanocomposites, nanocapas e interfases. Este trabajo también producirá una base sólida para definir y preparar 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 instrumentales y en la definición de standards para las 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 e 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 research.



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 (subwavelength 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.



Nanoingeniería de láminas de óxido de titanio para el desarrollo de materiales con aplicaciones avanzadas **Nanoengineered Titania thin films for advanced Materials Applications**

Código/Code:	STREP Project NMP3-CT-2006-032583 NATAMA
Periodo/Period:	01-10-2006 / 31-09-2009
Organismo Financiador/Financial source:	Unión Europea
Importe total/Total amount:	188.176 €
Investigador responsable/Research head:	González-Elipe, A.R.
Componentes/Research group:	Espinós, J.P., Barranco, A., Cotrino, J. Yubero, F., Romero, P., Rico, V.

El principal objetivo de este proyecto consiste en inducir nuevas propiedades físico-químicas y ópticas en láminas delgadas de óxido de titanio mediante el desarrollo de estructuras con arquitecturas más complejas (por ejemplo, “nanotubos” de óxido de titanio ordenados espacialmente), estructuras tipo “nanocomposite” (con aplicaciones como sensores de estado sólido, uniones electrónicas o semiconductores) o bien con estructuras de baja dimensionalidad (por ejemplo, láminas ultra-finas de óxido de titanio dopadas con hetero-átomos o decoradas con nanopartículas). Las motivaciones que rigen este proyecto son de naturaleza científica, estratégica y económica. El rango de aplicaciones abarca desde la protección medioambiental y de la salud hasta el diseño de recubrimientos de alta especialización relacionados especialmente con propiedades foto-catalíticas y super-hidrofílicas del óxido de titanio. No obstante, tampoco se puede desdeñar el más que presumible aumento de la demanda de mercado de este material, especialmente después del desarrollo que se está experimentando en los últimos años en el control y diseño de la nano-estructura de las láminas de óxido de titanio, fundamentalmente en el intento de ampliar su rango de actividad foto-catalítica hacia la zona espectral del visible. El desarrollo, control y explotación de esta gran variedad de propiedades (foto-catalíticas en el rango del visible, foto-electroquímicas, foto-conductoras, foto-magnéticas, comportamiento como sensores, respuesta fotovoltaica, respuesta al “mojado”) son de gran importancia para las compañías de la UE en áreas de la salud y de protección medioambiental (depuración de aire y agua), en el diseño de materiales avanzados (recubrimientos), en sistemas que fomenten el desarrollo sostenible (materiales fotovoltaicos) y en temáticas de seguridad nacional y personal (sensores avanzados, mecanismos de desactivación de agentes biológicos).

The objective of this project is to investigate the new chemical, physical and optical properties which can be induced in titania thin films by exploiting novel nanoarchitectures (for example, spatially ordered titania nanotubes) and nanocomposites (controlled heterojunctions, doping with solid state sensitizers, nanostructured composite semiconductors) and novel low dimensional structures (ultra-thin titania films doped with hetero-atoms or decorated with nanoparticles). The motivations of the project are scientific, strategic and economics. Present applications range from health and environment protection to specialized coatings, mainly in connection with the photocatalytic and super-hydrophilicity properties of titania. However a very large increase in the market, by at least one order of magnitude, is expected as a result of recent advances in the ability to nanostructure titania films, especially with respect to shifting their photoactivity into the visible region of the spectrum—an attribute that will hugely enhance their practical application. These new multifunctional properties include photocatalytic oxidation or reduction activity under visible light, photoelectrochemical behaviour, photoconductivity, photochromism and photomagnetic switching, sensing behaviour, photovoltaic response and controlled and “switchable” wetting behaviour. Exploitation of these properties is of strategic importance to EU companies in the fields of health and environment protection (air and water purification), advanced materials (surface coatings), sustainable energy production (photovoltaic materials) and national and personal security (advanced sensors operable under ambient conditions, devices for deactivation of biological agents).



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 fibrillation to generate fibrous collagenous cords with high tensile strength and wear-resistance.



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 desarrollado 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.



Control de 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 orgánicos 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 modifications 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 nanomateriales will be integrated in different configurations and whose absorption and emission will be experimentally and theoretically studied.



Desarrollo de estrategias para la preparación y optimización de materiales altamente fotoactivos **Development of photocatalytic-materials highly activ in the visible for environmental applications**

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

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 nano-sized 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.



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.



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 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 new 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.



Aplicación de una Nueva Generación de Materiales Cerámicos Bioderivados a Procesos Industriales de Filtración a Altas Temperaturas y Presión (BIOFIL) New Generation of Bioderivated Ceramic Materials Applied to Industrial Filtration Processes at High Temperatures and Pressure

Código/Code:	CIT-120000-2008-16
Periodo/Period:	21-07-2008 / 9-05-2009
Organismo Financiador/Financial source:	Ministerio de Ciencia e Innovación
Importe total/Total amount:	241.530 €
Investigador responsable/Research head:	Martínez Fernández, J.
Componentes/Research group:	Ramírez de Arellano-López, A., Miranda, H., Valera Fera, F.

RESUMEN / ABSTRACT

El objetivo principal del proyecto es la implementación de una tecnología alternativa para la filtración en caliente a altas temperatura y presión de gas de síntesis procedente de la gasificación de biomasa. Para ello se caracterizarán, optimizarán y diseñarán filtros cerámicos bioSiC, fabricados a partir de diversas técnicas/sistemas con base de madera, que ofrezcan soluciones a los problemas operacionales actuales experimentados en las unidades de gasificación.

The main project's aim is to implement a n alternative technology for high temperature and pressure synthesis gas filtration from biomass gasification. In order to that, bioSiC ceramic filters fabricated from several techniques/systems wood based, will be characterized, optimized and designed, to provide solution to actual operational problems in gasification units.



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, J.
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.



Desarrollo de materiales compuestos con aplicaciones estructurales y/o funcionales basados en sistemas metal-boro-carbono-nitrógeno **Development of composites for structural and/or functional applications based on metal-boron-carbon-nitrogen systems**

Código/Code:	MAT2006-04911 (Plan Nacional)
Periodo/Period:	01-10-2006/ 30-9-2009
Organismo Financiador/Financial source:	Ministerio de Ciencia y Tecnología
Importe total/Total amount:	100.430 €
Investigador responsable/Research head:	Gotor Martínez, F.J.
Componentes/Research group:	Criado, J.M., Sayagués, M.J., Alcalá, M.D., Donoso, A., Palma, D.

RESUMEN / ABSTRACT

Para muchas aplicaciones estructurales y funcionales, la mejora en las propiedades de los materiales encaminada a conseguir elevadas prestaciones, una mejor tolerancia bajo condiciones experimentales severas o una mayor vida media requiere el desarrollo de materiales multicomponentes y multifásicos. Los carburos, nitruros y boruros metálicos, y sus correspondientes soluciones sólidas son materiales con importantes implicaciones tecnológicas. En un proyecto anterior (MAT2003-00184) se ha puesto de manifiesto que el tratamiento mecánico, una técnica de procesado en seco de materiales que permite la obtención de productos homogéneos a partir de mezclas de elementos, es una técnica muy prometedora para la síntesis de este tipo de materiales. En particular, dicha técnica permite un elevado control de la estequiometría de las soluciones sólidas pudiéndose abarcar un amplio rango de composiciones. Este método constituye asimismo una vía atractiva y simple de obtención de materiales compuestos con microestructura nanométrica. Nos proponemos en el presente proyecto utilizar la molienda reactiva en la síntesis de fases correspondientes a sistemas del tipo Metal-Boro-Carbono-Nitrógeno. Posteriormente, se desarrollarán nanocomposites in-situ (cermets y superaleaciones) basados en este tipo de compuestos por aleado mecánico en una sola etapa a partir de mezclas estequiométricas principalmente de elementos. El conformado y el procesado utilizando técnicas basadas en la radiación de microondas estarán encaminados a la optimización de las propiedades requeridas para distintas aplicaciones tecnológicas.

For many structural and functional applications, the design and processing of materials with enhanced high temperature capabilities or better resistance to severe environments require the development of multicomponent-multiphase systems. Stoichiometric and solid solution carbides, nitrides and borides are of high interest as high temperature structural materials. In a previous project (MAT2003-00184), we have shown that mechanical milling, a dry powder processing technique that allows production of homogeneous materials starting from elemental powder blends, is a promising method of synthesis of these advanced materials. In particular, monophasic carbonitride powders covering a wide composition range for different solid solutions were obtained. In addition, mechanical milling is a simple and well-adapted method to obtain composite materials having nanophase structure. In this project, the mechanochemical synthesis of phases belonging to Metal-Boron-Carbon-Nitrogen systems is proposed. Nanocomposite materials (cermets and superalloys) based on these materials will be developed by one-step milling processes using stoichiometric elemental powder blends. Microwave-assisted sintering methods will be optimised in order to attain the set of properties that must be targeted for specific technological applications.



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:	Cotrina 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 ópticamente 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 ópticamente 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 fotocromáticos, 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/nanostructure 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/nanostructure 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.



Reactores catalíticos de microcanales para la producción de hidrógeno a partir de alcoholes **Microchannel catalytic reactors for hydrogen production from alcohols**

Código/Code:	MAT2006-12386-C05-01 (Plan Nacional)
Periodo/Period:	01-10-2006/ 30-9-2009
Organismo Financiador/Financial source:	Ministerio de Ciencia y Tecnología
Importe total/Total amount:	326.342 €
Investigador responsable/Research head:	Odriozola, J.A.
Componentes/Research group:	Paúl, A., Centeno, M.A., Romero Sarria, F.

RESUMEN / ABSTRACT

Una de las tecnologías más prometedoras actualmente en el campo de la intensificación de procesos químicos y energéticos es la basada en la utilización de reactores de microcanales. Esta tecnología que internacionalmente se puede considerar emergente y por la que existe un importante interés industrial, no está en desarrollo a nivel nacional, hasta donde alcanza nuestro conocimiento.

Dicha tecnología es compleja y multidisciplinar por lo que exige profundizar en el estudio de los materiales implicados (metales y catalizadores principalmente) y en su preparación e interacciones (superficies e interfases).

El ahorro energético y el respeto ambiental están impulsando el diseño y fabricación de dispositivos para la producción de hidrógeno que sean compactos y adaptables a los medios de transporte. En este marco general, el objetivo fundamental de este proyecto es la construcción de reactores de microcanales para la producción de hidrógeno a partir de alcoholes centrandó la investigación en el comportamiento de los materiales del dispositivo (metales, soldaduras, catalizadores e interfases metal/catalizador) de tal modo que se puedan identificar los aspectos críticos para las distintas reacciones catalíticas implicadas en la producción de hidrógeno a partir de alcoholes: reformado al vapor, oxidación parcial de alcoholes, WGS (desplazamiento al gas de agua) y PrOx (oxidación preferencial de CO). La idoneidad de la tecnología de microcanales para este conjunto de reacciones radica en su carácter compacto y seguro junto con un excelente control térmico de las reacciones que permite selectividades inalcanzables por procesos convencionales.

The use of microchannel catalytic reactors for chemical processes intensification is one of the most promising technologies nowadays. This technology that in the international context can be considered as an emerging one is not, to our knowledge, under development in Spain.

The development of microchannel catalytic reactors, a complex a multidisciplinary technology, requires a deep study of the materials constituting the miniaturised device, both catalysts and metal hosts, as well as their preparation and interactions.

The environmental impact and the need to reduce energy inputs are favouring the design and fabrication of devices for hydrogen production that meet criteria for adaptability to transport vehicles while being compact. In this framework is established the main objective of this Project: the construction of microchannel catalytic reactors for hydrogen production from alcohols. The behaviour of the materials forming the catalytic device (metals, weldings, catalysts and metal/catalyst interfaces) will be the key point of the project in such a way that were possible to identify the critical points affecting the fabrication of microchannel reactors for the different catalytic reactions involved in hydrogen production from alcohols: steam reforming, partial oxidation of alcohols, water gas shift reaction (WGS) and preferential oxidation of CO (PrOx). The excellent thermal control of the reactions allowing process selectivity unaffordable for conventional processes as well as safety and compact character of microchannel catalytic reactors made these devices the ideal choice for hydrogen production in transportation vehicles.



Producción de gas de síntesis e hidrógeno mediante reformado de hidrocarburo con catalizadores nanoestructurados de níquel
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:	Caballero Martínez, A.
Componentes/Research group:	Holgado, J.P., González-Elipe, A.R., González de la Cruz, V.M., Pereñíguez, R.M.

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 último 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 ZrO₂ or Al₂O₃, 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.



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 interfaces.

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, bio-materials, 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.



Preparación de materiales multiferroicos por métodos mecanoquímicos y térmicos con control inteligente de temperatura **Preparation of multiferroic materials by mechanical alloying and thermal methods with smart temperature 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:	Diáñez Millán, M.J., Criado Luque, J.M.

RESUMEN / ABSTRACT

Los materiales multiferroicos, aquellos que presentan simultáneamente dos o más 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 estequiometría 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 descomposición 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 mecano-síntesis 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 caracterizarán en cuanto al estado de oxidación 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 claimed 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, microstructure 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.



Nanoingeniería de láminas de óxido de titanio para el desarrollo de materiales con aplicaciones avanzadas **Nanoengineered Titania thin films for advanced Materials Applications**

Código/Code:	MAT2007-29321-E (Ayuda Complementaria)
Periodo/Period:	02-09-2008 / 01-09-2009
Organismo Financiador/Financial source:	Ministerio de Educación y Ciencia
Importe total/Total amount:	55.000 €
Investigador responsable/Research head:	González-Elipe, A.R.
Componentes/Research group:	Espinós, J.P., Barranco, A., Cotrino, J. Yubero, F., Romero, P., Rico, V.

RESUMEN / ABSTRACT

El principal objetivo de este proyecto consiste en inducir nuevas propiedades físico-químicas y ópticas en láminas delgadas de óxido de titanio mediante el desarrollo de estructuras con arquitecturas más complejas (por ejemplo, “nanotubos” de óxido de titanio ordenados espacialmente), estructuras tipo “nanocomposite” (con aplicaciones como sensores de estado sólido, uniones electrónicas o semiconductores) o bien con estructuras de baja dimensionalidad (por ejemplo, láminas ultra-finas de óxido de titanio dopadas con hetero-átomos o decoradas con nanopartículas).

Las motivaciones que rigen este proyecto son de naturaleza científica, estratégica y económica. El rango de aplicaciones abarca desde la protección medioambiental y de la salud hasta el diseño de recubrimientos de alta especialización relacionados especialmente con propiedades foto-catalíticas y super-hidrofílicas del óxido de titanio. No obstante, tampoco se puede desdeñar el más que presumible aumento de la demanda de mercado de este material, especialmente después del desarrollo que se está experimentando en los últimos años en el control y diseño de la nano-estructura de las láminas de óxido de titanio, fundamentalmente en el intento de ampliar su rango de actividad foto-catalítica hacia la zona espectral del visible.

El desarrollo, control y explotación de esta gran variedad de propiedades (foto-catalíticas en el rango del visible, foto-electroquímicas, foto-conductoras, foto-magnéticas, comportamiento como sensores, respuesta fotovoltaica, respuesta al “mojado”) son de gran importancia para las compañías de la UE en áreas de la salud y de protección medioambiental (depuración de aire y agua), en el diseño de materiales avanzados (recubrimientos), en sistemas que fomenten el desarrollo sostenible (materiales fotovoltaicos) y en temáticas de seguridad nacional y personal (sensores avanzados, mecanismos de desactivación de agentes biológicos).

The objective of this project is to investigate the new chemical, physical and optical properties which can be induced in titania thin films by exploiting novel nanoarchitectures (for example, spatially ordered titania nanotubes) and nanocomposites (controlled heterojunctions, doping with solid state sensitizers, nanostructured composite semiconductors) and novel low dimensional structures (ultra-thin titania films doped with hetero-atoms or decorated with nanoparticles).

The motivations of the project are scientific, strategic and economics. Present applications range from health and environment protection to specialized coatings, mainly in connection with the photocatalytic and super-hydrophilicity properties of titania. However a very large increase in the market, by at least one order of magnitude, is expected as a result of recent advances in the ability to nanostructure titania films, especially with respect to shifting their photoactivity into the visible region of the spectrum—an attribute that will hugely enhance their practical application.

These new multifunctional properties include photocatalytic oxidation or reduction activity under visible light, photoelectrochemical behaviour, photoconductivity, photochromism and photomagnetic switching, sensing behaviour, photovoltaic response and controlled and “switchable” wetting behaviour. Exploitation of these properties is of strategic importance to EU companies in the fields of health and environment protection (air and water purification), advanced materials (surface coatings), sustainable energy production (photovoltaic materials) and national and personal security (advanced sensors operable under ambient conditions, devices for deactivation of biological agents).



Nuevo equipo para la medida de propiedades térmicas bajo presión uniaxial hasta 50 MPa y 700 K: Aplicación al estudio de materiales ferroelásticos
New device for the measurement of thermal properties under uniaxial stress up to 50 MPa and 700 K: Application to the study of ferroelastic materials

Código/Code:	FIS2006-04045
Periodo/Period:	1-10-2006/ 30-9-2009
Organismo Financiador/Financial source:	Ministerio de Ciencia y Tecnología
Importe total/Total amount:	55.660 €
Investigador responsable/Research head:	Del Cerro, J.
Componentes/Research group:	Ramos, S., Jiménez Fernández, J., Gallardo Cruz, M.C., Martín Olalla, J.M., Romero Landa, F.J., Manchado Ligoiz, J.

RESUMEN / ABSTRACT

Para la medida de calor específico y calor latente de muestras bajo presión uniaxial de hasta 50 MPa y un rango de temperatura entre 200 y 700 K. Este dispositivo utilizará el método de medida SMDTA desarrollado por el grupo y que se ha utilizado con éxito en rangos de temperatura y presión inferiores.

Con este equipo de investigación se estudiará la influencia de la presión uniaxial según la dirección [100] y [110] sobre el calor específico y el calor latente y sobre la fase intermedia del cristal ferroelástico fosfato de plomo, en la que coexiste la fase paraelástica con microdominios ferroelásticos.

Así mismo, con los calorímetros que actualmente se dispone y con el que se construirá se estudiará las transiciones de fase cúbica-tetragonal y tetragonal-ortorrómbica en la solución sólida titanato de estroncio- titanato de calcio para diferentes composiciones. Se analizará la anomalía de calor específico en ambas transiciones y el carácter continuo o discontinuo de la transición tetragonal-ortorrómbica. Se contrastarán los resultados con las previsiones teóricas deducidas a partir de las medidas de deformaciones espontáneas.

A new experimental device will be built for the specific heat and latent heat measurements under uniaxial stress up to 50 MPa and in the temperature range 200-700K. The technique to perform the measurements will be the method Square Modulated Differential Thermal Analysis (SMDTA), which has been developed by us and which has been successfully used for lower temperature and pressure. The techniques to build the sensors will be based on precision welding, high resolution soldering, ablation and micromachining by laser.

Using this new equipment, the influence of uniaxial stress along the crystallographic axis [100] and [110] on the specific heat and latent of ferroelastic lead phosphate will be studied. It will be also investigated the influence of the stress on the intermediate phase where the paraelastic phase and ferroelastic microdomains coexist.

On the other hand, using the calorimeters which are now available and the new one, we will study the cubic-tetragonal and the tetragonal- orthorhombic phase transitions in the solid solution strontium titanate-calcium titanate for several compositions. The specific heat anomaly and the discontinuous or continuous character of the tetragonal-orthorhombic phase transition will be analysed. The results will be compared to the theoretical previsions deduced from spontaneous strain measurements.



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

Código/Code:	MAT2007-65227 (Plan Nacional)
Periodo/Period:	01-10-2007 / 3-8- 2010
Organismo Financiador/Financial source:	Ministerio de Ciencia y Tecnología
Importe total/Total amount:	72.600 €
Investigador responsable/Research head:	Conde, A.
Componentes/Research group:	Conde, C.F., Millán, M., Borrego, J.M., Franco, V., Blázquez, J.S., Ipus, J.J.

RESUMEN / ABSTRACT

Se propone estudiar materiales magnéticos blandos (aleaciones amorfas y nanocristalinas y nanopulvos) 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 objectives 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.



Estuctura, 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 autoensambladas. Más concretamente en la contribución de eventos a escala molecular en la propiedades friccionales 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 microscopía 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 tuning 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 alkylamines, are complementary to describe the contribution of defects to friction.



Materials World Network: Ceramic Composites from Natural and Synthetic Scaffolds

Código/Code:	MAT2007-30141-E
Periodo/Period:	2008 / 2009
Organismo Financiador/Financial source:	Ministerio de Educación y Ciencia
Importe total/Total amount:	29.500 €
Investigador responsable/Research head:	Martínez Fernández, J.
Componentes/Research group:	Ramírez de Arellano-López, A., Jiménez Melendo, M.

RESUMEN / ABSTRACT

La estructura del SiC, con canales abiertos, proporciona una base de gran utilidad para posteriores infiltraciones, dando lugar a una nueva clase de materiales compuestos. A diferencia de los materiales reforzados con partículas, whiskers o fibras, en los que la dispersión y alineamientos son múltiples, el bioSiC aporta una preforma para la infiltración con metales para mejorar la resistencia mecánica y la conductividad eléctrica o térmica. El objetivo de este trabajo es establecer nuevas vías en la producción de materiales compuestos bioderivados. El proyecto será realizado en cooperación entre Northwestern University, Universidad de Sevilla, Universidad Politécnica de Madrid and el Ioffe Physico-Technical Institute en St. Petersburg.

The porous SiC structure, with its open channels, provides a useful scaffold for further infiltration resulting in a new class of composite materials. Unlike reinforcement by particles, whiskers or fibers, where dispersion and alignment challenges are many, bioSiC provides a template for infiltration of a metal for enhancing mechanical robustness, electrical or thermal conductivity. It is the goal of this work to establish new directions in composite materials produced with naturally derived scaffolds. The project on Ceramic Composites from Natural and Synthetic Scaffolds will be done in conjunction with Northwestern University, Universidad de Sevilla and Universidad Politécnica de Madrid in Spain and the Ioffe Physico-Technical Institute in St. Petersburg.



Mecanosíntesis de hidruros metálicos y perowskitas multiferróicas en un molino planetario de alta energía de molienda bajo presiones 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., Diáñez, 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.



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:	Colón Ibáñez, G.
Componentes/Research group:	Navío, JA., Macías, M., Hidalgo, MC., Maicu, M.

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.



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:	González-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, tempera-

ture 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-translational 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.



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 Car-tes, 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 “nanocomposites” 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); Università 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 priority 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); Università 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).



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 SiO₂ y el TiO₂, 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 (CrO₂), 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 huésped: 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 huésped y de infiltrado de la fase alojada en sus poros.

This project is focused to the synthesis 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 SiO₂ and TiO₂, 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 (CrO₂) 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 synthesis and deposition of films and their subsequent infiltration with active nanoparticles and molecules will be tested and developed.



Producción de H₂. Reactores de microcanales H₂ production. Microchannel catalytic reactors

Código/Code:	P06-TEP-01965 (Proyecto de Excelencia)
Periodo/Period:	01-01-2007 / 31-12- 2009
Organismo Financiador/Financial source:	Junta de Andalucía
Importe total/Total amount:	228.536 €
Investigador responsable/Research head:	Odriozola, J.A.
Componentes/Research group:	Centeno, M.A., Paúl, A., Bobadilla, L.

RESUMEN / ABSTRACT

Una de las tecnologías más prometedoras actualmente en el campo de la intensificación de procesos químicos y energéticos es la basada en la utilización de reactores de microcanales. Esta tecnología que internacionalmente se puede considerar emergente y por la que existe un importante interés industrial, no está en desarrollo a nivel nacional, hasta donde alcanza nuestro conocimiento.

Dicha tecnología es compleja y multidisciplinar por lo que exige profundizar en el estudio de los materiales implicados (metales y catalizadores principalmente) y en su preparación e interacciones (superficies e interfases).

El ahorro energético y el respeto ambiental están impulsando el diseño y fabricación de dispositivos para la producción de hidrógeno que sean compactos y adaptables a los medios de transporte. En este marco general, el objetivo fundamental de este proyecto es la construcción de reactores de microcanales para la producción de hidrógeno a partir de alcoholes centrandó la investigación en el comportamiento de los materiales del dispositivo (metales, soldaduras, catalizadores e interfases metal/catalizador) de tal modo que se puedan identificar los aspectos críticos para las distintas reacciones catalíticas implicadas en la producción de hidrógeno a partir de alcoholes: reformado al vapor, oxidación parcial de alcoholes, WGS (desplazamiento al gas de agua) y PrOx (oxidación preferencial de CO). La idoneidad de la tecnología de microcanales para este conjunto de reacciones radica en su carácter compacto y seguro junto con un excelente control térmico de las reacciones que permite selectividades inalcanzables por procesos convencionales.

The use of microchannel catalytic reactors for chemical processes intensification is one of the most promising technologies nowadays. This technology that in the international context can be considered as an emerging one is not, to our knowledge, under development in Spain.

The development of microchannel catalytic reactors, a complex a multidisciplinary technology, requires a deep study of the materials constituting the miniaturised device, both catalysts and metal hosts, as well as their preparation and interactions.

The environmental impact and the need to reduce energy inputs are favouring the design and fabrication of devices for hydrogen production that meet criteria for adaptability to transport vehicles while being compact. In this framework is established the main objective of this Project: the construction of microchannel catalytic reactors for hydrogen production from alcohols. The behaviour of the materials forming the catalytic device (metals, weldings, catalysts and metal/catalyst interfaces) will be the key point of the project in such a way that were possible to identify the critical points affecting the fabrication of microchannel reactors for the different catalytic reactions involved in hydrogen production from alcohols: steam reforming, partial oxidation of alcohols, water gas shift reaction (WGS) and preferential oxidation of CO (PrOx). The excellent thermal control of the reactions allowing process selectivity unaffordable for conventional processes as well as safety and compact character of microchannel catalytic reactors made these devices the ideal choice for hydrogen production in transportation vehicles.



Inertización de residuos tóxicos y radioactivos en una matriz de silicatos Immobilization 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 controlling the quantity and distribution of the tetrahedral active centers. They will be submitted to a set of chemical soft treatments in order to immobilize 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.



Nanopartículas magnéticas de metales nobles con funcionalización controlada para tratamientos de hipertermia
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 multidisciplinary 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 treat-

ments 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.



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., Diáñez, 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 TiO₂ 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)TiO₂ 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.



Nanopartículas magnéticas de metales nobles con funcionalización controlada para tratamientos de hipertermia **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 multidisciplinary 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.



Desarrollo de catalizadores de Ni nanoestructurados: Obtención de hidrógeno a partir de CH₄ 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:	Holgado Vázquez, J.P.
Componentes/Research group:	Caballero Martínez, A., Pereñíguez Rodríguez, R., González de la Cruz, V.M., Ternero Fernández, F., Espinós Manzorro, J.P., Baranco Quero, A.

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 correlation between physicochemical characteristics and functional properties as reforming catalysts and/or SOFCs anodes.



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



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

Periodo/ <i>Period</i> :	2007 / 2010
Organismo Financiador/ <i>Financial source</i> :	Centro para el Desarrollo Tecnológico Industrial (Programa CENIT) Ministerio de Industria (Contratos: INDO, S.A., TORRECID, DECOART)
Investigador responsable/ <i>Research head</i> :	González-Elipe, A.R.
Componentes/ <i>Research group</i> :	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 medioambientalmente 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 antialérgicos.
- 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-allergic 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.

OTROS PROYECTOS / OTHER PROJECTS**Desarrollo de capas transparentes de TiO₂ modificado con propiedades fotocatalíticas y de autolimpieza**

Código/Code: 200860I204
 Periodo/Period: 01-10-2008 / 31-12-2009
 Organismo Financiador/Financial source: CSIC
 Importe total/Total amount: 30.000 €
 Investigador responsable/Research head: Carmen Hidalgo López

Nuevos materiales y catalizadores para la producción y almacenamiento de hidrógeno a partir de hidruros complejos (MATH2)

Código/Code: 200460E643
 Periodo/Period: 01-11-2009 / 30-04-2011
 Organismo Financiador/Financial source: CSIC
 Importe total/Total amount: 34.000 €
 Investigador responsable/Research head: Asunción Fernández Camacho

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

Desarrollo de sensores ópticos para la verificación de la calidad del aceite

Código/Code: PET2007_0363_02 - OPN - PETRI
 Periodo/Period: 12-09-2008 / 11-09-2010
 Organismo Financiador/Financial source: Ministerio de Educación y Ciencia
 Investigador responsable/Research head: José Cotrino Bautista

AYUDAS DE LA JUNTA DE ANDALUCÍA A CONSOLIDACIÓN DE GRUPOS SUPPORT FROM THE JUNTA DE ANDALUCÍA TO RESEARCH GROUPS

FÍSICA, QUÍMICA Y MATEMÁTICAS / PHYSICS, CHEMISTRY AND MATHEMATICS

Código	Denominación	Responsable	Financiación
FQM121	Sólidos No Cristalinos	Conde Amiano, Alejandro	7.657,90 €
FQM123	Sólidos Cristalinos	Criado Vega, Alberto	8.709,08 €
FQM130	Propiedades Térmicas y Dielectricas de Sólidos	Del Cerro González, Jaime	3.520,80 €
FQM163	Propiedades Mecánicas de Sólidos	Domínguez Rodríguez, Arturo	16.123,01 €
FQM181	Fotocatálisis Heterogénea: Aplicaciones	Navío Santos, José Antonio	4.529,10 €
FQM187	Nuevos Materiales a Partir de Silicatos Naturales	Justo Erbez, Angel	6.021,48 €
FQM196	Superficies, Interfaces y Capas Finas	Rodríguez González-Elipe, Agustín	13.696,32 €
FQM212	Química del Estado Sólido	Castro Arroyo, Miguel Angel	7.009,71 €
FQM342	Materiales Biomiméticos y Multifuncionales	Martínez Fernández, Julián	12.832,06 €
FQM356	Nanomateriales Ópticos	Ocaña Jurado, Manuel	6.848,16 €

TECNOLOGÍA DE LA PRODUCCIÓN / TECHNOLOGY OF THE PRODUCTION

Código	Denominación	Responsable	Financiación
TEP106	Química de Superficies y Catálisis	Odriozola Gordón, José Antonio	14.444,90 €
TEP110	Reactividad de Sólidos	Criado Luque, José Manuel	8.445,54 €
TEP204	Materiales Avanzados	Sánchez Soto, Pedro José	3.054,43 €
TEP217	Materiales Nanoestructurados y Microestructura	Fernández Camacho, Asunción	15.275,72 €

2.2. CONVENIOS Y CONTRATOS / CONTRACTS AND AGREEMENTS

Investigación y desarrollo de aplicaciones nanotecnológicas en aglomerados de piedra

Periodo/Period:	08-03-2007 / 08-05-2009
Organismo Financiador/Financial source:	Consentino, S.A.
Importe total/Total amount:	112.120 €
Investigador responsable/Research head:	Francisco Yubero
Componentes/Research group:	Agustín R. González-Elipe, Juan Pedro Espinós, José Cotrino, Angel Barranco, Patricia del Arco

Gold based nanoparticles (NPs) for hyperthermia treatments

Periodo/Period:	01-10-2007 / 31-12-2009
Organismo Financiador/Financial source:	Midatech Andalucía, S.L.
Importe total/Total amount:	98.136 €
Investigador responsable/Research head:	Asunción Fernández
Componentes/Research group:	Miguel Angel Muñoz, Estefanía Guerrero, Cristina Rojas

Mejoras en la respuesta a condiciones ambientales extremas de condensadores de cinta metalizada

Periodo/Period:	16-11-2007 / 15-11-2009
Organismo Financiador/Financial source:	EPCOS Electronic Components, S.A.
Importe total/Total amount:	7.448 €
Investigador responsable/Research head:	José Cotrino Bautista

Estudio de la aplicación del borohidruro sódico como sistema de producción de hidrógeno (proyecto SAC-H2)

Periodo/Period:	01-10-2007 / 31-12-2009
Organismo Financiador/Financial source:	Hynergreen Technologies, S.A.
Importe total/Total amount:	116.000 €
Investigador responsable/Research head:	Asunción Fernández
Componentes/Research group:	Carlos López, Estefanía Guerrero, Miguel Angel Muñoz

Estudio de nanotecnologías en aplicaciones solares fotovoltaicas

Periodo/Period:	30-04-2007 / 01-05-2009
Organismo Financiador/Financial source:	Solucar Energía, S.A.
Importe total/Total amount:	69.600 €
Investigador responsable/Research head:	Agustín R. González-Elipe
Componentes/Research group:	Francisco Yubero, Juan Pedro Espinós, José Cotrino, Angel Barranco Quero

Investigación de nuevas reacciones y procesos industriales de descomposición de CO₂, empleando biomasa y mediante técnicas de plasma

Periodo/*Period*: 27-07-2007 / 27-05-2009
 Organismo Financiador/*Financial source*: Instalaciones Inabensa, S.A.
 Importe total/*Total amount*: 139.200 €
 Investigador responsable/*Research head*: José Cotrino Bautista
 Componentes/*Research group*: Agustín R. González-Elipe, Juan Pedro Espinós Manzorro, Francisco Yubero Valencia, Angel Barranco Quero

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
 Importe total/*Total amount*: 16.774,25 €
 Investigador responsable/*Research head*: Hernán Ruy Miguez
 Componentes/*Research group*: Mauricio Calvo Roggiani, Silvia Colodrero

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)
 Importe total/*Total amount*: 230.000 €
 Investigador responsable/*Research head*: Agustín R. González-Elipe
 Componentes/*Research group*: Juan Pedro Espinós, Francisco Yubero, José Cotrino, Angel Barranco, Alberto Palmero

Neovil: Análisis de posibles usos de NFUS-S en obra civil

Periodo/*Period*: 01-10-2007 / 21-12-2009
 Organismo Financiador/*Financial source*: Acciona Infraestructuras, S.A.
 Importe total/*Total amount*: 115.760 €
 Investigador responsable/*Research head*: José Manuel Criado
 Componentes/*Research group*: María Jesús Diánez Millán, Luis Pérez Maqueda, María Jesús Sayagués de Vega

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

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 Technologies, S.A.

Importe total/Total amount: 388.600 €

Investigador responsable/Research head: Agustín R. González-Elipe

Componentes/Research group: José Cotrino Bautista, Juan Pedro Espinós Manzorro, Angel Barranco Quero

Validación y experimentación en planta piloto de nuevas técnicas para la remediación y tratamiento de suelos industriales contaminados

Periodo/Period: 20-10-2008 / 30-06-2011

Organismo Financiador/Financial source: Befesa Gestión de Residuos Industriales

Importe total/Total amount: 50.714 €

Investigador responsable/Research head: María Dolores Alba Carranza

Componentes/Research group: Miguel Angel Castro Arroyo, Ana Isabel Becerro Nieto, María del Mar Orta

Estudio de aplicación de recubrimientos sobre modelos técnicos de nuevas superficies para construcción

Periodo/Period: 1-10-2008 / 31-03-2009

Organismo Financiador/Financial source: Consentino, S.A.

Importe total/Total amount: 27.800 €

Investigador responsable/Research head: Francisco Yubero Valencia

Componentes/Research group: Agustín R. González-Elipe, Juan Pedro Espinós Manzorro, José Cotrino Bautista, Angel Barranco Quero

Estudios de Superficie Específica en Compuestos de Calcio

Periodo/Period: 26-05-2009 / 26-08-2009

Organismo Financiador/Financial source: ARIES, S.A.

Importe total/Total amount: 1.740 €

Investigador responsable/Research head: Gerardo Colón Ibáñez

Componentes/Research group: Miguel Angel Centeno, Juan Carlos Millán

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

Importe total/Total amount: 127.368 €

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

2.3. TÉCNICAS Y EQUIPOS INSTRUMENTALES / TECHNIQUES AND EQUIPMENT

SERVICIOS DE INVESTIGACIÓN / RESEARCH SERVICES

SERVICIO DE DIFRACCIÓN Y FLUORESCENCIA DE RAYOS X X-RAY FLUORESCENCE AND DIFFRACTION SERVICE

La difracción de rayos X es una técnica de uso general para la identificación cualitativa y cuantitativa de sustancias cristalinas, permite además la medida de tamaño de cristalito, microtensiones, parámetros de red, etc. Con la cámara de alta temperatura, se pueden seguir directamente las transformaciones que sufren los materiales con el calentamiento, como pueden ser reacciones en estado sólido o cambios de fase.

La Fluorescencia de rayos X permite el análisis químico cualitativo y cuantitativo de materiales cristalinos y amorfos.

Este servicio funciona bajo la supervisión de dos responsables científicos del ICMS que mantienen unas líneas de investigación en relación con el uso de estos equipamientos y dispone de personal técnico asignado al equipo.

X-ray Diffraction is a general use technique to identify crystalline substances qualitatively and quantitatively, it also allows crystallite size measurement, microtensions, net parameters, etc. With the high-temperature chamber, it's possible to follow directly transformations suffered by heating materials, such as reactions in solid state or phase shifts. X-ray fluorescence allows qualitative and quantitative chemical analysis of crystalline and amorphous materials.

This service is under the supervision of two ICMS scientists, who keep research lines related to the use of this equipment and it has a technical personnel assigned to the equipment.

INSTRUMENTAL DISPONIBLE / AVAILABLE INSTRUMENTAL



- Difractómetro Siemens D501 [Diffractometer Siemens D501](#)
- Difractómetro Siemens D5000 con accesorio para ángulo rasante [Diffractometer with an accessory for slope angle \(Siemens D5000\)](#)
- Difractómetro Siemens D5000 dual, con accesorios para transmisión y capilares [Dual Diffractometer with accessories for transmission and capillaries \(Siemens D5000\)](#)
- Difractómetro Philips X'Pert con cámara de alta temperatura (1200°C) y detector sensible a la posición (10.5°) [Diffractometer with high temperature oven camera and equipped with detector sensible to position](#)
- Espectrómetro de Fluorescencia de Rayos X Siemens SRS3000 [X-Ray Fluorescence Spectrometer \(Siemens SRS3000\)](#)
- Prensa hidráulica manual hasta 15 toneladas [Manual hydraulic press up to 15 tons](#)
- Matrices para la preparación por compresión de muestras en polvo [Matrices to prepare powdered samples](#)

SERVICIO DE MICROSCOPIA ELECTRÓNICA DE BARRIDO SCANNING ELECTRONIC MICROSCOPY SERVICE

La microscopía electrónica de barrido es una técnica ampliamente utilizada para la caracterización estructural de muestras sólidas. Se puede obtener una gran variedad de información morfológica, y de composición química en todo tipo de materiales. Es de destacar su elevada resolución y gran profundidad de campo, lo que permite una visualización tridimensional.

Esta técnica abarca un amplio espectro de las áreas a estudiar, como la determinación morfológica de materiales, estudio de estados de agregación, estudio de microestructura de metales, determinación de cambios de composición, estudio de superficie, capas finas e interfases, identificación de minerales de pequeño tamaño, determinación de estratos en restauración, y un sin fin de aplicaciones.

Este servicio funciona bajo la supervisión de dos responsables científicos del ICMS que mantienen unas líneas de investigación en relación con el uso de estos equipamientos y dispone de personal técnico asignado al equipo.

Scanning electronic microscopy is a technique widely used in structural characterization of solid samples. We can obtain a great variety of information about morphology and chemical composition from all kind of materials. It's relevant its high resolution and the great depth of field and it allows a three-dimensional visualization.

This technique extends over many different areas of study, such as morphological determination of materials, study of aggregation states and of metals microstructure, determination of composition changes, study of surface, thin films and interphases; identification of small size minerals, determination of restoring strata and many other applications.

This service is under the supervision of two ICMS scientists who keep research lines related to the use of this equipment and it has a technical personnel assigned to the equipment.

INSTRUMENTAL DISPONIBLE / AVAILABLE INSTRUMENTAL



- Microscopio JEOL JSM-5400
Microscope JEOL JSM-5400
- Microscopio Hitachi S-4800 Microscope
Hitachi S-4800
- Sistema de análisis por energías dispersivas de rayos X (EDX)
X-Ray Dispersive Energy Analysis System (EDX)
- Metalizador de Oro
Gold Metalizer
- Laboratorio Fotográfico
Photographic laboratory

SERVICIO DE MICROSCOPIA ELECTRÓNICA DE TRANSMISIÓN TRANSMISSION ELECTRONIC MICROSCOPY SERVICE

La microscopía electrónica de transmisión es una técnica ampliamente utilizada para la caracterización estructural y química de materiales. Pudiéndose obtener información sobre morfología, tamaño de grano, composición química, grado de cristalinidad e identificación de fases cristalinas en todo tipo de materiales. La técnica permite asimismo análisis cuantitativo, estudios estructurales por microscopía de alta resolución y análisis espectroscópicos por pérdida de energía de electrones.

Este servicio funciona bajo la supervisión de dos responsables científicos del ICMS que mantienen unas líneas de investigación en relación con el uso de estos equipamientos y dispone de personal técnico asignado al equipo.

Scanning electronic microscopy is a technique widely used in structural characterization of solid samples. We can obtain a great variety of information about morphology and chemical composition from all kind of materials. It's relevant its high resolution and the great depth of field and it allows a three-dimensional visualization.

This technique extends over many different areas of study, such as morphological determination of materials, study of aggregation states and of metals microstructure, determination of composition changes, study of surface, thin films and interphases; identification of small size minerals, determination of restoring strata and many other applications.

This service is under the supervision of two ICMS scientists who keep research lines related to the use of this equipment and it has a technical personnel assigned to the equipment.

INSTRUMENTAL DISPONIBLE / AVAILABLE INSTRUMENTAL



- Microscopio Philips CM200 de alta resolución High resolution microscope Philips CM200
- Sistema de análisis por energías dispersivas (EDX) Analysis system by Energy Dispersive Spectroscopy (EDX)
- Espectrómetro de pérdidas de energía de electrones (PEELS-Gatan) Electron Energy Loss Spectrometre (PEELS-Gatan)
- Evaporador de carbón Carbon evaporator
- Cortadora de disco de diamante Diamond disc cutter
- Pulidora Polishing machine
- Cortadora ultrasónica Ultrasonic disc cutter
- Adelgazador cóncavo-convexo (dimple) Precision dimple grinder
- Adelgazador iónico Ion milling
- Laboratorio Fotográfico Photographic laboratory
- Disco de lijado y pulido controlado de muestras TEM specimen disc grinder
- Portamuestras de calentamiento Heating holder
- Portamuestras de frío Cooled specimen holder

SERVICIO DE ESPECTROSCOPIA DE FOTOELECTRONES PHOTOELECTRON SPECTROSCOPY SERVICE

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, 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.

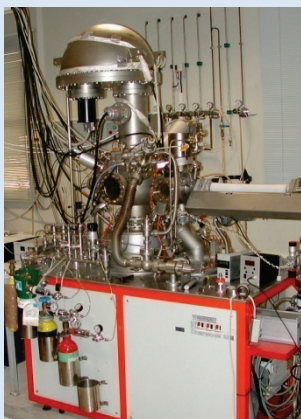
La característica más importante de la Espectroscopía de Fotoelectrones (XPS/ESCA) es el permitir diferenciar distintos estados de oxidación y/o situaciones del entorno (coordinación) de los átomos en las muestras sólidas analizadas así como el estudio de perfiles de composición combinando la técnica con el desbastado iónico empleando iones Ar⁺ acelerados. El límite de detección es del 0.5% para cada especie química

Typically the photoelectron spectroscopies (XPS/ESCA and AES) are powerful characterization techniques for the non-destructive quantitative analysis of the first atomic layers of solids (20-30 Å), what allows to get information on the chemical, physical and electronic properties of solid surfaces.

The technical interest of this information is very important in fields like corrosion, catalysts, surface treatments, flotation phenomena, adhesion, segregation in metallurgy, etc. The XPS/ESCA technique is actually a unique technique to solve all the problems arising in these technological fields.

The most important characteristic of the photoelectron spectroscopy (XPS/ESCA) is the possibility of differentiate different oxidation states and/or chemical coordination of the atoms in solid samples, as well as, the measurement of chemical composition depth profiling analysis by combining the technique with sputtering using Ar⁺ ion bombardment. The detection limit is around 0.5 atomic % for each chemical species.

INSTRUMENTAL DISPONIBLE / AVAILABLE INSTRUMENTAL



- Espectrómetro de Fotoelectrones "Leybold-Heraeus" mod. LHS-10/20. Photoelectron Spectrometer "Leybold-Heraeus" mod. LHS-10/20.
- Analizador multicanal EA200 Multichannel analyser EA200
- Sistema digital de Control del registro de los espectros Digital system to control the spectra register
- Precámara de tratamientos, en la que es posible someter a las muestras a tratamientos térmicos (-70 a +1000°C) bajo diversas atmósferas Treatment prechamber, where it is possible to submit the samples to thermal treatments under different atmospheres (-70 to +1000°C)
- Espectrómetro de Masas incorporado Built-in Mass Spectrometer
- Cañón de iones para bombardeo de las muestras con iones Ar⁺ acelerados a distintas energías (0.5-10 KV) Ion pipe to bombard samples with Ar⁺ ions accelerated at different energies (0.5-10 KV).

SERVICIO DE RESONANCIA MAGNÉTICA NUCLEAR EN ESTADO SÓLIDO NUCLEAR MAGNETIC RESONANCE IN SOLID STATE SERVICE

La Resonancia Magnética Nuclear en estado sólido es una técnica adecuada y cada vez más utilizada para la determinación estructural de materiales amorfos o poco cristalinos. Esta técnica se basa en el comportamiento de los momentos magnéticos de los núcleos bajo la influencia de medio. Por tanto, la posición, forma e intensidad de las señales están íntimamente relacionadas por el entorno químico del núcleo estudiado.

Este Servicio está bajo la dirección de una responsable científica del ICMS, la cual desarrolla líneas de investigación conexas con el mismo. Esta responsable, bajo cuya dirección está el técnico adscrito al Servicio, contribuye al desarrollo de líneas de investigación, solicita ayudas económicas para mantener y mejorar sus prestaciones y dirige en aquellos problemas o dudas que surgen dentro del Servicio.

Este Servicio de RMN del CICIC, funciona 24 horas al día todos los días del año. El espectrómetro RMN DRX-400 funciona tanto en su configuración para medidas de estado líquido (60% del tiempo) como en su configuración para medidas de estado sólido (40% del tiempo)

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 behaviour 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.

This Service is managed by a responsible scientist of the ICMS and there is a technical person who performs the measurements of the service. This scientist develops research lines connected with the service. Moreover, the responsible contributes to the development of the research projects, applies for economics aids and solves problems or doubts of the service.

This RMN service at CICIC work 24 hours a day every day. The DRX400 spectrometer works 60% of the time with the liquid configuration and the 40% of the time with its solid state configuration.

INSTRUMENTAL DISPONIBLE / AVAILABLE INSTRUMENTAL



- 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 N₂, 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 N₂, and with a temperature control system that allows to work at a range of 223 K - 373 K.

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 INSTRUMENTAL

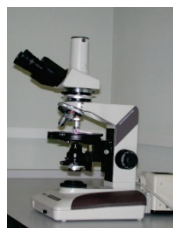
- Espectrómetro de descarga luminiscente LECO GDS 750A equipado con dos policromadores holográficos de 3600 y 1800 líneas respectivamente, óptica a vacío que permite el análisis en el UV y 43 fotomultiplicadores que permiten analizar los elementos indicados en la tabla mostrada abajo.

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

Resaltados en negro los elementos que se pueden analizar en el espectrómetro de descarga luminiscente LECO GDS 750A.

OTROS EQUIPOS / OTHER EQUIPMENT



- Analizador térmico diferencial y termogravimétrico (SETARAM TG-DTA 92) [Differential thermal and thermogravimetric analyzer \(SETARAM TG-DTA92\)](#)
- Analizador termogravimétrico (Perkin-Elmer, TGA-7) [Thermogravimetric analyzer \(Perkin-Elmer, TGA-7\)](#)
- Analizador de Carbono/Azufre LECO CS-200 [Carbon/Sulfur analyzer LECO CS-200](#)
- Análisis de gases (EGA) (hasta 1600 °C) [EGA \(up to 1600 °C\)](#)
- Analizador combinado de potencial "Z" y tamaño de partícula MALVERN ZETAMASTER Z [potential and particle size analyzer](#)
- Calorimetría de barrido diferencial (PERKIN-ELMER, DSC-7) [Differential scanning calorimeter \(PERKIN-ELMER, DSC-7\)](#)
- Calorímetros de conducción (2) para la medida precisa de calor específico y conductividad térmica de sólidos con campo eléctrico aplicado y con tensión mecánica uniaxial [Conductante calorimeters for thermal conductivity and specific heat determination](#)
- Difractómetro de Rayos X dual SIEMENS D-5000 para transmisión y reflexión [Dual X-ray diffractometer for transmission and reflection \(SIEMENS D-5000\)](#)
- Difractómetro de Rayos X SIEMENS D501 [X-ray diffractometer \(SIEMENS D501\)](#)
- Difractómetro SIEMENS D5000 equipado con sistema para difracción en película delgada [X-ray diffractometer equipped with thin film system \(SIEMENS D-5000\)](#)
- Difractómetros automáticos de RX para monocristal [X-ray diffractometer for single crystals](#)
- Dilatómetro diferencial ADAMEL LHOMARGY DI-24 [Differential dilatometer ADAMEL LHOMARGY DI-24](#)
- Equipo para el estudio de ciclos de histéresis eléctrica. Medida simultánea de propiedades térmicas y dieléctricas [Equipment for measurement of electric hysteresis cycles](#)
- Equipo para la medida precisa de resistividad, tensión eléctrica, constante dieléctrica y coeficiente piroeléctrico de monocristales y cerámicas dieléctricas [Equipment for measurement of resistivity, dielectric constant and piezoelectric coefficient of single crystals and ceramics](#)
- Espectrofotómetro de descarga luminiscente (GDS 750A LECO INST.) [Flow discharge spectrophotometer \(GDS 750A LECO INST.\)](#)
- Espectrofotómetro de infrarrojo por Transformada de Fourier (FT-IR) NICOLET 510 [FT-IR spectrometer \(NICOLET 510\)](#)
- Espectrofotómetro de infrarrojo por transformada de Fourier con accesorio de reflectancia difusa NICOLET 510P [FT-IR with diffuse reflectance accessory \(NICOLET 510P\)](#)
- Espectrómetro Raman, NICOLET 910 [Raman spectrometer NICOLET 910](#)
- Espectrómetro de resonancia magnética nuclear Bruker AMX-300 y DRX-400 [Nuclear magnetic resonance spectrometer Bruker AMX-300 and DRX-400](#)
- Espectrómetro de fluorescencia de rayos X (Siemens SRS3000) [X-ray fluorescence spectrometer \(Siemens SRS3000\)](#)

- Espectrómetro de masas [Mass spectrometer](#)
- Fuente de neutrones (acceso) [Access to neutron sources](#)
- Fuente de radiación sincrotrón (acceso) [Access to synchrotron radiation sources](#)
- Horno de Inducción LECO-Melt 6,6 μ p VAC High Frequency-Remelting Unit Lifumat 6,6 VAC
- Hornos y reactores [Ovens and reactor](#)
- Microscopio metalográfico NIKON modelo Optiphot [Metalographic microscope NIKON model](#)
- Microscopio de Fuerzas Atómicas TOPOMETRIX EXPLORER [Atomic force microscope TOPOMETRIX EXPLORER](#)
- Microscopio de infrarrojos NICPLAN [Infrared microscope NICPLAN](#)
- Microscopio electrónico de barrido JEOL equipado con un analizador de energía dispersiva de Rayos X [Scanning electron microscope JEOL with X-ray dispersive energy analyzer](#)
- Microscopio electrónico de transmisión Philips con accesorios EDX y EELS [Transmission electron microscope Philips with EDX and EELS accesories](#)
- Porosímetro de mercurio Fisons 4000 [Mercury porosimeter Fisons 4000](#)
- Sistemas INSTRON-1185 y INSTRON-8562 (velocidad de deformación constante) [INSTRON systems 1185 and 8562 \(constant deformation rate\)](#)
- Sistema de Ultra Alto Vacío Leybold-Heraeus LHS-10 y ESCALAB 210 para análisis AES, XPS, ISS [Ultra high vacuum spectrometers Leybold-Heraeus LHS-10 and ESCALAB 210 with accesories for AES, XPS and ISS](#)
- Sistema de fluencia dotado de horno de cromita [Fluence system with cromite oven](#)
- Sistemas de análisis Térmico a Velocidad Constante (ATVC) en alto vacío [ATVC analysis system in high vacuum](#)
- Trazador de ciclos de histéresis magnética (cuasi-estático) [Magnetic hysteresis tracer \(quasi-static\)](#)

PRODUCCIÓN CIENTÍFICA

SCIENTIFIC PRODUCTION



- 3.1.** Artículos publicados en Revistas SCI
Papers in SCI Journals
- 3.2.** Artículos publicados en Revistas no-SCI
Papers in non-SCI Journals
- 3.3.** Libros y otras publicaciones
Books and other publications
- 3.4.** Patentes
Patents
- 3.5.** Congresos y reuniones Internacionales
International congress and meetings
- 3.6.** Congresos y reuniones nacionales
National congress and Meetings
- 3.7.** Cursos
Courses
- 3.8.** Conferencias invitadas impartidas por personal del ICMS
Invited conferences by personnel of the ICMS
- 3.9.** Conferencias impartidas en el ICMS
Conferences in the ICMS
- 3.10.** Tesis doctorales
Doctor degree thesis
- 3.11.** Premios y Reconocimientos
Prizes and acknowledgements

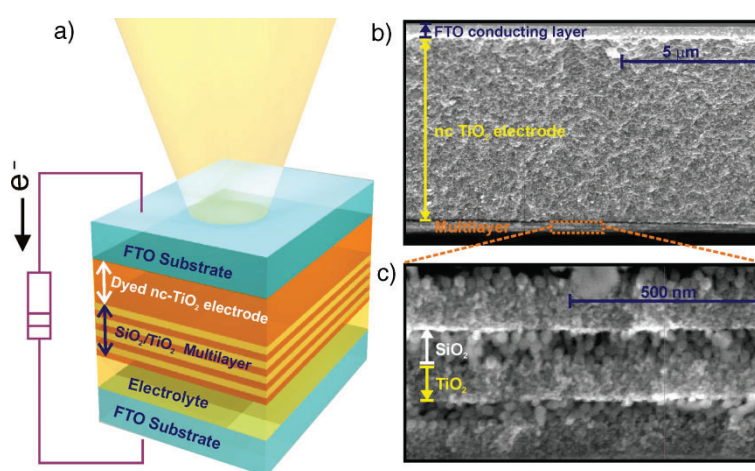
3.1. ARTÍCULOS PUBLICADOS EN REVISTAS SCI / PAPERS IN SCI JOURNALS

MATERIALES Y PROCESOS PARA SISTEMAS DE ENERGÍA SOSTENIBLE Y PROTECCIÓN DEL MEDIO AMBIENTE / MATERIALS AND PROCESSES FOR SUSTAINABLE ENERGY SYSTEMS AND ENVIRONMENT PROTECTION

Porous One-Dimensional Photonic Crystals Improve the Power-Conversion Efficiency of Dye-Sensitized Solar Cells

Colodrero, S; Mihi, A; Haggman, L; Ocaña, M; Boschloo, G; Hagfeldt, A; Miguez, H
Advanced Materials, **21** (2009) 764-770

The solar-to-electric power-conversion efficiency (71) of dye-sensitized solar cells can be greatly enhanced by integrating a mesoporous, nanoparticle-based, 1D photonic crystal as a coherent scattering layer in the device. The photogenerated current is greatly improved without altering the open-circuit voltage of the cell, while keeping the transparency of the cell intact. Improved average 77 values between 15% and 30% are attained.



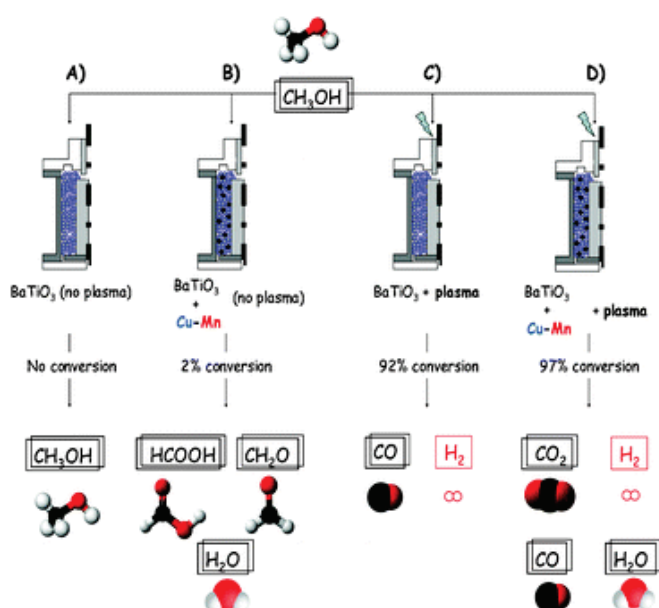
Design and microstructure of a DSSC coupled to a porous nanoparticle-based 1D PC. a) Scheme of the solar cell based on the 1D PC exposed to frontal illumination. b) FESEM image showing a cross-section of a dye-sensitized nc-TiO₂ electrode (total thickness indicated by the vertical yellow line) onto which a TiO₂-SiO₂ nanoparticle multilayer has been deposited (bottom of the image). c) Magnified view of the silica (spherical particles) and titania (smaller crystallites) layers composing the 1D PC.

Hybrid catalytic-DBD plasma reactor for the production of hydrogen and preferential CO oxidation (CO-PROX) at reduced temperatures

Rico, VJ; Hueso, JL; Cotrino, J; Gallardo, V; Sarmiento, B; Brey, JJ; Gonzalez-Elipe, AR

Chemical Communications (2009) 6192-6194

Dielectric Barrier Discharges (DBD) operated at atmospheric pressure and working at reduced temperatures ($T < 115$ degrees C) and a copper-manganese oxide catalyst are combined for the direct decomposition and the steam reforming of methanol (SRM) for hydrogen production and for the preferential oxidation of CO (CO-PROX).



Schematic representation of the reaction conditions and main products obtained during the direct decomposition of methanol in the hybrid catalyst-plasma reactor. A sketch of the mid-section DBD reactor combined with the BaTiO_3 beads and the copper-manganese catalyst is also included. (A) Reaction with BaTiO_3 in the absence of plasma; (B) Reaction with BaTiO_3 and the Cu-Mn catalyst in the absence of plasma; (C) Reaction with BaTiO_3 in the presence of plasma; (D) Reaction with BaTiO_3 and the Cu-Mn catalyst in the presence of plasma..

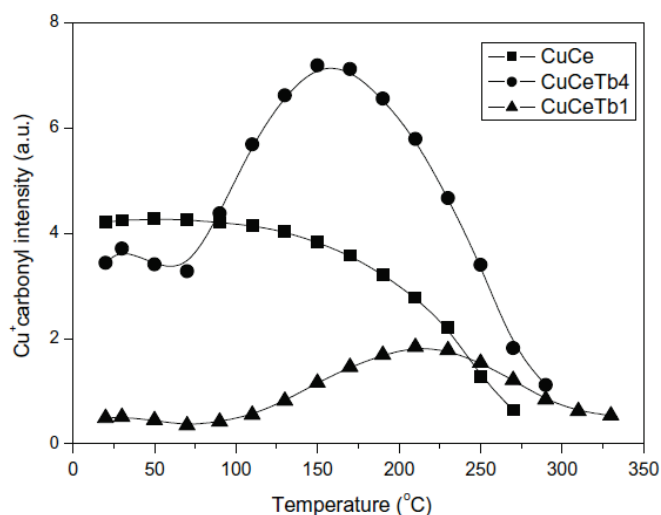
CO-TPR-DRIFTS-MS in situ study of $\text{CuO}/\text{Ce}_{1-x}\text{Tb}_x\text{O}_{2-y}$ ($x=0, 0.2$ and 0.5) catalysts: Support effects on redox properties and CO oxidation catalysis

Hornes, A; Bera, P; Camara, AL; Gamarra, D; Munuera, G; Martinez-Arias, A

Journal of Catalysis, **268** (2009) 367-375

Catalysts of copper oxide supported on CeO_2 and $\text{Ce}_{1-x}\text{Tb}_x\text{O}_{2-y}$ have been studied by temperature-programmed reduction employing CO as a reductant (CO-TPR) using a diffuse reflectance infrared Fourier transform spectroscopy (DRIFTS) cell as well as conventional tubular reactors in order to get insights into redox changes occurring in the course of interaction of the systems with CO. CO-TPR results collected in the classical way, i.e. starting

the temperature ramp after reactant gas equilibration at room temperature, suggest that the reduction of the copper species occurs at temperatures which decrease with the terbium content of the support. However, such result contrasts with CO oxidation activity of the systems under CO-PROX condition which follows just the opposite trend.



Evolution of the intensity of the Cu⁺-carbonyl species during the CO-TPR tests over the indicated samples.

FTIR study of photocatalytic degradation of 2-propanol in gas phase with different TiO₂ catalysts

Araña, J; Alonso, AP; Rodríguez, JMD; Colón, G; Navio, JA; Peña, JP
Applied Catalysis B-Environmental, **89** (2009) 204-213

The photocatalytic efficiency of different TiO₂ Catalysts in the degradation of 2-propanol in gas phase has been studied. The obtained efficiencies have been compared considering the distribution of rutile-anatase phases, surface area, particle size, distribution of surface hydroxyl groups and Bronsted or Lewis acid centres. The catalysts used were Degussa-P25 (TiO₂-P25), Hombikat, Millennium, Kemira and s/g-TiO₂, a catalyst prepared by a sol-gel method. The best photocatalytic behaviours have been obtained with those catalysts with higher surface area and the presence of only anatase phase (Hombikat and Millennium). A progressive deactivation of TiO₂-P25 and s/g-TiO₂ has been observed during the photocatalytic process. FTIR studies indicated that degradation mechanisms depended on the catalyst employed. Deactivation processes observed in TiO₂-P25 have been correlated with the formation of carboxylates. (C) 2008 Elsevier B.V. All rights reserved.

Ionic liquid templated TiO₂ nanoparticles as a support in gold environmental catalysis

Avellaneda, RS; Ivanova, S; Sanz, O; Romero-Sarria, F; Centeno, MA; Odriozola, JA
Applied Catalysis B-Environmental, **93** (2009) 140-148

This work presents the synthesis of a nanostructured titania support and its subsequent utilization for the gold particles deposition and application in the reaction of the CO oxidation. A functionalized ionic liquid has been used as a templating agent for the titanium

oxide synthesis resulting in a high specific surface nanostructured titania anatase. The as prepared support was then used for gold nanoparticles deposition without ionic liquid removal in order to study the possible role of the latter in the stabilization of the gold particles. The presence of ionic liquid in the catalysts results in an unusual catalytic behaviour-strong dependence on the presence of CO and changed kinetics and rate of oxidation. (C) 2009 Elsevier B.V. All rights reserved.

Influence of sulfur on the structural, surface properties and photocatalytic activity of sulfated TiO₂

Colon, G; Hidalgo, MC; Navio, JA; Kubacka, A; Fernandez-Garcia, M
Applied Catalysis B-Environmental, **90** (2009) 633-641

TiO₂ materials were prepared by sol-gel method and then impregnated with sulfuric acid and calcined using different temperatures and atmosphere (air and nitrogen). Systematic variation of these two experimental parameters makes possible to modulate the amount of surface sulfur from the impregnation procedure. The best photocatalyst for liquid phenol degradation was obtained after calcination at 700 degrees C in air, while gas toluene degradation optimum performance is obtained by calcination at 700 degrees C in nitrogen from 500 degrees C. Structural analysis of these materials by XRD, micro-Raman spectroscopy and FE-SEM shows that once calcined at 700 degrees C the material was a well-crystallized, high surface area anatase structure in all cases. The surface characterization by MR and XPS confirms the presence of a higher amount of sulfur species and acidic OH groups in samples partially calcined in nitrogen, and a low XPSO/Ti-atomic ratio with the O 1s peak shifted to higher binding energies (1.8 vs. 2 +/- 0.1 and 530.4 eV vs. 529.8 eV, respectively. against the reference materials) for samples calcined at 700 degrees C, temperature at which most of sulfate species have been evolved. The paper presents an attempt to correlate the contribution of the observed structural defects within the anatase sub-surface layers and surface acidity to the different photoactivity behaviour exhibited for phenol liquid phase and toluene gas phase photodegradation. (C) 2009 Elsevier B.V. All rights reserved.

Gold/hydroxyapatite catalysts Synthesis, characterization and catalytic activity to CO oxidation

Dominguez, MI; Romero-Sarria, F; Centeno, MA; Odriozola, JA
Applied Catalysis B-Environmental, **87** (2009) 245-251

This work reports the synthesis, characterization and catalytic activity for CO oxidation of gold catalysts supported on calcium hydroxyapatite. On both, the hydroxyapatite support and the gold-supported hydroxyapatite catalyst, the CO conversion shows a peak near 100% of conversion at room temperature. The generation of structural vacancies by interaction of CO with the solid provokes the formation of peroxide species in the presence of gaseous oxygen, which seems to be responsible of this high conversion of CO at room temperature. Moreover, the influence of the pre-treatment temperature on the activity has been observed and related with the elimination of carbonate species and the generation of structural defects in the apatite structure, which are able to modify the gold oxidation state. (C) 2008 Elsevier B.V. All rights reserved.

Manganese and iron oxides as combustion catalysts of volatile organic compounds

Duran, FG; Barbero, BP; Cadus, LE; Rojas, C; Centeno, MA; Odriozola, JA
Applied Catalysis B-Environmental, **92** (2009) 194-201

FeMn mixed oxides were prepared by the citrate method with Fe:Mn atomic ratio equal to 1:1, 1:3 and 3:1. The sample was characterized by means of specific surface area measurements, X-ray diffractometry (XRD), temperature programmed desorption of oxygen (O₂-DTP), temperature programmed reduction (TPR), X-ray fluorescence (XRF), transmission electron microscopy (TEM and SAED) and high resolution TEM (HREM). The characterization results demonstrated the formation of a Mn₂O₃-Fe₂O₃ solid solution. The catalytic performance in ethanol, ethyl acetate and toluene total oxidation on these samples was better than on Fe₂O₃ and Mn₂O₃ pure oxides. (C) 2009 Elsevier B.V. All rights reserved.

Water plasmas for the revalorisation of heavy oils and cokes from petroleum refining

Hueso, JL; Rico, VJ; Cotrino, J; Jimenez-Mateos, JM; Gonzalez-Elipe, AR
Environmental Science & Technology, **43** (2009) 2557-2562

This work investigates the possibility of using plasmas to treat high boiling point and viscous liquids (HBPVL) and cokes resulting as secondary streams from the refining of oil. For their revalorisation, the use of microwave (MW) induced plasmas of water is proposed, as an alternative to more conventional processes (i.e., catalysis, pyrolysis, combustion, etc.). As a main result, this type of energetic cold plasma facilitates the conversion at room temperature of the heavy aromatic oils and cokes into linear hydrocarbons and synthesis gas, commonly defined as syngas (CO + H₂ gas mixture). The exposure of the coke to this plasma also facilitates the removal of the sulfur present in the samples and leads to the formation on their surface of a sort of carbon fibers and rods network and new porous structures. Besides, optical emission measurements have provided direct evidence of the intermediates resulting from the fragmentation of the heavy oils and cokes during their exposure to the water plasma. Furthermore, the analysis of the mass spectra patterns suggests a major easiness to break the aromatic bonds mainly contained in the heavy oils. Therefore, an innovative method for the conversion of low value residues from oil-refining processes is addressed.

Experimental Demonstration of the Mechanism of Light Harvesting Enhancement in Photonic-Crystal-Based Dye-Sensitized Solar Cells

Colodrero, S; Mihi, A; Anta, JA; Ocana, M; Miguez, H
Journal of Physical Chemistry C, **113** (2009) 1150-1154

Herein, we report an experimental analysis of the photogenerated current of very thin and uniform dye-sensitized nanocrystalline titanium oxide (nc-TiO₂) electrodes coupled to high-quality one-dimensional photonic crystals. The effect of well-defined optical absorption resonances are detected both in optical spectroscopy and photogenerated current experiments, a clear correspondence between them being established. Our study demonstrates that light trapping within absorbing electrodes is responsible for the absorption enhancement that has previously been reported and unveils the mechanism behind it. We

prove that this effect improves significantly the power conversion efficiency of very thin electrodes.

Synthesis and Characterization of $Ce_{1-x}Eu_xO_{2-x/2}$ Mixed Oxides and Their Catalytic Activities for CO Oxidation

Hernandez, WY; Centeno, MA; Romero-Sarria, F; Odriozola, JA
Journal of Physical Chemistry C, **113** (2009) 5629-5635

A series of $Ce_{1-x}Eu_xO_{2-x/2}$ mixed oxides was synthesized by coprecipitation. The solids were characterized by means of XRF, S-BET, XRD, UV-vis, and Raman techniques, and their catalytic activities toward CO oxidation were tested. A solid solution, with CeO_2 F-type structure, is formed for europium contents (measured as Eu_2O_3 by XRF) $\leq 20\%$ wt. For higher contents, the solid solution is not formed, but a physical mixture is detected. The existence of oxygen vacancies in the solids with Eu_2O_3 contents between 3 and 17% wt was demonstrated by the presence of bands at 532 and 1275 cm^{-1} in their Raman spectra. The catalytic performances of the solids correlate with the amount of these punctual defects in the solid solution.

Effect of Sulfate Pretreatment on Gold-Modified TiO_2 for Photocatalytic Applications

Hidalgo, MC; Maicu, M; Navio, JA; Colon, G
Journal of Physical Chemistry C, **113** (2009) 12840-12847

The influence of sulfated pretreatment of TiO_2 on the structure, morphology, and dispersion of gold and photocatalytic properties of Au/TiO_2 were studied. Notable enhancements in the photocatalytic activity of TiO_2 were achieved by deposition of gold onto samples that had previously undergone sulfate treatment followed by high temperature calcination. The enhancement in activity can be attributed to the stronger bonding and improved electronic communication between gold particles and TiO_2 on defect rich surfaces as are found on sulfated samples after calcination at 700 degrees C. Two different methods for gold deposition were evaluated: chemical reduction by citrate and photodeposition. The citrate method produced more homogeneous and smaller gold particles with a better dispersion than photodeposition, which lead to greater increases in activity in the photocatalytic degradation of phenol when the former method was used for deposition on both sulfated and nonsulfated TiO_2 . The combination of sulfate pretreatment and gold deposition by chemical reduction was shown to be a good strategy to obtain gold/titania catalysts possessing homogeneous particle size and dispersion of the metal and a strong bonding between the Au and the TiO_2 surface.

W,N-Codoped TiO_2 -Anatase: A Sunlight-Operated Catalyst for Efficient and Selective Aromatic Hydrocarbons Photo-Oxidation

Kubacka, A; Bachiller-Baeza, B; Colon, G; Fernandez-Garcia, M
Journal of Physical Chemistry C, **113** (2009) 8553-8555

New W,N-doped TiO₂ anatase-based materials are synthesized having both unprecedented high activity and selectivity in the gas-phase partial oxidation of aromatic hydrocarbons using sunlight as excitation energy and molecular oxygen as oxidant.

Deposition of Al-Fe pillared bentonites and gold supported Al-Fe pillared bentonites on metallic monoliths for catalytic oxidation reactions

Martinez, LM; Dominguez, MI; Sanabria, N; Hernandez, WY; Moreno, S; Molina, R; Odriozola, JA; Centeno, MA

Applied Catalysis A-General, **364** (2009) 166-173

Al-Fe pillared bentonite and gold supported on Al-Fe pillared bentonite catalysts deposited on Fecralloy monoliths have been prepared, characterized and tested in two oxidation reactions: gaseous oxidation of CO and phenol oxidation in aqueous medium. The deposition of the solid on the metallic substrate does not alter its structural characteristics. The use of monoliths improves the activity in both reactions and offers the additional advantage to facilitate the separation of the catalyst from the reaction medium. (C) 2009 Elsevier B.V. All rights reserved.

ZnO activation by using activated carbon as a support: Characterisation and photoreactivity

Melián, EP; Diaz, OG; Rodriguez, JMD; Colón, G; Araña, J; Melian, JH; Navio, JA; Peña, JP

Applied Catalysis A-General, **364** (2009) 174-181

The effect of the mixing ZnO with different portions of activated carbon (AC) has been studied. The resulting catalysts were characterised and evaluated in the photocatalytic decomposition of aqueous pollutants. Changes in the catalyst colour and in the FTIR vibration bands of the surface hydroxyl groups were recorded. nu OH vibrations were shifted to lower wavenumbers as AC loading increased, demonstrating modification of the acid-base character of the catalysts. Laser scattering studies showed that AC loading leads to smaller ZnO particles. BET surface area measurements and scanning electron micrograph (SEM) analysis showed agglomeration of ZnO particle pores in the AC structure. Results showed that in addition to a synergistic effect of the AC-ZnO combination, AC content modifies the ZnO particle properties and consequently photocatalytic behaviour. This was evident in phenol degradation experiments where changes in the concentration profiles of the catechol and hydroquinone degradation intermediates, were observed. However, the AC-ZnO catalysts were less efficient than pure ZnO in the degradation of 2,4-dichlorophenol (DCP). This seems to be due to the strong adsorption of the DCP molecule on AC, resulting in lower diffusion to the catalytic ZnO and thus a lower rate of photocatalysis. (C) 2009 Elsevier B.V. All rights reserved.

Pillared clays with Al-Fe and Al-Ce-Fe in concentrated medium: Synthesis and catalytic activity

Sanabria, NR; Centeno, MA; Molina, R; Moreno, S

Applied Catalysis A-General, **356** (2009) 243-249

This paper proposes a new methodology for the modification of clays with the mixed Al-Fe and Al-Ce-Fe systems, which involves the synthesis of solid polymeric precursors and their use as pillaring agents in the modification of clays. The process of intercalation of clay with Al-13, Al-13 + Fe and Al-13 + Ce + Fe nitrate was performed using ultrasound. The pillaring agents Al-13, Al-13 + Fe and Al-13 + Ce + Fe were characterized by XRF, XRD, SEM and Al-27 NMR techniques, and pillared clays were characterized by XRF, XRD and N₂ adsorption to 77 K. The catalytic properties of pillared clays were evaluated using catalytic wet peroxide oxidation of phenol in dilute aqueous medium, demonstrating activity comparable to that of solids modified by the conventional method. (C) 2009 Elsevier B.V. All rights reserved.

Integration of methanol steam reforming and combustion in a microchannel reactor for H₂ production: A CFD simulation study

Arzamendi, G; Dieguez, PM; Montes, M; Centeno, MA; Odriozola, JA; Gandia, LM
Catalysis Today, **143** (2009) 25-31

A computational fluid dynamics (CFD) study of the thermal integration of the steam reforming of methanol (SRM) and the combustion of methanol in a catalytic microchannel reactor is presented. This issue is of interest for in situ H₂ production for portable power units based on low-temperature PEM fuel cells. Three-dimensional simulations have been carried out under relevant conditions for the SRM reaction that have shown that microreactors allow achieving complete methanol reforming and combustion at space velocities as high as 50,000 h⁻¹, with selectivities for H₂ above 99% at relatively low temperatures in the 270-290 degrees C range. (C) 2008 Elsevier B.V. All rights reserved.

Cationic (V, Mo, Nb, W) doping of TiO₂-anatase: A real alternative for visible light-driven photocatalysts

Kubacka, A; Colon, G; Fernandez-Garcia, M
Catalysis Today, **143** (2009) 286-292

In this article we investigate the structure-activity link of anatase-type Ti-M (M = V, Mo, Nb, and W) mixed oxides used for toluene photo-oxidation under sunlight-type excitation. An analysis of the local and long-range structural and electronic characteristics of the mixed oxides show that only structurally highly homogeneous anatase-type oxides with electronic properties exclusively leading to a band gap decrease drive to efficient visible light-driven photocatalysts. Within our microemulsion preparation method, this only occurs for Ti-V and Ti-W series of samples. The isoelectronic (V⁴⁺) substitution of Ti⁴⁺ ions at the anatase lattice is characterized by a low solubility limit (ca. 2.5 at. %), and drives to a limited modification of the band gap and to a moderate enhancement of the photo-activity with respect to bare titania reference systems. W presence at anatase cation positions occurs with concomitant presence of cation vacancies derived by the charge imbalance between the W⁶⁺ and Ti⁴⁺ species. A unique W-vacancy local arrangement is detected by the structural characterization, leading to both an important band gap decrease and enhancement of the photo-activity upon sunlight excitation. (C) 2008 Elsevier B.V. All rights reserved.

Wetting angles and photocatalytic activities of illuminated TiO₂ thin films

Rico, V; Romero, P; Hueso, JL; Espinos, JP; Gonzalez-Elipe, AR
Catalysis Today, **143** (2009) 347-354

TiO₂ thin films have been prepared by physical vapour deposition (PVD) and plasma enhanced chemical vapour deposition (PECVD) to study the UV-induced photo-activity of this material. Wetting angle variations and photo-catalytic activity for the degradation of dyes upon UV illumination have been compared for thin films with different crystalline structure (amorphous, rutile and anatase), microstructure (columnar, compact, etc.) and porosities as estimated from the Values of their refraction indices and their direct assessment with a quartz crystal monitor. The surface of the thin films became superhydrophilic upon UV light irradiation and then it recovered its original state by keeping the samples in the dark. Wetting angle decays follow very similar kinetics for amorphous and crystalline films, independently of their actual porosities. By contrast the photo-catalytic activity was very dependent on the crystalline structure of the films (anatase > rutile > amorphous) and on their porosities. The different behaviour depicted by the films with regard to these two properties suggests that they respond to different though related mechanisms and that they cannot be considered as equivalent when trying to prove the photo-activity of TiO₂. (C) 2008 Published by Elsevier B.V.

Larnite powders and larnite/silica aerogel composites as effective agents for CO₂ sequestration by carbonation

Santos, A; Ajbary, M; Morales-Florez, V; Kherbeche, A; Pinero, M; Esquivias, L
Journal of Hazardous Materials, **168** (2009) 1397-1403

This paper presents the results of the carbonation reaction of two sample types: larnite (Ca₂SiO₄) powders and larnite/silica aerogel composites, the larnite acting as an active phase in a process of direct mineral carbonation. First, larnite powders were synthesized by the reaction of colloidal silica and calcium nitrate in the presence of ethylene glycol. Then, to synthesize the composites, the surface of the larnite powders was chemically modified with 3-aminopropyltriethoxysilane (APTES), and later this mixture was added to a silica sol previously prepared from tetraethylorthosilicate (TEOS). The resulting humid gel was dried in an autoclave under supercritical conditions for the ethanol. The textures and chemical compositions of the powders and composites were characterized. The carbonation reaction of both types of samples was evaluated by means of X-ray diffraction and thermogravimetric analysis. Both techniques confirm the high efficiency of the reaction at room temperature and atmospheric pressure. A complete transformation of the silicate into carbonate resulted after submitting the samples to a flow of pure CO₂ for 15 min. This indicates that for this reaction time, 1 t of larnite could eliminate about 550 kg Of CO₂. The grain size, porosity, and specific surface area are the factors controlling the reaction. (C) 2009 Elsevier B.V. All rights reserved.

Methane steam reforming in a microchannel reactor for GTL intensification: A computational fluid dynamics simulation study

Arzamendia, G; Dieguez, PM; Montes, M; Odriozola, JA; Sousa-Aguiar, EF; Gandia, LM
Chemical Engineering Journal, **154** (2009) 168-173

The integration of the steam reforming and combustion of methane in a catalytic microchannel reactor has been simulated by computational fluid dynamics (CFD). Two models including 4 or 20 square microchannels of 20 mm of length and 0.7 mm of side have been developed. It has been assumed that a thin and homogeneous layer of an appropriate catalyst has been uniformly deposited onto the channels walls. The kinetics of the steam reforming of methane (SRM), water-gas shift (WGS) and methane combustion in air have been incorporated into the models. This has allowed simulating the effect of the gas streams space velocities, catalyst load, steam-to-carbon (S/C) ratio and flow arrangement on the microreformer performance. The results obtained illustrate the potential of microreactors for process intensification: complete combustion of methane is achieved at gas hourly space velocities (GHSV) as high as 130,000 h⁻¹. As concerns the SRM, methane conversions above 97% can be obtained at high GHSV of 30,000 h⁻¹ and temperatures of 900-950 degrees C. Under these conditions selectivity for syngas is controlled by the WGS equilibrium. (C) 2009 Elsevier B.V. All rights reserved.

AISI 304 Austenitic stainless steels monoliths for catalytic applications

Martinez, LM; Sanz, O; Dominguez, MI; Centeno, MA; Odriozola, JA
Chemical Engineering Journal, **148** (2009) 191-200

The thermal treatments of austenitic stainless steels monoliths were studied in order to generate a highly homogeneous and rough oxide scale strongly attached to the base alloy, which will subsequently ensure the good adherence of the catalysts. In this work it has been shown that the morphology integrity and, homogeneity of the scale are strongly influenced by the temperature and time of treatment. Washcoating method was Used to deposit oil the monolith surface a Au/CeO₂ catalyst. The drying procedure turned out to be the most critical variable for the adherence and homogeneity of the catalytic ceria layer, while the ceria colloid concentrations in the starting aqueous dispersion seems to have only a threshold effect. The monolithic reactors containing Au/CeO₂ layers are active in the oxidation of CO. (C) 2008 Elsevier B.V. All rights reserved.

Aluminium anodisation for Au-CeO₂/Al₂O₃-Al monoliths preparation

Sanz, O; Martinez, LM; Echave, FJ; Dominguez, MI; Centeno, MA; Odriozola, JA; Montes, M
Chemical Engineering Journal, **151** (2009) 324-332

The anodisation of aluminium monoliths was performed in order to generate an alumina layer that ensures a good adherence of the catalysts. In this study, it is demonstrated that the morphology of the produced alumina layer depends on time, temperature, current density and concentration of the selected electrolyte. When anodisation process with the extreme conditions was applied (30 degrees C, 50 min, 2A dm⁻²) and 2.6 M of sulphuric acid) a significant cracks were obtained and used to fix the subsequent catalytic coatings. The washcoating method was used to cover the monoliths with colloidal solutions of CeO₂ and/or Au-CeO₂ catalysts. The resulting monolithic catalysts were tested in the CO oxidation reaction being 1%Au-CeO₂ containing system the most active. The structured catalyst prepared this way changed neither the textural nor the catalytic properties of the deposited catalytic powders. (C) 2009 Elsevier B.V. All rights reserved.

Near-ambient X-ray photoemission spectroscopy and kinetic approach to the mechanism of carbon monoxide oxidation over lanthanum substituted cobaltites

Hueso, JL; Martinez-Martinez, D; Caballero, A; Gonzalez-Elipe, AR; Mun, BS; Salmeron, M
Catalysis Communications, **10** (2009) 1898-1902

We have studied the oxidation of carbon monoxide over a lanthanum substituted perovskite ($\text{La}_{0.5}\text{Sr}_{0.5}\text{CoO}_{3-d}$) Catalyst prepared by spray pyrolysis. Under the assumption of a first-order kinetics mechanism for CO, it has been found that the activation energy barrier of the reaction changes from similar to 80 to similar to 40 kJ mol⁻¹ at a threshold temperature of ca. 320 degrees C. In situ XPS near-ambient pressure (similar to 0.2 torr) shows that the gas phase oxygen concentration over the sample decreases sharply at ca. 300 degrees C. These two observations suggest that the oxidation of CO undergoes a change of mechanism at temperatures higher than 300 degrees C. (c) 2009 Elsevier B.V. All rights reserved.

Redox chemistry of gold in a Au/FeOx/CeO₂ CO oxidation catalyst

Penkova, A; Chakarova, K; Laguna, OH; Hadjiivanov, K; Saria, FR; Centeno, MA; Odriozola, JA
Catalysis Communications, **10** (2009) 1196-1202

Calcination and evacuation of a Au/FeOx/CeO₂ catalyst at 573 K leads to reduction of the deposited gold to metal. This metal state is stable under oxygen and only at 573 K some metal atoms are oxidized to Au delta+ sites (Au+ cations situated on metal gold particles). However, even at room temperature, gold is readily oxidized in a CO + O-2 mixture producing, in addition to the Au delta+ sites, some isolated Au+ cations. (C) 2009 Elsevier B.V. All rights reserved.

Chemical and electronic interface structure of spray pyrolysis deposited undoped and Al-doped ZnO thin films on a commercial Cz-Si solar cell substrate

Gabas, M; Barrett, NT; Ramos-Barrado, JR; Gota, S; Rojas, TC; Lopez-Escalante, MC
Solar Energy Materials And Solar Cells, **93** (2009) 1356-1365

We have studied differences in the interface between undoped and Al-doped ZnO thin films deposited on commercial Si solar cell substrates. The undoped ZnO film is significantly thicker than the Al-doped film for the same deposition time. An extended silicate-like interface is present in both samples. Transmission electron microscopy (TEM) and photoelectron spectroscopy (PES) probe the presence of a zinc silicate and several Si oxides in both cases. Although Al doping improves the conductivity of ZnO, we present evidence for Al segregation at the interface during deposition on the Si substrate and suggest the presence of considerable fixed charge near the oxidized Si interface layer. The induced distortion in the valence band, compared to that of undoped ZnO, could be responsible for considerable reduction in the solar cell performance. (C) 2009 Elsevier B.V. All rights reserved.

Chemical reactivity of argillaceous material in engineered barrier Rare earth disilicate formation under subcritical conditions

Alba, MD; Chain, P; Orta, MM
Applied Clay Science, **43** (2009) 369-375

The Deep Geological Repository (DGR) is the most internationally accepted option for the storage of high radioactive wastes. This confinement is based on the multibarrier concept where the engineered barrier is crucial for the safety of the repository. Nowadays, bentonite is accepted as the best argillaceous material in the engineered barrier of DGR. Additionally to its well-known physical role, a chemical interaction between lutetium, as actinide simulator, and the smectite has been demonstrated. The aim of this paper is the study of the hydrothermal reaction of smectite and a wide set of rare earth cations as trivalent actinide simulators. Saponite was submitted to hydrothermal treatment at 300 degrees C with a solution of REE³⁺ cations (REE=Sc, Lu, Y, Sm, Nd and La). The products were analyzed by XRD, NMR and electron microscopy. Under hydrothermal conditions, saponite formed rare earth silicates. The final products and the reactivity of saponite depend on, among other factors, the nature of those cations. (C) 2008 Elsevier B.V. All rights reserved.

Rare-earth disilicate formation under Deep Geological Repository approach conditions

Alba, MD; Chain, P; Orta, MM
Applied Clay Science, **46** (2009) 63-68

The Deep Geological Repository (DGR) concept involves the placement of long-lived radioactive waste in rooms excavated deep. The major responsibility of the disposal safety falls on the Engineered Barrier System (EBS). The main constituent of EBS is bentonite that prevents the release of radioactive nuclei by physical and chemical mechanisms. The physical mechanism is expected to fault with the weathering of the bentonite while the chemical mechanisms have been only proved at 300 degrees C. It is the aim of this paper to explore the feasibility of the chemical mechanism at temperatures closer to the DGP conditions and to shed light on the mechanism of transformation of the argillaceous materials of the EBS in rare-earth disilicate phases. Saponite was submitted to hydrothermal reaction at 175 degrees C and 150 degrees C with different solutions of REE³⁺ cations (REE = Sc, Lu, Y, Sm, Nd and La). The products were analyzed by XRD, NMR and electron microscopy. At conditions close to the DGP, the saponite was able to form rare-earth silicates. The formation of the disilicate phase, as final product, needs a set of stages and oxyorthosilicate as precursor. (C) 2009 Elsevier B.V. All rights reserved.

Characterization of sepiolite-gel-based formulations for controlled release of pesticides

Maqueda, C; Partal, P; Villaverde, J; Perez-Rodriguez, JL
Applied Clay Science, **46** (2009) 289-295

Novel controlled release formulations (CRFs) were developed for reducing leaching of herbicides and contamination of groundwater. The herbicide metribuzin (MTB) was entrapped within a sepiolite-gel matrix using a novel and ultrasound-based technique. Different sepiolite/herbicide matrices (either as a gel or as a powder after freeze-drying) were prepared with pesticide loading between 28.6 and 9.1%. The release of MTB from the control released formulations into water was retarded when compared with commercial formulation (CF), except in the case of the sepiolite-gel-based formulations with lower amounts of sepiolite. The rheological properties and microstructure of these formulations were examined in detail. FRIR spectra showed that there was no evidence of herbicide inside the sepiolite tunnels. The SEM micrograph of the sepiolite-gel-based formulations showed the fibrous morphology typical of sepiolite and no separate particles of MTB were found. However, the chemical analysis by EDX confirmed the presence of S, N, and C, which were attributed to MTB, together with the fibers of sepiolite. Rheological characterization indicated that samples containing MTB develops a microstructure. which is irrespective of concentration above 1 mass % sepiolite. There was a good agreement between the microstructure characteristics and MTB release behavior. (C) 2009 Elsevier B.V. All rights reserved.

Study of ground and unground leached vermiculite

Maqueda, C; Perez-Rodriguez, JL; Subrt, J; Murafa, N
Applied Clay Science, **44** (2009) 178-184

Grinding of clays modifies their surfaces and can significantly affect their leaching behaviour. The acid reaction of vermiculite from Santa Olalla (Huelva, Spain) with HCl at various concentrations was affected by grinding and acid concentration. The acid leaching of ground vermiculite for 3 min with 1 M HCl solution at 80 degrees C for 24 h removed MgO and Al₂O₃ almost completely, leaving a residue containing SiO₂ and Fe₂O₃. X-ray diffraction analysis showed the presence of akaganeite (beta-FeOOH) and an amorphous phase (silica). Porosity studies showed a very high specific surface area for ground samples compared with unground vermiculite samples, attributed to the presence of iron in the residue coming from structural iron. High resolution transmission electron microscopy (HRTEM) confirmed the presence of iron oxyhydroxides embedded in the silica material. The particle morphology of the iron oxides corresponded well to akaganeite microcrystals precipitated from solution. The leached vermiculite residue also contained Cl⁻ and a small amount of Ti⁴⁺, which were accumulated into the akaganeite microcrystals. (C) 2009 Elsevier B.V. All rights reserved.

Fibrous MnO₂ Nanoparticles with (2 x 2) Tunnel Structures. Catalytic Activity in the Total Oxidation of Volatile Organic Compounds

Dominguez, MI; Navarro, P; Romero-Sarria, F; Frias, D; Cruz, SA; Delgado, JJ; Centeno, MA; Montes, M; Odriozola, JA
Journal of Nanoscience and Nanotechnology, **9** (2009) 3837-3842

Manganese oxides having 2 x 2 tunnel structures (cryptomelanes) have been synthesized by a milling method in order to test their efficiency as catalysts for the abatement of volatile organic compounds, using toluene as probe molecule. These materials present excellent textural properties, arising from the nanofiber morphology and were active for

toluene total oxidation. DRIFTS of the adsorbed phase allow proposing the role of lattice oxygen in the catalytic reaction.

Reactivity of $\text{LaNi}_{1-y}\text{Co}(y)$ O_{3-delta} Perovskite Systems in the Deep Oxidation of Toluene

Pereniguez, R; Hueso, JL; Holgado, JP; Gaillard, F; Caballero, A
Catalysis Letters, **131** (2009) 164-169

In the present work we have evaluated the oxidation of toluene over different lanthanum perovskites with a general composition of $\text{LaNi}_{1-y}\text{Co}(y)$ O_{3-delta}. These catalysts, prepared by a spray pyrolysis method, have been characterised by XRD, BET and FE-SEM techniques. Additional experiments of temperature programmed desorption of O₂, reduction in H₂ and X-ray absorption spectroscopy were also performed in order to identify the main surface oxygen species and the reducibility of the different perovskites. The catalytic behaviour toward the oxidation of toluene (as a model for VOCs compounds) was evaluated in the range 100-600 A degrees C, detecting a total conversion for all the samples below 400 A degrees C and higher activities for the cobalt-containing perovskites. The catalytic behaviour of these samples is consistent with a suprafacial mechanism, with the alpha-type oxygen playing an active role in the oxidation reaction.

Co₃O₄ + CeO₂/SiO₂ Catalysts for n-Hexane and CO Oxidation

Todorova, S; Kadinov, G; Tenchev, K; Caballero, A; Holgado, JP; Pereniguez, R
Catalysis Letters, **129** (2009) 149-155

Two-component Co-Ce samples deposited onto SiO₂ have been prepared, characterized and tested in the reaction of complete n-hexane and CO oxidation. It was established that cerium enhanced the catalytic activity of cobalt in the reaction of n-hexane oxidation, although this depended on the sequence of cobalt and cerium introduction. Co-impregnation of Co and Ce resulted in a close interaction between Co₃O₄ and CeO₂ leading to more surface oxygen species available and, therefore, a better reactivity.

Degradation of n-Butyl tin Chlorides in Waters. A Comparative Assessment of the Process by Photo-assisted and Chemical- treatment Methods

Navio, JA; Cerrillos, C; Macias, M
Journal of Advanced Oxidation Technologies, **12** (2009) 158-163

The degradation of aqueous n-butyl tin by several selected advanced oxidation technologies (AOTs) was studied and comparisons made between the processes. UV-photolytic and TiO₂-photoassisted oxidation and treatment with chemical oxidants (hydrogen peroxide, hypochlorite) were thus evaluated in terms of their action upon n-butyltin chlorides in water.

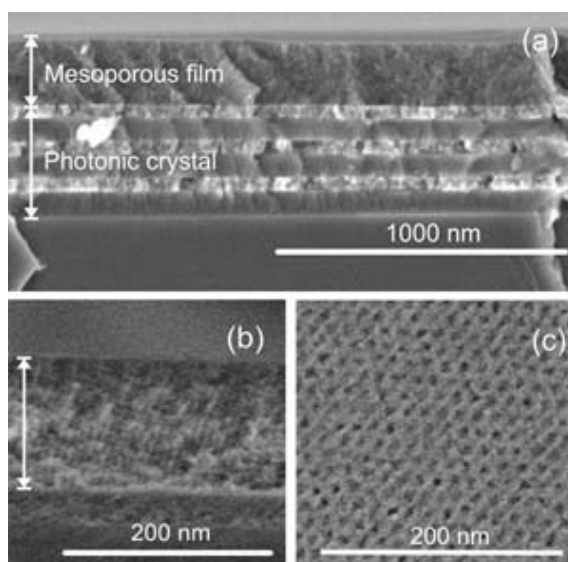
RECUBRIMIENTOS Y FUNCIONALIZACIÓN QUÍMICA DE SUPERFICIES CHEMICAL FUNCTIONALISATION OF SURFACES AND COATINGS

Mesostructured Thin Films as Responsive Optical Coatings of Photonic Crystals

Hidalgo, N; Calvo, ME; Miguez, H

Small, 5 (2009) 2309-2315

A synthetic route is presented to attain high-optical-quality multilayered structures that residtfront coupling ordered mesoporous titanium oxide thin films to the surface of a dense one-dimensional photonic crystal. Such architectures present spectrally well-defined photon resonant modes localized in the outer coating that finely respond to physicochemically induced modifications of its pore volume. The potential of these porous coatings in detection of environmental changes through variations of the photonic response of the ensemble is demonstrated by performing isothermal optical reflectance measurements under controlled vapor-pressure conditions.



FESEM characterization. a) Cross section of a dense SiO₂-TiO₂ multilayer coated with a mesostructured TiO₂ film. b) Detail of the mesostructured film in which the ordered pore planes can be seen. c) Top view of the TiO₂ mesoporous coating, in which the open pores can be clearly distinguished



Molding with nanoparticle-based one-dimensional photonic crystals: a route to flexible and transferable Bragg mirrors of high dielectric contrast

Calvo, ME; Sobrado, OS; Lozano, G; Miguez, H

Journal of Materials Chemistry, **19** (2009) 3144-3148 | journal cover

Self-standing, flexible Bragg mirror films of high refractive index contrast and showing intense and wide Bragg peaks are herein presented. Nanoparticle-based one-dimensional photonic crystals are used as templates to infiltrate a polymer, which provides the multilayer with mechanical stability while preserving the dielectric contrast existing in the mold. Such films can be lifted off the substrate and used to coat another surface of arbitrary shape.

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

Lozano, GS; Dorado, LA; Depine, RA; Miguez, H

Journal of Materials Chemistry, **19** (2009) 185-190

Recent advances in the comprehension of the growth dynamics of colloidal crystal films opens the door to rational design of experiments aiming at fabricating lattices in which the density of intrinsic defects is minimized. Since such imperfections have a dramatic effect on scattered light of wavelength smaller than the lattice constant, the evaluation of the experimental optical response at those energy ranges, based on the comparison to rigorous calculations, is identified as the most sensitive guide to accurately evaluate the progress towards the actual realization of defect-free colloidal crystals.

Growth of Crystalline TiO₂ by Plasma Enhanced Chemical Vapor Deposition

Borras, A; Sanchez-Valencia, JR; Widmer, R; Rico, VJ; Justo, A; Gonzalez-Eliphe, AR

Crystal Growth & Design, **9** (2009) 2868-2876

TiO₂ thin films in the form of anatase have been prepared by plasma enhanced chemical vapor deposition (PECVD) at 523 K as the substrate temperature and a low working pressure. The study of the microstructure and texture of the films at different stages of deposition show that their growth follows the Kolmogorov's model developed to describe the evolution of crystalline films from a saturated homogeneous medium. An additional characteristic feature of the growth process by PECVD is the formation of different crystalline domains, particularly at low deposition rates. The effects of this parameter and of the characteristics of the substrate on the growing process are also addressed.

Incorporation and Thermal Evolution of Rhodamine 6G Dye Molecules Adsorbed in Porous Columnar Optical SiO₂ Thin Films

Sanchez-Valencia, JR; Blaszczyk-Lezak, I; Espinos, JP; Hamad, S; Gonzalez-Elipe, AR; Barranco, A
Langmuir, **25** (2009) 9140-9148

Rhodamine 6G (Rh6G) dye Molecules have been incorporated into transparent and porous SiO₂ thin films prepared by evaporation at glancing angles. The porosity of these films has been assessed by analyzing their water adsorption isotherms measured for the films deposited on a quartz crystal monitor. Composite Rh6G/SiO₂ thin films were prepared by immersion of a SiO₂ thin film into a solution of the dye at a given pH. It is found that the amount of Rh6G molecules incorporated into the film is directly dependent on the pH of the solution and can be accounted for by a model based on the point of zero charge (PZC) concepts originally developed for colloidal oxides. At low pHs, the dye molecules incorporate in the form of monomers, while dimers or higher aggregates are formed if the pH increases. Depending on the actual preparation and treatment conditions, they also exhibit high relative fluorescence efficiency. The thermal stability of the composite films has been also investigated by characterizing their optical behavior after heating in an Ar atmosphere at increasing temperatures up to 275 degrees C. Heating induces a progressive loss of active dye molecules, a change in their agglomeration state, and an increment in their relative fluorescence efficiency. The obtained Rh6G/SiO₂ composite thin films did not disperse the light and therefore can be used for integration into optical and photonic devices.

Optically Active Luminescent Perylene Thin Films Deposited by Plasma Polymerization

Blaszczyk-Lezak, I; Aparicio, FJ; Borrás, A; Barranco, A; Alvarez-Herrero, A; Fernandez-Rodriguez, M; Gonzalez-Elipe, AR
Journal of Physical Chemistry C, **113** (2009) 431-438

This work reports about the preparation of plasma polymerized thin films of perylene with thicknesses similar to 30-150 nm and their characterization by different methods and the analysis of their optical properties. Highly absorbent and fluorescent films have been obtained by this method that combines the Sublimation of the perylene molecules and their controlled polymerization by the interaction with remote Ar plasma. The polymeric films are very flat with a root mean square (rms) roughness in the range 0.3-0.4 nm. In contrast with the sublimated layers of perylene that present a high scattering of light, the polymerized films depict the well-defined absorption bands in the region 400-450 nm and fluorescence spectra of the perylene molecule at similar to 475 nm. The films are formed by a matrix formed by cross-linked fragments of perylene and intact molecules that confer the observed optical properties to this material. The optical and microstructural characteristics of this type of thin films and the possibility to perform their deposition by using lithographic procedures make them suitable for their integration into photonic components for various applications. A preliminary study of the use of these films as an optical sensor of NO₂ is also presented.

Wetting Angles on Illuminated Ta₂O₅ Thin Films with Controlled Nanostructure

Rico, V; Borrás, A; Yubero, F; Espinos, JP; Frutos, F; Gonzalez-Elipe, AR
Journal of Physical Chemistry C, **113** (2009) 3775-3784

Ta₂O₅ thin films with different nanostructure and surface roughness have been prepared by electron evaporation at different angles between the evaporation source and the substrates. Large variation of refraction indexes (*n*) from 1.40 to 1.80 were obtained by changing the geometry of evaporation and/or by annealing the evaporated films at increasing temperatures up to 1000 degrees C to make them crystalline. Very flat and compact thin films (*n* = 2.02) were also obtained by assisting the growth by bombardment with O²⁺ ions of 800 eV kinetic energy. A similar correlation has been found between the wetting contact angle of water and the roughness of the films for the evaporated and evaporated + annealed samples, irrespective of their procedure of preparation and other microstructural characteristics. When the films were illuminated with UV light of $h\nu > E_g = 4.2$ eV (*E_g*, band gap energy of Ta₂O₅), their surface became superhydrophilic (contact angle < 10 degrees) in a way quite similar to those reported for illuminated TiO₂ thin films. The rate of transformation into the superhydrophilic state was smaller for the crystalline than for the amorphous films, suggesting that in Ta₂O₅ the size of crystal domains at the surface is an important parameter for the control of this kinetics. Changes in the water contact angle on films illuminated with visible light were also found when they were subjected to implantation with N²⁺ ions of 800 eV kinetic energy. The origin of this photoactivity is discussed in terms of the electronic band gap states associated with the nitrogen-implanted atoms. The possibility of preparing antireflective and self-cleaning coatings of Ta₂O₅ is discussed.

Chemical State of Nitrogen and Visible Surface and Schottky Barrier Driven Photoactivities of N-Doped TiO₂ Thin Films

Romero-Gomez, P; Rico, V; Borrás, A; Barranco, A; Espinos, JP; Cotrino, J; Gonzalez-Elipé, AR
Journal of Physical Chemistry C, **113** (2009) 13341-13351

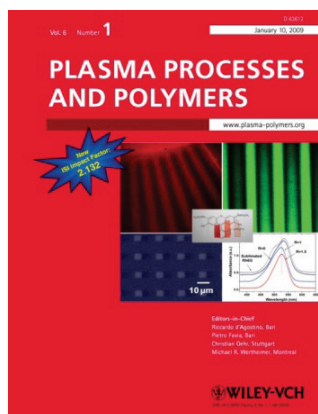
N-doped TiO₂ thin films have been prepared by plasma enhanced chemical vapor deposition and by physical vapor deposition by adding nitrogen or ammonia to the gas phase. Different sets of N-doped TiO₂ thin films have been obtained by changing the preparation conditions during the deposition. The samples have been characterized by X-ray diffraction, Raman, UV-vis spectroscopy, and X-ray photoemission spectroscopy (XPS). By changing the preparation conditions, different structures, microstructures, and degrees and types of doping have been obtained and some relationships have been established between these film properties and their visible light photoactivity. The N1s XP spectra of the samples are characterized by three main features, one tentatively attributed to Ti-N (i.e., nitride with a binding energy (BE) of 396.1 eV) and two others with BEs of 399.3 and 400.7 eV, tentatively attributed to nitrogen bonded simultaneously to titanium and oxygen atoms (i.e., Ti-N-O like species). By controlling the deposition conditions it is possible to prepare samples with only one of these species as majority component. It has been shown that only the samples with Ti-N-O like species show surface photoactivity being able to change their wetting angle when they are illuminated with visible light. The presence of these species and an additional complex structure formed by a mixture of anatase and rutile phases is an additional condition that is fulfilled by the thin films that also present photocatalytic activity with visible light (i.e., surface and Schottky barrier driven photoactivities). The relationships existing between the reduction state of the samples and the formation of Ti-N or Ti-N-O like species are also discussed.

Changing the physical and chemical properties of titanium oxynitrides $TiN_{1-x}O_x$ by changing the composition

Graciani, J; Hamad, S; Sanz, JF

Physical Review B, **80** (2009) 184112-1-184112-10

The stability and structural properties of titanium oxynitrides, $TiN_{1-x}O_x$, of different compositions are theoretically analyzed by means of first-principles periodic density-functional calculations. We show that at $x=0.55-0.6$ there is a change in the preferred structure from that of NaCl type to the alpha-TiO arrangement. For the NaCl-type structure the cell volume increases with x while it decreases with x for the alpha-TiO structure. The bulk moduli are always much larger for NaCl-type structures than for alpha-TiO and they decrease as the amount of O increases, moving from 280 GPa for TiN to 226 GPa for TiO (NaCl-type structure) or 197 GPa for alpha-TiO. Changes in the electronic structure with the composition are also considered. In general we found that in the two types of structure (NaCl and alpha-TiO), both the band gap and the ionic character increase with the O concentration.



Luminescent and Optical Properties of Nanocomposite Thin Films Deposited by Remote Plasma Polymerization of Rhodamine 6G

Aparicio, FJ; Borrás, A; Blaszczyk-Lezak, I; Groning, P; Alvarez-Herrero, A; Fernandez-Rodriguez, M; Gonzalez-Elise, AR; Barranco, A

Plasma Processes and Polymers, **6** (2009) 17-26 | journal cover

Mechanically stable and insoluble fluorescent thin films have been deposited by sublimating Rhodamine 6G laser dye in the downstream region of a low-power microwave ECR plasma using an experimental set-up designed to control the interaction of the dye molecule with the glow discharge. The use of reactive organosilane plasmas allows to control the dye distribution inside the matrix, leading to solid nanocomposite thin films containing non-aggregated dye molecules. The suppression of aggregates is a key issue to avoid fluorescence quenching. The obtained nanocomposite films are interesting because of their strong absorption and high fluorescence emission. In addition, they can be patterned using in situ plasma treatments in order to produce optically functional devices.

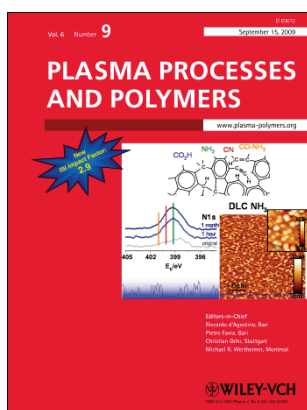
Thermal Evolution of WC/C Nanostructured Coatings by Raman and In Situ XRD Analysis

El Mrabet, S; Abad, MD; Lopez-Cartes, C; Martinez-Martinez, D; Sanchez-Lopez, JC

Plasma Processes and Polymers, **6** (2009) S444 - S449

In this work, a series of WC/C nanostructured films were deposited on silicon substrates by changing the ratio of sputtering power applied to graphite and WC magnetron sources (P_C/P_{WC} : 0, 0.1, 0.5, 1). The thermal stability of WC/C coatings was followed in situ by means of X-ray diffraction measurements up to 1100 °C in vacuum (10^{-1} Pa). Initially, the film microstructure is composed of nanocrystalline WC_{1-x} and W_2C phases. As the P_C/P_{WC} ratio

increases the crystallinity decreases, and WC_{1-x} becomes the predominant phase from $P_C/P_{WC} = 0.1$. The results show that the structural evolution with temperature of all studied layers depends essentially on their initial phase and chemical composition (determined by the synthesis conditions: ratio P_C/P_{WC}). The coating deposited at $P_C/P_{WC} = 0$ reveals a transformation of W_2C phase into W and W_3C phases at 400 degrees C. However, the samples with P_C/P_{WC} greater than 0 exhibits an improved thermal stability up to 600-700 °C where the WC_{1-x} begins to transform into W_2C and WC phases. At 900 °C, WC is the predominant phase, especially for those coatings prepared with higher ratios. Further annealing above 1000 °C yields W as the foremost phase. The thermal behaviour was later studied by means of Raman spectroscopy measurements at certain temperatures where the main changes in phase composition were observed. Particularly, a fitting analysis was carried out on the D and G bands typical of disordered and amorphous carbon. The changes induced during heating are discussed in terms of the positions of D and G lines, and full width at half maximum (FWHM).



Formation of Nitrogen Functional Groups on Plasma Treated DLC

Lopez-Santos, C; Yubero, F; Cotrino, J; Contreras, L; Barranco, A; Gonzalez-Elipe, AR

Plasma Processes and Polymers, 6 (2009) 555-565 | journal cover

Diamond like carbon (DLC) thin films have been exposed to different nitrogen containing plasmas. A dielectric barrier discharge (DBD) at atmospheric pressure and a microwave discharge (MW) at low pressure using N_2 and mixtures Ar^+NH_3 have been compared. Optical Emission and X-ray Photoelectron spectroscopies, Atomic Force Microscopy and contact angle

measurements have been used for this study. A DBD with Ar^+NH_3 is the most efficient method for DLC functionalization. Films treated with this plasma presented the highest concentration of amine groups as determined by derivatization with 4-chlorobenzaldehyde. All the treated samples underwent a significant aging with time. The efficiency of the different plasmas for DLC functionalization is discussed in the light of the intermediate species detected in the plasma.

Surface nanostructuring of TiO_2 thin films by ion beam irradiation

Romero-Gomez, P; Palmero, A; Yubero, F; Vinnichenko, M; Kolitsch, A; Gonzalez-Elipe, AR

Scripta Materialia, 60 (2009) 574-577

This work reports a procedure to modify the surface nanostructure of TiO_2 anatase thin films through ion beam irradiation with energies in the keV range. Irradiation with N^+ ions leads to the formation of a layer with voids at a depth similar to the ion-projected range. By setting the ion-projected range a few tens of nanometers below the surface of the film, well-ordered nanorods appear aligned with the angle of incidence of the ion beam. Slightly different results were obtained by using heavier (S^+) and lighter (B^+) ions under similar conditions. (C) 2008 Acta Materialia Inc. Published by Elsevier Ltd. All rights reserved.

Porosity and microstructure of plasma deposited TiO₂ thin films

Borras, A; Sanchez-Valencia, JR; Garrido-Molinero, J; Barranco, A; Gonzalez-Elipse, AR
Microporous and Mesoporous Materials, **118** (2009) 314-324

The microstructure of TiO₂ thin films prepared by plasma enhanced chemical vapour deposition has been assessed by using water adsorption-desorption isotherms measured by means of a quartz crystal monitor (QCM). Thin films have been deposited by using titanium tetraisopropoxide as a precursor and by changing different experimental parameters of the deposition procedure such as temperature of the substrate, pressure, and gas composition in the plasma. The films were characteristic of different microstructures that, according to their scanning electron micrographs, have been categorized as columnar, homogeneous and crystalline. They also have different refraction indices with values between 1.95 and 2.41. Water and toluene adsorption isotherms have been measured by means of a QCM monitor for the films heated in vacuum to remove the water previously adsorbed in their pores. The analysis of the adsorption-desorption isotherms by means of the so called "t-plots" and the determination of the pore size distribution curves rendered that the three kinds of microstructures presented different kinds of isotherms and water adsorption behaviours. Columnar films consisted of micro- and meso-pores had a very high adsorption hysteresis at low pressures. Homogeneous films only had micropores and presented no adsorption hysteresis. Crystalline films consisted of both micro- and meso-pores but had no adsorption hysteresis at low pressures. A zone scheme has been proposed to account for the microstructure of the films depending on the plasma conditions utilized. The implications of the different water adsorption behaviours of the films for the determination of their refraction indices are discussed. (C) 2008 Elsevier Inc. All rights reserved.

Gold nanoparticles on silica monospheres modified by amino groups

Penkova, A; Blanes, JMM; Cruz, SA; Centeno, MA; Hadjiivanov, K; Odriozola, JA
Microporous and Mesoporous Materials, **117** (2009) 530-534

Silica monospheres with a diameter of 330 nm modified with aminosilane compounds of three different basicities have been prepared. Surface coverage of the silica with an organic compound leads to an increase of the point of zero charge (PZC) of the silica surface from 2.1 to 5.1, 6.5 and 7.2 values, depending on the amine used. From these silicas, gold-containing catalysts have been prepared by a deposition-precipitation method at the same pH as the PZC of the support. The best results have been obtained using 3-(Diethoxymethylsilyl) propylamine as a modifying agent, which has allowed obtaining a good dispersion of the gold particles with an average size of 3.8 nm. (c) 2008 Elsevier Inc. All rights reserved.

WC/a-C nanocomposite thin films: Optical and electrical properties

Abad, MD; Sanchez-Lopez, JC; Cusnir, N; Sanjines, R
Journal of Applied Physics, **105** (2009) 033510- 033510-6

WC/amorphous carbon (a-C) thin films were deposited by dual magnetron sputtering from individual WC and graphite targets. The influence of film composition and microstructure on the optical and electrical properties was investigated. As evidenced by x-ray photoelectron

spectroscopy and grazing angle x-ray diffraction measurements, the WC/a-C films are composite materials made of hexagonal W_2C and/or cubic beta- WC_{1-x} nanocrystallites embedded in (a-C) matrix. The optical properties were studied by spectroscopic ellipsometry and the electrical resistivity was measured by the van der Pauw method between 20 and 300 K. Both the optical and the electrical properties of the WC/a-C films are correlated with the chemical composition and microstructure evolution caused by a-C addition. The optical properties of $W_2C/a-C$ and $\beta-WC_{1-x}/a-C$ films with a-C content ≤ 10 at. % are explained by modeling their dielectric functions by a set of Drude-Lorentz oscillators. Further increase in a-C content leads only to the formation of $\beta-WC_{1-x}/a-C$ nanocomposite structures and their optical properties progressively evolve to those of a-C single phase. The electrical resistivity as a function of the temperature of all the films exhibits a negative temperature coefficient of resistivity. Theoretical fitting using the grain-boundary scattering model shows that the transport properties are mainly limited by the grain size and electron mean free path parameters.

Nanoindentation of TiO_2 thin films with different microstructures

Gaillard, Y; Rico, VJ; Jimenez-Pique, E; Gonzalez-Elipe, AR
Journal of Physics D-Applied Physics, **42** (2009) 145305

A series of nanoindentation tests has been carried out with TiO_2 films produced by physical vapour deposition (PVD) under different conditions. Films with different microstructures and crystallographic structures have been prepared by changing experimental parameters such as the temperature of the substrate, the deposition angle (by the so-called glancing angle physical vapour deposition, GAPVD) or by exposing the growing film to a beam of accelerated ions. The obtained results of hardness and Young's modulus depict interesting correlations with the microstructure and structure of the films providing a general picture for the relationships between these characteristics and their mechanical properties. Different models have been used to extract Young's modulus and hardness parameters from the experimental nanoindentation curves. The obtained results are critically discussed to ascertain the ranges of validity of each procedure according to the type of sample investigated.

Electrical characteristics of mixed Zr-Si oxide thin films prepared by ion beam induced chemical vapor deposition at room temperature

Ferrer, FJ; Frutos, F; Garcia-Lopez, J; Jimenez, C; Yubero, F
Thin Solid Films, **517** (2009) 5446-5452

Mixed Zr-Si oxide thin films have been prepared at room temperature by ion beam decomposition of organometallic volatile precursors. The films were flat and amorphous. They did not present phase segregation of the pure single oxides. A significant amount of impurities (-C-, -CH_x, -OH, and other radicals coming from partially decomposed precursors) remained incorporated in the films after the deposition process. This effect is minimized if the At content in the O-2/Ar bombarding gas is maximized. Static permittivity and breakdown electrical field of the films were determined by capacitance-voltage and current-voltage electrical measurements. It is found that the static permittivity increases non-linearly from -4 for pure SiO_2 to similar to 15 for pure ZrO_2 . Most of the dielectric failures in the films were due to extrinsic breakdown failures. The maximum breakdown electrical field decreases from similar

to 10.5 MV/cm for pure SiO₂ to similar to 45 MV/cm for pure ZrO₂. These characteristics are justified by high impurity content of the thin films. In addition, the analysis of the conduction mechanisms in the formed dielectrics is consistent to Schottky and Poole-Frenkel emission for low and high electric fields applied, respectively. (C) 2009 Elsevier B.V. All rights reserved.

Influence of the microstructure on the mechanical and tribological behavior of TiC/a-C nanocomposite coatings

Martinez-Martinez, D; Lopez-Cartes, C; Fernandez, A; Sanchez-Lopez, JC
Thin Solid Films, **517** (2009) 1662-1671

The performance of protective thin films is clearly influenced by their microstructure. The objective of this work is to study the influence of the structure of TiC/a-C nanocomposite coatings with a-C contents ranging from similar to 0% to 100% on their mechanical and tribological properties measured by ultramicroindentation and pin-on-disks tests at ambient air, respectively. The microstructure evolves from a polycrystalline columnar structure consisting of TiC crystals to an amorphous and dense TiC/a-C nanocomposite structure when the amount of a-C is increased. The former samples show high hardness, moderate friction and high wear rates, while the latter ones show a decrease in hardness but an improvement in tribological performance. No apparent direct correlation is found between hardness and wear rate, which is controlled by the friction coefficient. These results are compared to the literature and explained according to the different film microstructures and chemical bonding nature. The film stress has also been measured at the macro and micro levels by the curvature and Williamson-Hall methods respectively. Other mechanical properties of the coating such as resilience and toughness were evaluated by estimating the H^3/E^{*2} and H/E^* ratios and the percentage of elastic work (W_e). None of these parameters showed a tendency that could explain the observed tribological results, indicating that for self-lubricant nanocomposite systems this correlation is not so simple and that the assembly of different factors must be taken into account. (C) 2008 Elsevier B.V. All rights reserved.

High deposition rates of uniform films in tetramethylsilane-based plasmas generated by elementary microwave sources in matrix configuration

Latrasse, L; Lacoste, A; Sanchez-Lopez, JC; Bes, A; Rayar, M; Pelletier, J
Surface & Coatings Technology, **203** (2009) 2343-2349

Plasma scaling up can be achieved by distributing elementary microwave plasma sources on planar rectangular networks. These so-called matrix plasmas can generate uniform sheets of plasma over a wide argon pressure range, from 7.5 to 750 Pa, with densities between 10^{12} and 10^{13} cm⁻³ in order to estimate the capabilities of matrix plasmas for PACVD processing in terms of deposition rate and uniformity, SiOCH and SiNCH films were deposited using TMS (tetramethylsilane), as the organic gas precursor of silicon, mixed with oxygen or nitrogen flows. Plasmas of O₂ / TMS and N₂ / TMS gas mixtures can be sustained between 5 and 25 Pa. Variations in the deposition rate as a function of microwave power and nitrogen partial pressure are reported. Thickness uniformity of SiOCH and SiNCH films was measured across a silicon wafer. The obtained deposition rates exceed 1.3 μm/min and the films present a uniformity better than 5% on 75 mm diameter silicon wafers. Composition of the films has also

been analyzed by XPS as a function of process parameters: microwave input power, composition of gas mixture, and N_2 partial pressure. In particular, these analyses have shown a very low yield of nitrogen incorporation when using N_2 gas as nitrogen precursor and high Si and Si-Si bonding contents in the films, probably due to a strong fragmentation of the TMS precursor in the high density plasma. (C) 2009 Elsevier B.V. All rights reserved.

Thermogravimetric and in situ SEM characterisation of the oxidation phenomena of protective nanocomposite nitride films deposited on steel

Mege-Revil, A; Steyer, P; Thollet, G; Chiriac, R; Sigala, C; Sanchez-Lopez, JC; Esnouf, C
Surface & Coatings Technology, **204** (2009) 893-901

The lifetime of TiN coatings is often limited by its poor resistance to high temperatures. For an optimized addition of silicon, both mechanical and physico-chemical properties are enhanced, owing to the formation of a nanocomposite structure. In this study, pure Ti and TiSi (80/20) targets were arc-evaporated to produce hard, single-layered coatings. Magnetron sputtered SiN_x films were also synthesized for a comparison purpose. The nanocomposite structure was determined by XRD and TEM, and its efficiency regarding the mechanical properties was confirmed by nanohardness measurements. Through thermogravimetric experiments it is shown that in isothermal and dynamic conditions, the chemical stability inherent to SiN_x controls the oxidation behaviour of TiSiN. However, in thermal cycling conditions TiSiN withstands efficiently temperature variations whereas SiN_x does not. The aim of this study is to understand the role of SiN_x on the oxidation of the TiSiN nanocomposite film. For this purpose, an in situ approach of the oxidation phenomena is detailed, based on experiments performed in an environmental scanning electron microscope (ESEM) operating in controlled pressure mode up to 1000 °C. ESEM, used in real-time oxidative conditions, has been proved to be an efficient tool to characterise the mechanism of degradation. The successive steps of the attack throughout the in situ oxidation process are as follows: oxidation first initiates at coating defects (open pores and droplets), then spreads to the whole surface. The whole flaking of the film that is observed at the microscopic scale during the cooling step proves the poor thermal fatigue resistance of SiN_x . This strong propensity to cracking is explained on the basis of thermo-mechanical considerations. The nanocomposite structure thus combines the chemical stability inherent to the SiN_x matrix with the beneficial thermo-mechanical properties associated to TiN nanograins. (C) 2009 Elsevier B.V. All rights reserved.

Metal carbide/amorphous C-based nanocomposite coatings for tribological applications

Sanchez-Lopez, JC; Martinez-Martinez, D; Abad, MD; Fernandez, A
Surface & Coatings Technology, **204** (2009) 947-954

This paper tries to assess the factors governing the tribological behaviour of different nanocomposite films composed by metallic carbides (MeC) mixed with amorphous carbon (a-C). Different series of MeC/a-C coatings (with Me: Ti(B) and W) were prepared by magnetron sputtering technique varying the power applied to the graphite target in order to tailor the carbon content into the films. A deep investigation of the chemical and structural features at the nano-scale is carried out by X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), electron energy-loss spectroscopy (EELS) and Raman spectroscopy techniques in order

to establish correlations with the tribological properties measured by a pin-on-disk tribometer in ambient air. The analysis of the counterfaces by Raman confocal microscopy after the friction tests is used to follow the chemical phenomena occurring at the contact area responsible of the observed friction behaviour. The importance of determining the fraction of C atoms in the amorphous phase (X_{a-c}) is highlighted as a key-parameter to control the tribological properties. A comparative analysis of the mechanical and tribological performance of the three systems (TiC/a-C, WC/a-C, TiBC/a-C) is done and conclusions are obtained concerning the friction and wear mechanism involved. (C) 2009 Elsevier B.V. All rights reserved.

Comparative investigation of TiAlC(N), TiCrAlC(N), and CrAlC(N) coatings deposited by sputtering of MAX-phase $Ti_{2-x}Cr_xAlC$ targets

Shtansky, DV; Kiryukhantsev-Korneev, PV; Sheveyko, AN; Mavrin, BN; Rojas, C; Fernandez, A; Levashov, EA

Surface & Coatings Technology, **203** (2009) 3595-3609

A comparative investigation of the structure and properties of TiAlC(N), TiCrAlC(N), and CrAlC(N) coatings deposited by sputtering of MAX-phase $Ti_{2-x}Cr_xAlC$ targets (where $x = 0, 0.5, 1, 3$, and 2) in an Ar atmosphere or in a gaseous mixture of Ar + N_2 is presented. The coatings were characterized in terms of their structure, elemental and phase composition, hardness, elastic modulus, elastic recovery, thermal stability, friction coefficient, wear rate, corrosion, and high-temperature oxidation resistance. The structure of the coatings was studied by means of X-ray diffraction, scanning and transmission electron microscopy, X-ray photoelectron spectroscopy, glow discharge optical emission spectroscopy, electron energy loss spectroscopy, and Raman spectroscopy. To evaluate the thermal stability and oxidation resistance, the coatings were annealed either in vacuum or in air at temperatures 600-1200 °C. The results obtained show that the TiAlCN coatings possess high hardness of 32-35 GPa, low friction coefficient against WC-Co well below 0.25, high thermal stability up to 1200 °C, and superior performance in dry milling tests against high Cr steel. Meanwhile, the coatings with high Cr content demonstrated improved oxidation resistance up to 1000 °C and superior electrochemical behavior, but their mechanical and tribological properties were deteriorated. (C) 2009 Elsevier B.V. All rights reserved.

Tribological carbon-based coatings: An AFM and LFM study

Martinez-Martinez, D; Kolodziejczyk, L; Sanchez-Lopez, JC; Fernandez, A

Surface Science, **603** (2009) 973-979

In this work some carbon-based coatings were studied by atomic force microscopy (AFM) and lateral force microscopy (LFM) techniques in order to evaluate their microstructure and friction properties at the micro and nanoscale. With this aim, four samples were prepared by magnetron sputtering: an amorphous carbon film (a-C), two nanocomposites TiC/a-C with different phase ratio (similar to 1:1 and similar to 1:3) and a nanocrystalline TiC sample. Additionally, a highly oriented pyrolytic graphite (HOPG) and an amorphous hydrogenated carbon coating (a-C:H) were included to help in the evaluation of the influence of the roughness and the hydrogen presence respectively. The topography (roughness) of the samples was studied by AFM, whereas LFM was used to measure the friction properties at the

nanoscale by two different approaches. Firstly, an evaluation of possible friction contrast on the samples was done. This task was performed by subtraction of forward and reverse images and lately confirmed by the study of lateral force profiles in both directions and the histograms of the subtraction images. Secondly, an estimation of the average friction coefficient over the analysed surface of each sample was carried out. To take into account the tip evolution/damaging, mica was used as a reference before and after each sample (hereafter called sandwich method), and samples-to-mica friction ratios were calculated. The LFM was shown to be a useful tool to characterise a mixture of phases with different friction coefficients. In general, the friction ratios seemed to be dominated by the amorphous carbon phase, as it was impossible to distinguish among samples with different proportions of the amorphous phase (friction ratios between 1.5 and 1.75). Nevertheless, it could be concluded that the differences in friction behaviour arose from the chemical aspects (nature of the phase and hydrogen content) rather than surface characteristics, since the roughness (R_a values up to 5.7 nm) does not follow the observed trend. Finally, the Ogletree method was employed in order to calibrate the lateral force and estimate the friction coefficient of our samples. A good agreement was found with macroscopic and literature values going from similar to 0.3 for TiC to similar to 0.1 for pure carbon. (C) 2009 Elsevier B.V. All rights reserved.

Vibrational spectroscopy characterization of magnetron sputtered silicon oxide and silicon oxynitride films

Godinho, V; Denisov, VN; Mavrin, BN; Novikova, NN; Vinogradov, EA; Yakovlev, VA; Fernandez-Ramos, C; de Haro, MCJ; Fernandez, A
Applied Surface Science, **256** (2009) 156-164

Vibrational (infrared and Raman) spectroscopy has been used to characterize SiO_xN_y and SiO_x films prepared by magnetron sputtering on steel and silicon substrates. Interference bands in the infrared reflectivity measurements provided the film thickness and the dielectric function of the films. Vibrational modes bands were obtained both from infrared and Raman spectra providing useful information on the bonding structure and the microstructure (formation of nano-voids in some coatings) for these amorphous (or nanocrystalline) coatings. X-ray photoelectron spectroscopy (XPS) and scanning electron microscopy (SEM) analysis have also been carried out to determine the composition and texture of the films, and to correlate these data with the vibrational spectroscopy studies. The angular dependence of the reflectivity spectra provides the dispersion of vibrational and interference polaritons modes, what allows to separate these two types of bands especially in the frequency regions where overlaps/resonances occurred. Finally the attenuated total reflection Fourier transform infrared measurements have been also carried out demonstrating the feasibility and high sensitivity of the technique. Comparison of the spectra of the SiO_xN_y films prepared in various conditions demonstrates how films can be prepared from pure silicon oxide to silicon oxynitride with reduced oxygen content. (C) 2009 Elsevier B.V. All rights reserved.

Structural characteristics and morphology of Sm_xCe_{1-x}O_{2-x/2} thin films

Hartmanova, M; Jergel, M; Mansilla, C; Holgado, JP; Zemek, J; Jurek, K; Kundracik, F
Applied Surface Science, **255** (2009) 9085-9091

Effect of the deposition temperature (200 and 500 degrees C) and composition of $\text{Sm}_x\text{Ce}_{1-x}\text{O}_{2-x/2}$ ($x = 0, 10.9-15.9$ mol%) thin films prepared by electron beam physical vapor deposition (EB-PVD) and Ar^+ ion beam assisted deposition (IBAD) combined with EB-PVD on structural characteristics and morphology/microstructure was investigated. The X-ray photoelectron spectroscopy (XPS) of the surface and electron probe microanalysis (EPMA) of the bulk of the film revealed the dominant occurrence of Ce^{4+} oxidation state, suggesting the presence of CeO_2 phase, which was confirmed by X-ray diffraction (XRD). The Ce^{3+} oxidation states corresponding to Ce_2O_3 phase were in minority. The XRD and scanning electron microscopy (SEM) showed the polycrystalline columnar structure and a rooftop morphology of the surface. Effects of the preparation conditions (temperature, composition, IBAD) on the lattice parameter, grain size, perfection of the columnar growth and its impact on the surface morphology are analyzed and discussed. (C) 2009 Elsevier B.V. All rights reserved.

Growth Mechanism and Chemical Structure of Amorphous Hydrogenated Silicon Carbide (a-SiC:H) Films Formed by Remote Hydrogen Microwave Plasma CVD From a Triethylsilane Precursor: Part 1

Wrobel, AM; Walkiewicz-Pietrzykowska, A; Ahola, M; Vayrynen, IJ; Ferrer-Fernandez, FJ; Gonzalez-Elipe, AR

Chemical Vapor Deposition, **15** (2009) 39-46

Amorphous hydrogenated silicon carbide (a-SiC:H) films are produced by remote microwave hydrogen plasma (RHP)CVD using triethylsilane (TrES) as the single-source precursor. The reactivity of particular bonds of the precursor in the activation step is examined using tetraethylsilane as a model compound for the RHP-CVD experiments. The susceptibility of a TrES precursor towards film formation is characterized by determining the yield of RHP-CVD and comparing it with that of the trimethylsilane precursor. The effect of substrate temperature (T-s) on the rate of the RHP-CVD process, chemical composition, and chemical structure of the resulting a-SiC:H films is reported. The substrate temperature dependence of the film growth rate implies that film growth is independent of the temperature and RHP-CVD is a mass transport-limited process. The examination of the a-SiC:H films, performed by means of X-ray photoelectron spectroscopy (XPS), elastic recoil detection analysis (ERDA), and Fourier transform infrared absorption spectroscopy (FTIR), reveals that the increase in the substrate temperature from 30 degrees C to 400 degrees C causes the elimination of organic moieties from the film and the formation of a Si-carbidic network structure. On the basis of the results of the structural study, the chemistry involved in film formation is proposed.

Molecular dynamics simulation of the effect of pH on the adsorption of rhodamine laser dyes on TiO_2 hydroxylated surfaces

Hamad, S; Sanchez-Valencia, JR; Barranco, A; Mejias, JA; Gonzalez-Elipe, AR

Molecular Simulation, **35** (2009) 1140-1151

We have carried out a study of adsorption, on the (101) surface of anatase TiO_2 , of two industrially relevant rhodamine molecules [rhodamine 6G (R6G) and rhodamine 800 (R800)] employing molecular dynamics. These theoretical studies have shown that R6G must adsorb on surfaces under basic conditions. Moreover, the adsorption of this molecule shows a

strong dependence upon the pH of the system, i.e. under basic conditions the adsorption energy is quite high, under neutral conditions the adsorption energy is lower and under acidic conditions an even lower adsorption energy indicates that there must be very little adsorption under such conditions. By contrast, for R800, there is little dependence of the adsorption energy upon the pH, suggesting that the amount of adsorption of these molecules is little affected by this parameter. These theoretical results are in qualitative agreement with the experimental results consisting of the incorporation of these dye molecules into porous thin films.

Phase separation of carboxylic acids on graphite surface at submonolayer regime

Alba, MD; Bickerstaffe, AK; Castro, MA; Clarke, SM; Medina, S; Millan, C; Orta, MM; Pavon, E; Perdigon, AC

European Physical Journal-Special Topics, **167** (2009) 151-156

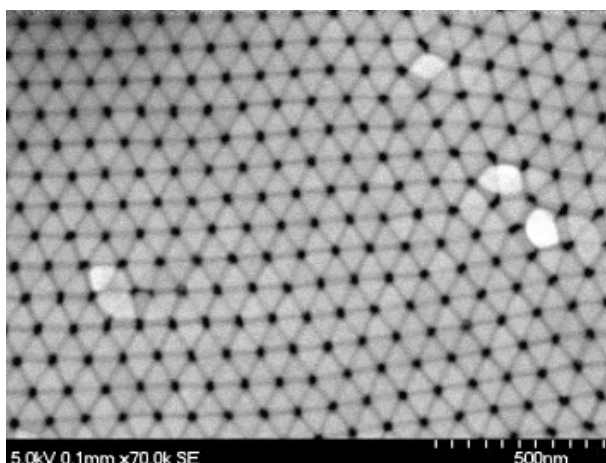
Mixing behaviour of solid crystalline monolayers adsorbed onto graphite from different mixtures of undecanoic and dodecanoic acids at submonolayer coverage has been investigated. X-ray diffraction measurements have been collected from a variety of compositions as a function of temperature. An extensive phase separation is found for all the compositions - the scattering patterns characteristic of the pure material crystalline structures being preserved across the entire composition range. The temperature dependence of the monolayer melting points and their depression is also clearly indicative of separation of the two surface components, in clear contrast to that expected if the two carboxylic acids mixed ideally in the monolayer.

NANOPÁRTICULAS Y NANOCOMPOSITOS PARA APLICACIONES TECNOLÓGICAS NANOPARTICLES AND NANOCOMPOSITOS FOR TECHNOLOGICAL APPLICATIONS

Fabrication of ordered crystalline zirconium nanoporous membranes by an one-step procedure

Marquez, F; Morant, C; Pirota, KR; Borrás, A; Sanz, JM; Elizalde, E
Nano Today, 4 (2009) 21-26

Crystalline porous zirconium membranes were obtained by physical vapor deposition on AAO templates at room temperature. These membranes were found to have similar hexagonal nanohole arrays as the template and high crystallinity. The pore size of the synthesized metallic membranes could be controlled during the synthesis through appropriate parameters in the experimental procedure. (C) 2008 Elsevier Ltd. All rights reserved.



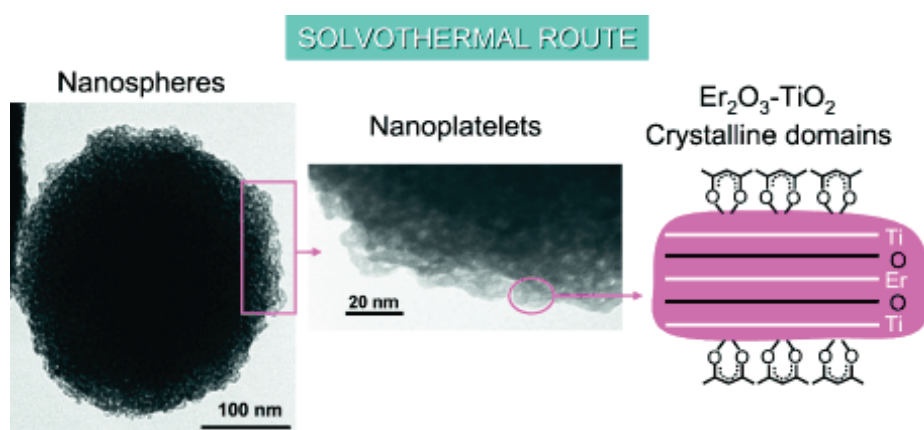
HRSEM image of a zirconium membrane, detached from the AAO template, with a mean nanohole size of 40 nm.

Self-Assembling of Er₂O₃-TiO₂ Mixed Oxide Nanoplatelets by a Template-Free Solvothermal Route

Julian-Lopez, B; Martos, M; Ulldemolins, N; Odriozola, JA; Cordoncillo, E; Escribano, P
Chemistry-A European Journal, 15 (2009) 12426-12434

An easy solvothermal route has been developed to synthesize the first mesoporous Er₂O₃-TiO₂ mixed oxide spherical particles composed of crystalline nanoplatelets, with high surface area and narrow pore size distribution. This synthetic strategy allows the preparation of materials at low temperature with interesting textural properties Without the use of surfactants, as well as the control of particle size and shape. TEM and Raman analysis confirm the formation of nanocrystalline Er₂O₃-TiO₂ mixed oxide. Mesoscopic ordered porosity is reached through the thermal decomposition of organic moieties during the synthetic process, thus leading to a template-free methodology that can be extended to other nanostructured

materials. High specific surface areas (up to $313 \text{ m}^2\text{g}^{-1}$) and narrow pore size distributions are achieved in comparison to the micrometric material synthesized by the traditional sol-gel route. This study opens new perspectives in the development, by solvothermal methodologies, of multifunctional materials for advanced applications by improving the classical pyrochlore properties (magnetization, heat capacity, catalysis, conductivity, etc.). In particular, since catalytic reactions take place on the surface of catalysts, the high surface area of these materials makes them promising candidates for catalysts. Furthermore, their spherical morphology makes them appropriate for advanced technologies in, for instance, ceramic inkjet printers.



Control over morphology and tailored pore structure without templates has been achieved for Er₂O₃-TiO₂ materials through an easy solvothermal route (see picture). The mixed oxide is composed of crystalline nanoplatelets organized into mesoporous spherical particles. The high specific surface area of these materials makes them promising candidates for catalysts

Control over the Structural and Optical Features of Nanoparticle-Based One-Dimensional Photonic Crystals

Calvo, ME; Sanchez-Sobrado, O; Colodrero, S; Miguez, H
Langmuir, **25** (2009) 2443-2448

Herein we present a detailed analysis of the effect of the spin-coating protocol over the optical properties of nanoparticle-based one-dimensional photonic crystals. Based on these results, we provide a reliable synthetic route to attain high-quality porous multilayers in which the effect of imperfections is minimized and whose Bragg diffraction can be precisely tuned over the entire visible and near-infrared spectrum. We present a systematic study of the effect of the acceleration ramp and final rotation speed over the structural and optical quality of these materials. This allows us to relate the structural variations observed with the different relative importance of fluid flow and solvent evaporation on the thinning of each layer in the stack for the different deposition conditions employed.

Light generation at the anomalous dispersion high energy range of a nonlinear opal film

Botey, M; Maymo, M; Molinos-Gomez, A; Dorado, L; Depine, RA; Lozano, G; Mihi, A; Miguez, H; Martorell, J

Optics Express, **17** (2009) 12210-12216

We study experimentally and theoretically light propagation and generation at the high energy range of a close-packed fcc photonic crystal of polystyrene spheres coated with a nonlinear material. We observe an enhancement of the second harmonic generation of light that may be explained on the basis of amplification effects arising from propagation at anomalous group velocities. Theoretical calculations are performed to support this assumption. The vector KKR method we use allows us to determine, from the linear response of the crystal, the behavior of the group velocity in our finite photonic structures when losses introduced by absorption or scattering by defects are taken into account assuming a nonzero imaginary part for the dielectric constant. In such structures, we predict large variations of the group velocity for wavelengths on the order or smaller than the lattice constant of the structure, where an anomalous group velocity behavior is associated with the flat bands of the photonic band structure. We find that a direct relation may be established between the group velocity reduction and the enhancement of a light generation processes such as the second harmonic generation we consider. However, frequencies for which the enhancement is found, in the finite photonic crystals we use, do not necessarily coincide with the frequencies of flat high energy bands. (C) 2009 Optical Society of America

Linear and third-order nonlinear optical responses of multilayered Ag:Si₃N₄ nanocomposites

Toudert, J; Fernandez, H; Babonneau, D; Camelio, S; Girardeau, T; Solis, J

Nanotechnology, **20** (2009) 475705

The linear and third-order nonlinear responses of tailored Si₃N₄/Ag/Si₃N₄ trilayers and (Si₃N₄/Ag)(n)/Si₃N₄ multilayers grown by alternating ion-beam sputtering have been studied by combining complementary characterization techniques such as transmission electron microscopy, spectroscopic ellipsometry and degenerate four-wave mixing. The linear optical response dominated by the surface plasmon resonance of Ag nanoparticles has been measured over the whole visible range while the third-order nonlinear susceptibility has been probed at the surface plasmon resonance wavelength. Due to the weak in-plane interaction between Ag nanoparticles, the linear and nonlinear optical responses of the Si₃N₄/Ag/Si₃N₄ trilayers are mainly influenced by the size and shape of the nanoparticles. A maximum value of 1.1×10^{-7} esu has been found at 635 nm for the effective third-order nonlinear susceptibility of the trilayer with the highest amount of silver. The linear optical response of the (Si₃N₄/Ag)(n)/Si₃N₄ multilayers is shown to be dominated by the surface plasmon resonance of isolated layers of weakly interacting nanoparticles at wavelengths shorter than 600 nm whereas a contribution due to vertical interactions has been shown for higher wavelengths. Below the vertical percolation threshold, their nonlinear optical response at the surface plasmon resonance wavelength is similar to the one of an isolated assembly of nanoparticles, and the effective third-order nonlinear susceptibility is slightly increased by decreasing the thickness of the Si₃N₄ spacer.

Diffusion-driven superplasticity in ceramics: Modeling and comparison with available data

Gomez-Garcia, D; Zapata-Solvas, E; Dominguez-Rodriguez, A; Kubin, LP
Physical Review B, **80** (2009) 214107-214107-9

The discovery of superplasticity in ceramics polycrystals led to debates about whether or not earlier models developed for metallic polycrystals can apply to these systems. In particular, all existing models require some mobility of lattice or grain-boundary dislocations whereas such activity is not observed in most ceramic systems. A model is presented that accounts for the occurrence of superplasticity in the absence of dislocation motion. It is based on a mechanism of grain-boundary sliding by pure-shear motion under stationary conditions, which is accommodated by lattice or grain-boundary diffusion. The prediction of this model regarding the temperature dependences of the stress exponent and of the effective activation energy are found in agreement with experimental results and literature data on five ceramic systems where dislocation activity could not be recorded: beta-SiAlON polycrystals, Al-doped SiC polycrystals, nanocrystalline MgO, yttria-tetragonal zirconia polycrystals, and alumina ceramics polycrystals.

Bonding Structure and Mechanical Properties of Ti-B-C Coatings

Abad, MD; Caceres, D; Pogozhev, YS; Shtansky, DV; Sanchez-Lopez, JC
Plasma Processes and Polymers, **6** (2009) S107–S112

Nanocomposite coatings combining hard phases (TiB₂, TiC) with an amorphous carbon (a-C) were developed to provide a good compromise between mechanical and tribological properties for M2 steels used in a wide variety of applications such as cutting tools, bearings and gear mechanisms. A combined d.c.-pulsed and r.f.-magnetron deposition process was used to deposit nanocomposite TiBC/a-C coatings with a variable content of carbon matrix phase. Chemical composition was determined by electron energy loss spectroscopy (EELS) and X-ray photoelectron spectroscopy (XPS). Transmission electron microscopy (TEM) revealed that the coatings microstructure is rather amorphous with small nanocrystals of TiC and/or TiB₂ (not possible to differentiate by diffraction techniques). Investigation of the chemical bonding environment by XPS and EELS allows us to confirm the presence of titanium-boron and titanium-carbon bonds together with free a-C. Coatings exhibited hardness values (H) of 25-29 GPa, effective Young modulus (E*) of 310-350 GPa, H/E* ratios over 0.080 and resistance to plastic deformation (H³/E*²) from 0.15 to 0.20. Tribological properties of the coatings were characterized by a pin-on-disk tribometer using steel and WC balls at high contact stresses (1.1 and 1.4 GPa respectively). Friction coefficients were reduced from 0.6 to 0.2 by increasing the content of free carbon without reduction of the hardness (around 28 GPa), by self-lubricant effects. The tribo-mechanical data are revised according to the phase composition and chemical bonding inside the nanocomposites.

Thermal Stability and Oxidation Resistance of Nanocomposite TiC/a-C Protective Coatings

Martinez-Martinez, D; Lopez-Cartes, C; Gago, R; Fernandez, A; Sanchez-Lopez, JC
Plasma Processes and Polymers, **6** (2009) S462 - S467

Nanocomposite films composed by small crystallites of hard phases embedded in an amorphous lubricant matrix have been extensively studied as protective coatings. These kinds of coatings have often to work in extreme environments, exposed to high temperatures (above 800-900 °C), and/or oxidizing/corrosive atmospheres, which may resist. As a result, it is important to study the behavior of such coatings at high temperatures (thermal stability) and in the presence of oxygen (oxidation resistance). In this sense, we have selected a TiC/a-C nanocomposite coating with good mechanical and tribological properties in order to do several thermal tests under three different environments: high vacuum (10^{-6} mbar), low vacuum (10^{-1} mbar), and air. Our observations allow us to establish that the film microstructure is stable at least up to 1000 °C in high vacuum. When oxygen is present, the practical temperature of use is reduced at 700 °C (low partial pressure) and 300 °C (air) by formation of Ti oxides and C removal.

M-Doped Al₂TiO₅ (M=Cr, Mn, Co) Solid Solutions and their Use as Ceramic Pigments

Dondi, M; Lyubenova, TS; Carda, JB; Ocana, M

Journal of The American Ceramic Society, **92** (2009) 1972-1980

New ceramic pigments based on the tialite (Al₂TiO₅) structure, doped with Co (pink), Cr (green), or Mn (brown), were prepared through the pyrolysis of aerosols followed by calcination of the obtained powders at 1400 degrees C. The expected decomposition of Al₂TiO₅ into a mixture of Al₂O₃ and TiO₂ on refiring was inhibited by Cr-doping and also by co-doping with Mg the Mn- or Co-doped samples. Microstructure and phase evolution during pigment preparation were monitored by scanning electron microscopy and XRPD. Unit cell parameters of tialite were determined by Rietveld refinement of the X-ray diffraction patterns, revealing in all cases the formation of solid solutions where the solubility of dopants in the Al₂TiO₅ lattice followed the trend Co < Mn < Cr. The valence state and possible location of dopants in the tialite lattice were investigated by X-ray photoelectron spectra and diffuse reflectance spectroscopies, which suggested the presence of Cr³⁺ ions in a large interstitial site of the tialite lattice with a distorted octahedral geometry, and of Mn³⁺ and Co²⁺ ions in the Al³⁺ octahedral sites of the tialite lattice in the former case, and in both Al³⁺ and Ti⁴⁺ octahedral sites in the latter. Testing the ceramic glazes assessed the technological behavior of pigments, which found that the color stability was reasonably good for the Mn-doped tialite and the Cr-doped pigment, although the latter suffered a small loss of green hue. The Co-doped pigment was found to be not stable in glazes, undergoing a cobalt-leaching effect.

Synthesis by pyrolysis of aerosols and ceramic application of Cr-doped CaYAlO₄ red-orange pigments

Lyubenova, TS; Carda, JB; Ocana, M

Journal of The European Ceramic Society, **29** (2009) 2193-2198

The synthesis of red-orange Cr-doped YCaAlO₄ Pigments has been improved (softer thermal conditions and lower environmental impact) and optimised by using the pyrolysis of aerosols method. We also study the crystallochemical features of the Cr chromophore with special emphasis on its oxidation state which has not been yet clarified, finding that Cr(III) and Cr(IV) species are present in the octahedral and interstitial tetrahedral sites of the YCaAlO₄ lattice, respectively. Finally, the applicability of this system as ceramic pigment was tested

using conventional industrial glazes. A change from orange to pink shades was detected after glaze firing, which is mainly attributed to the Cr³⁺ to Cr⁴⁺ oxidation.

Self-lubricating Ti-C-N nanocomposite coatings prepared by double magnetron sputtering

Martinez-Martinez, D; Lopez-Cartes, C; Justo, A; Fernandez, A; Sanchez-Lopez, JC
Solid State Sciences, **11** (2009) 660-670

This paper is devoted to the development of Ti(C,N)-based nanocomposite protective coatings consisting of nanocrystals of a hard phase (TiN or TiC_xN_y) embedded in an amorphous carbon-based matrix (a-C or a-CN_x). The objective here is the achievement of a good compromise between the mechanical and tribological properties by the appropriate control of the hard/soft phase ratio and the microstructural characteristics of the film. To achieve this purpose, dual magnetron sputtering technique was employed following two different strategies. In the first one, we use Ti and graphite targets and Ar/N₂ gas mixtures, while in the second case, TiN and graphite targets are sputtered in an Ar atmosphere. By changing the sputtering power applied to each magnetron, different sets of samples are prepared for each route. The effect of the bias voltage applied to the substrate is also studied in some selected cases. The mechanical and tribological properties of the films are characterized and correlated with the microstructure, crystallinity and phase composition. The establishment of correlations enables the development of advanced coatings with tailored mechanical and tribological properties for desired applications. (C) 2008 Elsevier Masson SAS. All rights reserved.

Percolation of the organic phase in hybrid organic-inorganic aerogels

Morales-Florez, V; Toledo-Fernandez, JA; de la Rosa-Fox, N; Pinero, M; Esquivias, L
Journal of Sol-Gel Science and Technology, **50** (2009) 170-175

The properties (texture, mechanical behaviour, etc.) of hybrid organic-inorganic silica aerogels change dramatically when the concentration of the organic additive is varied from a given value. It has been known for several years that this critical concentration is around 40% of the total weight of silica present in the sample. We have made use of a new structural model to conclude that this concentration of 40% by weight corresponds to the percolation threshold of the organic phase.

Experimental and computational studies of ZnS nanostructures

Hamad, S; Woodley, SM; Catlow, CRA
Molecular Simulation, **35** (2009) 1015-1032

We review the experimental and computational studies of nanoparticulate ZnS, a system that has received much attention recently. We describe in detail how the nanoparticle structures evolve with increasing size. The results of the computational studies reveal intriguing families of structures based on spheroids, which have the greater stability for clusters with less than 50 ZnS pairs. More complex structures are predicted for larger systems, such as double bubbles, BCT nanoparticles and nanotubes.

DIAGNÓSTICO Y EVALUACIÓN DE MATERIALES RELACIONADOS CON EL PATRIMONIO HISTÓRICO Y CULTURAL **DIAGNOSIS AND EVALUATION OF MATERIALS IN RELATION WITH HISTORICAL AND CULTURAL HERITAGE**

Study of the gilding technique used in polychromed stones and ceramics by dedicated laboratory-made micro X-ray diffraction and complementary techniques

Duran, A; Perez-Rodriguez, JL; de Haro, MCJ

Analytical and Bioanalytical Chemistry, **394** (2009) 1671-1677

This work describes the use of a new dedicated laboratory-made micro X-ray diffraction system for detecting the phases present in cross-sections of artworks. As an example, the phases present in samples from gilding ceramics and stone sculptures from the heritage of Seville (Spain) were successfully detected using this new system, which takes advantage of various devices developed for synchrotron radiation, and is complemented by the information provided by other techniques.

Characterization of illuminated manuscripts by laboratory-made portable XRD and micro-XRD systems

Duran, A; Perez-Rodriguez, JL; Espejo, T; Franquelo, ML; Castaing, J; Walter, P

Analytical and Bioanalytical Chemistry, **395** (2009) 1997-2004

Illuminated Arabic manuscripts have been studied, employing two laboratory-made X-ray diffraction (XRD) systems developed recently in the C2RMF laboratory. The validity of the μ -XRD and XRD portable systems for the study of this type of artworks has been demonstrated. A common observation in all the analyses is the presence of calcite and rutile; also, hematite, goethite, cinnabar, brass, anatase and barite were detected in the various colours. Differences between the results obtained by both techniques due to acquisition mode are discussed. In addition, other techniques such as X-ray fluorescence (XRF) and micro-Raman were used for the complete characterization of the manuscripts.

Study of metallic components of historical organ pipes using synchrotron radiation X-ray microfluorescence imaging and grazing incidence X-ray diffraction

Herrera, LK; Justo, A; Munoz-Paez, A; Sans, JA; Martinez-Criado, G

Analytical and Bioanalytical Chemistry, **395** (2009) 1969-1975

A comparative study of the composition and microstructure of two different brass alloys from reed pipes, one from a Spanish baroque organ and the other from a modern one, was carried out. This study allowed us to determine the procedure followed to produce the brass used to make ancient reed pipes. Moreover the distribution and correlation of lead and other trace elements present into the main component of the brass, the copper and zinc phases, of the historical tongues and shallots were established. This chemical composition was compared with that of a tongue from a twentieth-century organ. The whole study was accomplished using a combination of laboratory and synchrotron radiation techniques. X-ray

fluorescence was the technique used to obtain elemental and chemical imaging of the main phases and the trace elements at a sub-micrometer scale.

Advanced combined application of μ -X-ray diffraction/ μ -X-ray fluorescence with conventional techniques for the identification of pictorial materials from Baroque Andalusia paintings

Herrera, LK; Montalbani, S; Chiavari, G; Cotte, M; Sole, VA; Bueno, J; Duran, A; Justo, A; Perez-Rodriguez, JL

Talanta, **80** (2009) 71-83

The process of investigating paintings includes the identification of materials to solve technical and historical art questions, to aid in the deduction of the original appearance, and in the establishment of the chemical and physical conditions for adequate restoration and conservation. In particular, we have focused on the identification of several samples taken from six famous canvases painted by Pedro Atanasio Bocanegra, who created a very special collection depicting the life of San Ignacio, which is located in the church of San Justo y Pastor of Granada, Spain. The characterization of the inorganic and organic compounds of the textiles, preparation layers, and pictorial layers have been carried out using an XRD diffractometer, SEM observations, EDX spectrometry, FT-IR spectrometry (both in reflection and transmission mode), pyrolysis/gas chromatography/mass spectrometry and synchrotron-based μ -X-ray techniques. In this work, the advantages over conventional X-ray diffraction of using combined synchrotron-based μ -X-ray diffraction and μ -X-ray fluorescence in the identification of multi-layer paintings is demonstrated. (C) 2009 Elsevier B.V. All rights reserved.

Comparison between micro-Raman and micro-FTIR spectroscopy techniques for the characterization of pigments from Southern Spain Cultural Heritage

Franquelo, ML; Duran, A; Herrera, LK; de Haro, MCJ; Perez-Rodriguez, JL

Journal of Molecular Structure, **924-26** (2009) 404-412

An extensive overview of the complementary use of micro-FTIR and micro-Raman spectroscopy in the Cultural Heritage studies is described in this work. The samples have been prepared using the cross-section technique. This technique allows the examination of a large portion of a single paint layer in its original condition. A variety of pigments from samples belonging principally to the Cultural Heritage of Southern Spain were characterized by micro-Raman spectroscopy using visible excitation sources and micro-FTIR spectroscopy. The pigments studied comprise blue (azurite, ultramarine blue, Prussian blue), red (vermilion, haematite, red ochre, red lead, etc.), ochre and yellow (goethite, orpiment, realgar, etc.), green (malachite, copper resinate), and white (calcite, gypsum, white lead, titanium white, barite, lithopone) pigments, among others. An orientation is given for their appropriate and unequivocal characterization. Characterization by micro-FTIR and micro-Raman presents difficulties with some pigments. In these cases, analysis by EDX solves most of these doubts. The combined use of both spectroscopic techniques, together with SEM-EDX microanalysis, provides one of the most useful methods in the characterization (and possible dating) of materials used in Cultural Heritage. (C) 2009 Published by Elsevier B.V.

Hg/Sn amalgam degradation of ancient glass mirrors

Herrera, LK; Duran, A; Franquelo, ML; Justo, A; Perez-Rodriguez, JL
Journal of Non-Crystalline Solids, **355** (2009) 1980-1983

Tin amalgam, which is obtained by pouring mercury onto a sheet of tin, has been used in the production of reflective coatings for mirrors. The corrosion processes of the amalgam layer were investigated in several mirrors from historical buildings located in southern Spain using SEM/EDS, XPS, and GID. Mercury and Sn⁴⁺ are present as spheres on the amalgam surface due to the evaporation process (similar to 5 nm). The profile shows a mixture of Sn²⁺ and Sn⁴⁺. The original amalgam was composed of a binary alloy of tin and mercury (Hg_{0.1}Sn_{0.9}) and metallic tin. In this paper the tin oxidation mechanism of the amalgam is described. Liquid mercury is volatile and evaporates slowly, leaving fine tin particles that oxidize easily, forming tin monoxide (SnO) and tin dioxide (SnO₂). The mercury-rich phase accelerates the corrosion of the tin-rich phase. (C) 2009 Elsevier B.V. All rights reserved.

Surface analysis and materials characterization for the study of biodeterioration and weathering effects on cultural property

Herrera, LK; Videla, HA
International Biodeterioration & Biodegradation, **63** (2009) 813-822

Several methods for material characterization and surface analysis such as scanning electron microscopy (SEM), energy dispersion X-ray analysis (EDX), environmental scanning electron microscopy (ESEM), petrographic analyses, Mossbauer spectroscopy (MS), conventional X-ray diffraction (XRD), grazing incidence diffraction (GID), Roman spectroscopy (RS), other spectroscopic techniques like X-ray photoelectron spectroscopy (XPS), reflection electron energy-loss spectroscopy (REELS) and advanced combined applications of synchrotron based mu-X-ray diffraction/mu-X-ray fluorescence (SR-mu XRD/mu XRF) can be used for assessing weathering and biodeterioration effects on materials (such as stone buildings, metallic artefacts, pigments, mixtures, and processes) of cultural property. Molecular biology techniques to identify the microbial components of biofilms are also described. Different examples of the use of these methods in the field of cultural property preservation are presented. (C) 2009 Elsevier Ltd. All rights reserved.

Study by grazing incident diffraction and surface spectroscopy of amalgams from ancient mirrors

Herrera, LK; Duran, A; Franquelo, ML; Gonzalez-Elipse, AR; Espinos, JP; Rubio-Zuazo, J; Castro, GR; Justo, A; Perez-Rodriguez, JL
Central European Journal of Chemistry, **7** (2009) 47-53

Characterization of four amalgam surfaces, with different alteration degrees from Andalusia historical mirrors, has been carried out by grazing-incidence X-ray diffraction (GIXRD), and other spectroscopic techniques (SEM/EDX, XPS, and REELS). The combination of all these techniques allows determining the corrosion state of the amalgams. The results show that the amalgams are composed in all cases of a binary alloy of tin and mercury. As mercury has high vapour pressure at RT, it slowly segregates and eventually evaporates, it leaves finely

divided particles of tin that easily can be oxidize, forming tin monoxide (SnO) and tin dioxide (SnO₂). In one of the samples, most of the amalgam remains unoxidized, since Hg_{0.1}Sn_{0.9} and metallic Sn phases are the major components; in two other samples, Hg_{0.1}Sn_{0.9} and Sn phases are not detected while SnO₂ and SnO phases appear. Finally, in the last studied sample, only SnO₂ phase is detected. The surface analyses of these samples by XPS show that, for most of them an unique chemical species (Sn⁴⁺) is found.

Study of degradation processes of metals used in some artworks from the cultural heritage of Andalusia, Spain

Duran, A; Herrera, LK; de Haro, MCJ; Perez-Rodriguez, JL; Justo, A
Revista de Metalurgia, **45** (2009) 277-286

The study of the alteration processes of metals, Such as lead, bronze, iron and tin-mercury alloys, used in some of the most important chosen artefacts of Andalusian Cultural Heritage is the main objective of this paper. Hydrocerussite and cerussite were detected in lead seals stored in a hole of cardboard. Bronze is altered to atacamite by environmental contamination, which is also responsible for the formation of rust from iron. Corrosion of the tin-mercury surface of amalgam mirrors produces tin monoxide and tin dioxide and releases liquid mercury from the solid phase.

Modern methods for materials characterization and surface analysis to study the effects of biodeterioration and weathering on buildings of cultural heritage

Herrera, LK; Le Borgne, S; Videla, HA
International Journal of Architectural Heritage, **3** (2009) 74-91

Several methods for material characterization and surface analysis - such as scanning electron microscopy (SEM), environmental scanning electron microscopy (ESEM), atomic force microscopy (AFM), confocal laser microscopy (CLM), energy dispersion X-ray (EDX) analysis, X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), petrographic analyses, Mossbauer spectroscopy (MS), and synchrotron X-ray diffraction (SR-XRD)-can be used for assessing weathering and biodeterioration effects on stone monuments and buildings of the cultural heritage. Novel DNA-based molecular biology techniques to identify the microbial components of damaging biofilms are also described. This article presents the pros and cons of these methods illustrated in some cases with studies made on the Ibero American cultural heritage.

MICROESTRUCTURA Y PROPIEDADES FÍSICAS DE MATERIALES MICROSTRUCTURE AND MAGNETIC PROPERTIES OF MATERIALS

Optical Analysis of the Fine Crystalline Structure of Artificial Opal Films

Lozano, G; Dorado, LA; Schinca, D; Depine, RA; Miguez, H

Langmuir, **25** (2009) 12860-12864

Herein, we present a detailed analysis of the Structure of artificial opal films. We demonstrate that, rather than the generally assumed face centered cubic lattice of spheres, opal films are better approximated by rhombohedral assemblies of distorted colloids. Detailed analysis of the optical response in a very wide spectral range ($0.4 \leq a/\lambda \leq 2$, where a is the conventional lattice constant), as well as at perpendicular and off-normal directions, unambiguously shows that the interparticle distance coincides very approximately with the expected diameter only along directions contained in the same close-packed plane but differs significantly in directions oblique to the $[1\ 1\ 1]$ one. A full description of the real and reciprocal lattices of actual opal films is provided, as well as of the photonic band structure of the proposed arrangement. The implications of this distortion in the optical response or the lattice are discussed.

A new generation of bio-derived ceramic materials for medical applications

Gonzalez, P; Borrajo, JP; Serra, J; Chiussi, S; Leon, B; Martinez-Fernandez, J; Varela-Feria, FM; de Arellano-Lopez, AR; de Carlos, A; Munoz, FM; Lopez, M; Singh, M

Journal of Biomedical Materials Research Part A, **88A** (2009) 807-813

A new generation of bio-derived ceramics can be developed as a base material for medical implants. Specific plant species are used as templates on which innovative transformation processes can modify the chemical composition maintaining the original biostructure. Building on the outstanding mechanical properties of the starting lignocellulosic templates, it is possible to develop lightweight and high-strength scaffolds for bone substitution. In vitro and in vivo experiments demonstrate the excellent biocompatibility of this new silicon carbide material (bioSiC) and how it gets colonized by the hosting bone tissue because of its unique interconnected hierarchic porosity, which opens the door to new biomedical applications.

Correlation between microstructure and temperature dependence of magnetic properties in $\text{Fe}_{60}\text{Co}_{18}(\text{Nb}, \text{Zr})(6)\text{B}_{15}\text{Cu}_1$ alloy series

Blazquez, JS; Franco, V; Conde, CF; Conde, A; Ferenc, J; Kulik, T; Kiss, LF

Journal of Applied Physics, **105** (2009) 093928-093935

Temperature dependence of magnetic properties of nanocrystalline $\text{Fe}_{60}\text{Co}_{18}\text{Cu}_1\text{B}_{15}\text{Nb}_{6-x}\text{Zr}_x$ ($x=0, 3, 6$) alloys has been studied at different stages of devitrification. Transmission electron microscopy shows nanocrystals of the size similar to 5 nm, which remains almost constant along the nanocrystallization process. Curie temperature of the residual amorphous

phase decreases as nanocrystallization progresses for all the studied alloys. Thermal dependence of the exchange stiffness constant is obtained from the measurement of specific magnetization and coercivity as a function of crystalline fraction and temperature for the three studied alloys. (C) 2009 American Institute of Physics.

Influence of the demagnetizing field on the determination of the magnetocaloric effect from magnetization curves

Caballero-Flores, R; Franco, V; Conde, A; Kiss, LF

Journal of Applied Physics, **105** (2009) 07A919-07A919-3

The influence of the demagnetizing factor (N) on the magnetic entropy change ($\Delta S-M$) curves is studied for materials with a second order phase transition. For this purpose, a soft magnetic amorphous ribbon is measured for different orientations of the magnetic field with respect to the plane of the sample. For temperatures below the Curie temperature ($T-C$), the increase in N causes a decrease in $\Delta S-M$, while for temperatures above $T-C$ no change in the shape of the curves has been found for the different orientations, as expected. In order to eliminate this influence of N and compare the $\Delta S-M(T)$ curves for samples with different shapes, the recently proposed universal curve for the magnetocaloric effect can be used. (C) 2009 American Institute of Physics.

The magnetocaloric effect in materials with a second order phase transition: Are T-C and T-peak necessarily coincident?

Franco, V; Conde, A; Kuz'min, MD; Romero-Enrique, JM

Journal of Applied Physics, **105** (2009) 07A917-07A917-3

Using the Arrott-Noakes equation of state it is shown that the Curie point ($T-C$) and the temperature where the magnetic entropy change is maximum (T -peak) coincide only in the mean field approximation, but the Heisenberg model implies that T -peak $>$ $T-C$ even for homogeneous materials. The distance between T -peak and $T-C$ increases with applied magnetic field following a power law. In both cases, $T-C$ corresponds to a singular point in the temperature dependence of the magnetic entropy change. The field dependence of the magnetic entropy change is exactly the same at the Curie temperature and at the temperature of the peak. (C) 2009 American Institute of Physics.

Field dependence of the adiabatic temperature change in second order phase transition materials: Application to Gd

Franco, V; Conde, A; Romero-Enrique, JM; Spichkin, YI; Zverev, VI; Tishin, AM

Journal of Applied Physics, **106** (2009) 103911-103911-4

The field dependence of the adiabatic temperature change ΔT -ad of second order phase transition materials is studied, both theoretically and experimentally. Using scaling laws, it is demonstrated that, at the Curie temperature, the field dependence of ΔT -ad is characterized by H^{-1}/Δ . Therefore, as the magnetic entropy change $\Delta S-M$ follows a $H^{(1-\alpha)}/\Delta$ power law, these two dependencies coincide only in the case of a mean field

model. A phenomenological construction of a universal curve for ΔT_{ad} is presented, and its theoretical justification is also given. This universal curve can be used to predict the response of materials in different conditions not available in the laboratory (extrapolations in field or temperature), for enhancing the resolution of the data and as a simple screening procedure for the characterization of materials. (C) 2009 American Institute of Physics.

Magnetocaloric response of Fe₇₅Nb₁₀B₁₅ powders partially amorphized by ball milling

Ipus, JJ; Blazquez, JS; Franco, V; Conde, A; Kiss, LF
Journal of Applied Physics, **105** (2009) 123922-123922-6

The magnetocaloric response of mechanically alloyed Fe₇₅Nb₁₀B₁₅ powders was studied for samples with different amorphous and nanocrystal volume fractions. Thermomagnetic properties scale following a Ω^3 law for different milling processes, where Ω is the milling frequency. Curie temperature of the amorphous phase increases as the amorphous fraction increases due to its progressive enrichment in B. The peak magnetic entropy change, $\Delta S_M(p_k)$, as well as the refrigerant capacity increase with increasing amorphous fraction. The field dependence of $\Delta S_M(p_k)$ can be explained by the multiphase character of the studied samples. (c) 2009 American Institute of Physics.

Properties of Ti(C,N) cermets synthesized by mechanically induced self-sustaining reaction

Cordoba, JM; Sanchez-Lopez, JC; Aviles, MA; Alcalá, MD; Gotor, FJ
Journal of The European Ceramic Society, **29** (2009) 1173-1182

The properties of TiC_xN_{1-x}/(Ni or Co) cermets sintered by a pressureless method from powder mixtures, and obtained for the first time by a mechanically induced self-sustaining reaction process (MSR), were studied. The hardness, toughness, friction and wear coefficients, and oxidation resistance were determined. It was shown that cermets obtained from powdered materials synthesized in one single MSR step possessed improved mechanical properties, similar to those obtained in cermets with more complex bulk compositions. Higher wear resistances were observed in cermets whose hard phase was richer in carbon. The oxidation resistance of the cermets depended primarily on the binder composition. This resistance was better for those cermets with cobalt as the binder. Superior oxidation resistance was displayed when small amounts of W or Mo were incorporated into the binder. (C) 2008 Elsevier Ltd. All rights reserved.

The hydrothermal conversion of kaolinite to kalsilite: Influence of time, temperature, and pH

Becerro, AI; Escudero, A; Mantovani, M
American Mineralogist, **94** (2009) 1672-1678

Kalsilite (the low-temperature form of KAlSiO_4) is used as the precursor of leucite, an important component in porcelain-fused-to-metal and ceramic-restoration systems, and it has also been proposed as a high-thermal expansion ceramic for bonding to metals. The present study reports the hydrothermal synthesis and characterization of pure kalsilite from kaolinite in subcritical conditions, as well as the characterization of the intermediate products by means of XRD, Si-29 and Al-27 MAS NMR, IR, SEM, and TEM. Effects of time, temperature, and pH on the reaction products are analyzed. The experimental data indicate that pure kalsilite is obtained after hydrothermal treatment of kaolinite at 300 degrees C for 12 h in 0.5 M KOH solution. Longer reaction times increase the crystallinity of the structure, whereas lower reaction times give rise to the metastable ABW-type KAlSiO_4 polymorph. Lower temperatures are not sufficient to produce kalsilite, but zeolite W is obtained instead as the unique reaction product. Finally, the pH of the aqueous solution in contact with kaolinite is an important parameter for the synthesis of kalsilite, which must be ≥ 13.70 .

Mineralogical stability of phyllosilicates in hyperalkaline fluids: Influence of layer nature, octahedral occupation and presence of tetrahedral Al

Becerro, AI; Mantovani, M; Escudero, A
American Mineralogist, **94** (2009) 1187-1197

Mineralogical changes in a set of phyllosilicates, differing in their layer nature, chemical composition, octahedral character, and Al content of the tetrahedral sheet, were analyzed after hydrothermal reaction in an alkaline solution. The composition of the alkaline solution was selected to simulate the First stage of cement degradation [NaOH-KOH-Ca(OH)_2]. The reaction products have been analyzed by XRD, Si-21 and Al-21 MAS NMR spectroscopy, SEM/EDX, and TEM. The results indicate that the main factor influencing the stability of the clays is the occupation of the octahedral sheet such that all trioctahedral members withstand the alkaline attack, whereas most of the dioctahedral clays suffer a complete dissolution and crystallization of new phases. Second, clays with Al in the tetrahedral sheet of their layers are shown to be less stable than those with a pure Si tetrahedral sheet.

Memory effect in triglycine sulfate induced by a transverse electric field: specific heat measurement

Gallardo, MC; Martin-Olalla, JM; Romero, FJ; del Cerro, J; Fugiel, B
Journal of Physics-Condensed Matter, **21** (2009) 025902

The influence of a transverse electric field on the specific heat of triglycine sulfate (TGS) has been studied. The specific heat of TGS has been measured on heating the sample from the ferroelectric to the paraelectric phase after prolonged application of transverse electric field (i.e. perpendicular to the ferroelectric axis). It is shown that the specific heat of TGS can 'remember' the temperature T_s at which the transverse field was previously applied.

Dielectric, calorimetric and elastic anomalies associated with the first order I4/mcm <-> Pbcm phase transition in (Ca, Sr)TiO₃ perovskites

Manchado, J; Romero, FJ; Gallardo, MC; del Cerro, J; Darling, TW; Taylor, PA; Buckley, A; Carpenter, MA

Journal of Physics-Condensed Matter, **21** (2009) 295903

Conduction calorimetry has been used to determine with high precision the latent heat and variation in heat capacity which accompany the first order I4/mcm <-> Pbcm phase transition in perovskites with compositions (Ca_{1-x}Sr_x)TiO₃, x = 0.65, 0.68, 0.74 (CST65, CST68, CST74). In CST65 (CST68), the latent heat is dissipated/absorbed over a temperature interval of similar to 11 K (similar to 6 K), which is centred on similar to 292 K (similar to 258 K) during cooling and similar to 302 K (similar to 270 K) during heating. The magnitude of the latent heat diminishes with increasing SrTiO₃ content and was not detected in CST74. Integration of the latent heat and excess heat capacity yields small excess entropies, which are consistent with the structural changes being displacive rather than order-disorder in origin. Resonant ultrasound spectroscopy measurements on the same CST65 sample as used for dielectric and calorimetric measurements through the same temperature intervals have allowed quantitative correlations to be made with the bulk modulus, shear modulus and acoustic dissipation parameter, Q(-1). The dielectric anomaly and changes in Q(-1) can be understood as being linear combinations of the properties of the separate I4/mcm and Pbcm phases in proportion to their volume fractions across the two-phase field. A change of only similar to 0.5-1 GPa has been detected in the bulk modulus but the shear modulus softens by similar to 5-8 GPa as the transition interval is approached from above and below. This shear mode softening presumably reflects clustering and/or phonon softening in both the I4/mcm and Pbcm structures. This pattern of structure-property relations could be typical of first order transitions in perovskites where there is no group/subgroup relationship between the high and low symmetry phases.

First order phase transition in deuterated triglycine selenate under an electric field: experimental study and analysis in the frame of Landau theory

Romero, FJ; Gallardo, MC; del Cerro, J

Journal of Physics-Condensed Matter, **21** (2009) 155902

The influence of electric fields lower than the critical field in the ferroelectric phase transition in deuterated triglycine selenate has been studied by means of thermal and dielectric properties. The latent heat, specific heat and dielectric constant have been measured and compared to the theoretical expectations from the Landau theory under an electric field. A full agreement has been found on cooling experiments.

Stability of phyllosilicates in Ca(OH)₂ solution: Influence of layer nature, octahedral occupation, presence of tetrahedral Al and degree of crystallinity

Mantovani, M; Escudero, A; Alba, MD; Becerro, AI

Applied Geochemistry, **24** (2009) 1251-1260

This paper presents the results of a comprehensive investigation of the interaction of layered silicates with $\text{Ca}(\text{OH})_2$ in hydrothermal conditions. The study is intended to evaluate the stability of the clay buffer in radioactive waste repositories, at the intermediate stages of concrete leaching, when the pH is controlled by the dissolution of portlandite. The influence of layer nature, octahedral occupation, presence of tetrahedral Al and degree of crystallinity will be assessed by analysing the behaviour of a set of well-selected phyllosilicates and using the combined capabilities of Si-29 and Al-27 MAS-NMR spectroscopy, powder X-ray diffraction and SEM/EDX. The results show that the main factor affecting the stability of the clay is the octahedral occupation, so that trioctahedral phyllosilicates are much more stable than dioctahedral ones. The nature and expandability of the layer does not seem to much influence the stability of the clay, so that a 2:1 expandable phyllosilicate shows the same stability as a chemically analogous 1:1 non-expandable phyllosilicate. However other factors like the poor crystallinity of the starting material or the presence of Al in the tetrahedral sheet of trioctahedral phyllosilicates weaken the clay structure in alkaline conditions and favour the transformation towards other phases. (C) 2009 Elsevier Ltd. All rights reserved.

Supersaturated solid solution obtained by mechanical alloying of 75% Fe, 20% Ge and 5% Nb mixture at different milling intensities

Blazquez, JS; Ipus, JJ; Millan, M; Franco, V; Conde, A; Oleszak, D; Kulik, T
Journal of Alloys and Compounds, **469** (2009) 169-178

Mechanical alloying process of $\text{Fe}_{75}\text{Ge}_{20}\text{Nb}_5$ composition has been Studied at different milling frequencies from initial pure powder mixture to the development of a single bcc phase (supersaturated solid solution). As an intermediate state, an intermetallic phase is formed, which disappears after further milling or after thermal treatment (ascribed to an endothermic process at 700-800 K). A preferential partition of Nb and Ge to the boundaries between nanocrystals of bcc Fe-Ge-Nb supersaturated solid solution is observed from X-ray diffraction (XRD) and Mossbauer results. (C) 2008 Elsevier B.V. All rights reserved.

Specific heat measurements on amorphous and nanocrystalline $\text{Al}_{88}\text{Y}_5\text{Ni}_5\text{Co}_2$

Blazquez, JS; Millan, M; Conde, CE; Conde, A; Latuch, J; Kulik, T
Journal of Alloys and Compounds, **478** (2009) 19-21

Specific heat at constant pressure, C-P, was measured on amorphous and nanocrystalline $\text{Al}_{88}\text{Y}_5\text{Ni}_5\text{Co}_2$ alloys from differential scanning calorimetry experiments. Linear behavior of C-P versus temperature from 323 to 423 K is explained by conduction electrons contribution and dilatation correction factor. Results indicate that the Fermi energy increases as nanocrystallization progresses, although the estimated values are clearly lower than those found for crystalline Al. (C) 2008 Elsevier B.V. All rights reserved.

Synthesis of complex carbonitride powders $\text{TiyMT}_{1-y}\text{CxN}_{1-x}$ (M-T: Zr, V, Ta, Hf) via a mechanically induced self-sustaining reaction

Cordoba, JM; Aviles, MA; Sayagues, MJ; Alcalá, MD; Gotor, FJ
Journal of Alloys and Compounds, **482** (2009) 349-355

The machinability of materials is a dynamic field with enormous implications in different industrial sectors because manufacturers are constantly looking for improvements that can increase the overall productivity. Manufacturers of cutting tool inserts need to develop products that can perform at higher speeds and last longer under increasingly rigorous operating conditions. It has been revealed that cermets may exhibit better properties and performances when solid solution of multiple hard compounds is added instead of a mixture of several binary ones. In this work, a mechanically induced self-sustaining reaction (MSR) is described as a suitable synthesis method to obtain a wide range of different new quaternary carbonitride systems by milling mixtures of elemental powders of transition metals and graphite in a nitrogen atmosphere. Characterization was carried out using X-ray powder diffraction, elemental analysis, energy dispersive X-ray analysis (EDX), scanning and transmission electron microscopy and electron diffraction (ED). (C) 2009 Elsevier B.V. All rights reserved.

Preferential Co partitioning to alpha-Fe in nanocrystalline CoFeNbB alloys by Mn addition

Millan, M; Blazquez, JS; Conde, CF; Conde, A; Lozano-Perez, S; Ochin, P
Journal of Non-Crystalline Solids, **355** (2009) 109-113

Influence of Mn addition on the microstructure and hyperfine parameters of amorphous and nanocrystalline Co₆₀(FeMn)₍₁₈₎Nb₆B₁₆ alloys has been studied. Although Mn addition does not yield significant differences in crystallization kinetics and in the phases formed after each transformation, it seriously affects the partitioning of Co during nanocrystallization. Whereas for Mn free alloy Co is homogeneously distributed throughout the amorphous matrix and the nanocrystals, in Mn containing alloy Co is enriched in the alpha-FeCo nanocrystals. This fact prevents the exhaustion in Fe of the amorphous matrix and the crystalline volume fraction achieved at the end of nanocrystallization in the case of Mn containing alloy is similar to 20% higher than in the Mn free alloy. (c) 2008 Elsevier B.V. All rights reserved.

The influence of a minority magnetic phase on the field dependence of the magnetocaloric effect

Franco, V; Caballero-Flores, R; Conde, A; Dong, QY; Zhang, HW
Journal of Magnetism And Magnetic Materials, **321** (2009) 1115-1120

The field dependence of the magnetic entropy change can be used to detect the existence of a minority magnetic phase without experimentally reaching its Curie temperature. In this work, we present results that could suggest a breakdown of the recently proposed universal behaviour of the magnetocaloric effect in materials with a second-order magnetic phase transition in some La-containing samples. The behaviour of the outlier La-containing materials is an evidence of the existence of minority phases, preventing the construction of the universal curve with a single reference temperature. However, the use of two reference temperatures avoids this difficulty and allows applying the universal curve for practical

purposes even with the presence of the minority phase. (C) 2008 Elsevier B.V. All rights reserved.

FePd melt-spun ribbons and nanowires: Fabrication and magneto-structural properties

Prida, VM; Vega, V; Franco, V; Llamazares, JLS; Perez, MJ; Santos, JD; Escoda, L; Sunol, JJ; Hernando, B

Journal of Magnetism and Magnetic Materials, **321** (2009) 790-792

Fe-30% Pd alloys in ribbon and nanowire geometry have been prepared. Ribbon samples were produced by the melt-spinning technique in the Ar environment. FePd nanowires, having about 35 nm in diameter, 105 nm inter-nanowires distance and around 4 μm in length, were synthesized into nanoporous anodic alumina membranes as templates. Energy dispersive X-ray microanalysis of ribbons shows an average atomic composition of Fe (73.2%) and Pd (26.8%). The X-ray diffraction at RT analysis was performed on both surfaces, free and wheel side, of the melt-spun ribbon. It shows the coexistence of two phases: fct and bct FePd, but with differences between both surfaces consisting the existence of Fe oxides (Fe₂O₃ and Fe₃O₄) and a textured 200 reflection in the free side. Heating and cooling thermomagnetic curves exhibit a reversible behaviour from RT to 720 K, but around 770 K a clear irreversible transformation takes place. (C) 2008 Elsevier B.V. All rights reserved.

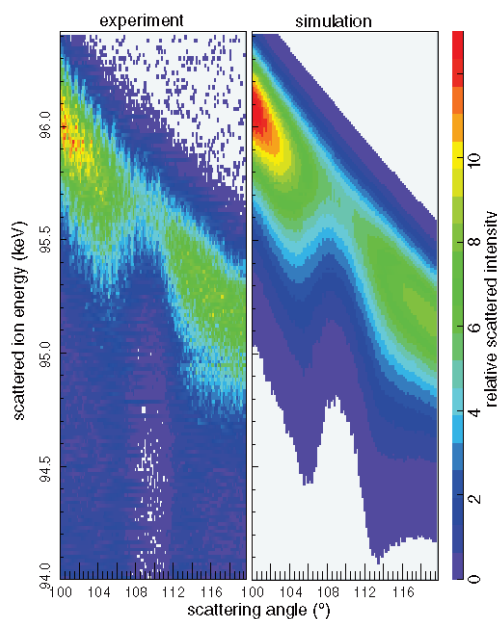
OTROS / OTHERS

Direct Observation and Theory of Trajectory-Dependent Electronic Energy Losses in Medium-Energy Ion Scattering

Hentz, A; Parkinson, GS; Quinn, PD; Munoz-Marquez, MA; Woodruff, DP; Grande, PL; Schiwietz, G; Bailey, P; Noakes, TCQ

Physical Review Letters, **102** (2009) 96103-96106

The energy spectrum associated with scattering of 100 keV H⁺ ions from the outermost few atomic layers of Cu(111) in different scattering geometries provides direct evidence of trajectory-dependent electronic energy loss. Theoretical simulations, combining standard Monte Carlo calculations of the elastic scattering trajectories with coupled-channel calculations to describe inner-shell ionization and excitation as a function of impact parameter, reproduce the effects well and provide a means for far more complete analysis of medium-energy ion scattering data.



Two-dimensional map of scattered-ion intensities as a function of scattering-angle and scattered-ion energy around the [011] blocking dip (at 109.5°) for $\bar{4}\bar{1}\bar{1}$ incidence of 100 keV H⁺ ions on Cu(111). The raw experimental data are compared with the theoretical simulation.

General Quantum-Mechanical Study on the Hydrolysis Equilibria for a Tetravalent Aquaion: The Extreme Case of the Po(IV) in Water

Ayala, R; Martinez, JM; Pappalardo, RR; Paez, AM; Marcos, ES

Journal of Physical Chemistry B, **113** (2009) 487-496

A systematic study of the different hydrolyzed species derived from the hydrated Po(IV) in water, $[\text{Po}(\text{H}_2\text{O})(n)(\text{OH})(m)]^{(4-m)}$ for $1 \leq m \leq 4$, and $4 \leq m + n \leq 9$, has been carried out by means of quantum mechanical computations. The effects of outer solvation shells have been included using a polarizable continuum dielectric model. For a fixed number of hydroxyl groups, the preferred hydration number for the Po(IV) can be determined in terms of Gibbs energy. It is shown that the hydration number (n) systematically decreases with the increase in the number of hydroxyl groups (m) in such a way the total coordination number ($n + m$) becomes smaller, being 9 in the aquocomplex and 4 in the neutral hydroxo-complex. Free energies for the hydrolysis processes involving Po(IV) complexes and a different number of hydroxyl groups have been computed, revealing the strong tendency toward hydrolysis exhibited by these complexes. The predominant species of Po(IV) in aqueous solutions are ruled by a dynamical equilibrium involving aggregates containing in the first coordination shell OH- groups and water molecules. Although there is not experimental information to check the theoretical predictions, theoretical computations in Solution seem to suggest that the most likely clusters are $[\text{Po}(\text{H}_2\text{O})(5)(\text{OH})(2)]^{(2+)}$ and $[\text{Po}(\text{H}_2\text{O})(4)(\text{OH})(2)]^{(2+)}$. The geometry of the different clusters is ruled by the trend of hydroxyl groups to be mutually orthogonal and to promote a strong perturbation of the water molecule in trans-position by lengthening the Po-H₂O distances and tilting the corresponding bond angle. A general thermodynamic cycle is defined to compute the Gibbs free energy associated to the formation of the different hydrolyzed forms in solution. From it, the estimates of pK(a) values associated to the different protolytic equilibria are provided and discussed. Comparison of the relative values of pK(a) along a hydrolysis series with the experimental values for other tetravalent cations supports its consistency.

Chemical Reactions in 2D: Self-Assembly and Self-Esterification of 9(10),16-Dihydroxypalmitic Acid on Mica Surface

Heredia-Guerrero, JA; San-Miguel, MA; Sansom, MSP; Heredia, A; Benitez, JJ
Langmuir, **25** (2009) 6869-6874

9(10),16-Dihydroxypalmitic acid (diHPA) is a particularly interesting polyhydroxylated fatty acid (1) because it is the main monomer of cutin, the most abundant biopolyester in nature, and (2) because the presence of a terminal and a secondary hydroxyl group in midchain positions provides an excellent model to study their intermolecular interactions in a confined phase such as self-assembled layers. In this study we have combined atomic force microscopy (AFM), X-ray photoelectron spectroscopy (XPS), attenuated total reflection Fourier transform infrared (ATR-FT-IR) spectroscopy, as well as molecular dynamics (MD) simulations to conclude that the self-assembling of diHPA molecules on mica is a layer by layer process following a Brunauer-Emmett-Teller (BET) type isotherm and with the first layer growing much faster than the rest. Interactions between secondary hydroxyls reinforce the cohesive energy of the monolayer, while the presence of the terminal hydroxyl group is necessary to trigger the multilayered growth. Besides, XPS and ATR-FT-IR spectroscopies clearly indicate that spontaneous self-esterification occurs upon self-assembling. The esterification reaction is a prerequisite to propose a self-assembly route for the biosynthesis of cutin in nature. Molecular dynamics simulations have shown that internal molecular reorganization within the self-

assembled layers provides the appropriate intermolecular orientation to facilitate the nucleophilic attack and the release of a water molecule required by the esterification reaction.

Identification of hydrogen and deuterium at the surface of water ice by reflection electron energy loss spectroscopy

Yubero, F; Tokesi, K

Applied Physics Letters, **95** (2009) 084101- 084101-3

A nondestructive method to distinguish between hydrogen (H) and deuterium (D) at surfaces by reflection electron energy loss spectroscopy is presented. It is based on the analysis of the energy distributions of electrons elastically backscattered from surfaces containing H or D. We consider standard and deuterated water ices as test surfaces. The recoil energy of the backscattered electrons depends on the atomic mass of the targets, and the contributions of H, D, and O to the measured spectra can be easily separated. The results of Monte Carlo simulations corroborate the experimental findings.

Preferential Adsorption from Binary Mixtures on Graphite: The n-Decane-n-Heptan-1-ol System

Alba, MD; Castro, MA; Clarke, S; Medina, S; Messe, L; Millan, C; Orta, MM; Perdigon, AC

Journal of Physical Chemistry C, **113** (2009) 3176-3180

The competitive adsorption of n-decane and n-heptan-1-ol adsorbed from the binary liquid mixture onto graphite has been studied using differential scanning calorimetry, incoherent quasielastic neutron scattering, and H-1 and H-2 nuclear magnetic resonance. A solid monolayer is identified at all bulk solution compositions with a melting temperature that varies with bulk composition in a manner resembling the bulk behavior. Incoherent elastic neutron scattering, IQNS, and nuclear magnetic resonance, NMR, data indicate that decane is preferentially adsorbed onto the surface over most of the composition range, heptanol being the principal surface component only at very high heptanol concentrations. NMR is proved, for the first time, to be an efficient tool to provide independent information on each component of the system.

Synthesis and characterization of a plant cutin mimetic polymer

Heredia-Guerrero, JA; Heredia, A; Garcia-Segura, R; Benitez, JJ

Polymer, **50** (2009) 5633-5637

A mimetic polymer of plant cutin have been synthesized from 9,10,16-trihydroxyhexadecanoic (aleuritic) acid through a low temperature polycondensation reaction. Reaction conditions (solvent, catalyst, temperature, etc...) were studied and modified to optimize yield and product characteristics. The resulting polyaleurate polymer was characterized by Attenuated Total Reflection-Fourier Transform Infrared Spectroscopy (ATR-FTIR), Differential Scanning Calorimetry (DSC), X-ray Diffraction (XRD) and solid state C-13-Cross Polarization/Magic Angle Spinning Nuclear Magnetic Resonance (C-13-CP/MAS NMR). Mechanical and hydrodynamic properties were also investigated. In the average, the product

obtained is physically and chemically very similar to plant cutin (a hydrophobic polyester). However, a more detailed analysis of results reveals that polyaleurate framework is more rigid than natural cutin and with additional larger short-range ordered domains. Also, the synthetic polymer displays slightly different mechanical properties with respect to natural cutin. Additional hydrogen bonding within the framework of polyaleurate is considered to be responsible for such experimental observations. (C) 2009 Elsevier Ltd. All rights reserved.

Reversibility of La and Lu sorption onto smectites: Implications for the design of engineered barriers in deep geological repositories

Galunin, E; Alba, MD; Aviles, MA; Santos, MJ; Vidal, M
Journal of Hazardous Materials, **172** (2009) 1198-1205

The sorption reversibility of La and Lu (considered as actinide analogues) onto a set of smectites (bentonite FEBEX; hectorite, HEC; MX80; saponite, SAP; Otay montmorillonite, SCA-3; and Texas montmorillonite, STx-1) was studied to estimate actinide retention by smectites that are candidates for use as engineered barriers in deep geological repositories. The sorption distribution coefficients (K-d) and the reversibility parameters (desorption distribution coefficients (K-d,K-des), adjusted distribution coefficients (K-d,K-adj), and desorption rates (R-des)) were determined from batch tests in two ionic media: deionized water and Ca 0.02 mol L⁻¹. The latter simulates possible conditions due to the presence of concrete leachates. The results varied greatly depending on the ionic medium, the lanthanide concentration and the clay structure. The high values of K-d,K-des obtained (up to 1.1×10^5 and 9.2×10^4 Lkg⁽⁻¹⁾ for La and Lu in water, and 2.8×10^4 and 4.1×10^4 Lkg⁽⁻¹⁾ for La and Lu in the Ca medium) indicate the suitability of the tested smectites for lanthanide (and therefore, actinide) retention. Based on all the data, SCA-3, HEC and FEBEX clays are considered the best choices for water environments, whereas in Ca environments the suitable clays depended on the lanthanide considered. (C) 2009 Elsevier B.V. All rights reserved.

Sonication induced redox reactions of the Ojen (Andalucia, Spain) vermiculite

Poyato, J; Perez-Rodriguez, JL; Ramirez-Valle, V; Lurf, A; Wagner, FE
Ultrasonics Sonochemistry, **16** (2009) 570-576

Sonication in a 1: 1 mixture (volume ratio) of water and concentrated H₂O₂ (30%) is a soft method for particle size reduction of phyllosilicate minerals like vermiculites. Repeated sonication causes a particle size reduction to about 70 nm for the Santa Olalla and to 45 nm for the Ojen-vermiculite. In this context the question arises whether the strong oxidising effect of the hydrogen peroxide affects the oxidation state of the iron in the vermiculites. Therefore, the Fe³⁺/Fe-total ratio before and after sonication was determined by means of Mossbauer spectroscopy. Whereas this ratio was found to remain almost constant in the Santa Olalla vermiculite, it increased from 0.79 to 0.85 in case of the Ojen sample. In the latter case, the oxidation is accompanied by a decrease of the layer charge. Surprisingly, sonication in pure water leads to a decrease of the Fe³⁺/Fe-total ratio in the case of the Ojen-vermiculite, i.e., to an increase of the Fe²⁺ fraction to roughly twice the value before sonication. Again the Fe³⁺/Fe-total ratio of the Santa Olalla vermiculite remains unchanged. The surface area S-BET of the reduced Ojen-vermiculite amounts to 50 m²/g, which is close to the value obtained in

the presence of hydrogen peroxide. The results presented should be taken as a warning that particle size reduction by sonication may be accompanied by a change of the redox state and the layer charge of the material. (c) 2009 Elsevier B.V. All rights reserved.

Synthesis of MCM-22 zeolites of different Si/Al ratio and their structural, morphological and textural characterisation

Delitala, C; Alba, MD; Becerro, AI; Delpiano, D; Meloni, D; Musu, E; Ferino, I
Microporous and Mesoporous Materials, **118** (2009) 1-10

MCM-22 zeolites with Si/Al in the 9-46 range were synthesised in rotating autoclave and characterised by X-ray diffraction, H-1, Si-29 and Al-27 magic angle spinning nuclear magnetic resonance, scanning electron microscopy and nitrogen physisorption. For the Si/Al = 21, 30 and 46 samples both X-ray diffraction and scanning electron microscopy revealed the crystallisation of pure MCM-22. Besides the latter, crystals of ferrierite also formed during the synthesis of the Si/Al = 9 sample. Based on the H-1 MAS NMR spectra of dehydrated samples, the different proton species present on the MCM-22 samples were determined and quantified. Information about the incorporation of Al ions into the zeolite framework, as well as on the preferential crystallographic sites occupied in dependence on the Si/Al ratio of the sample, was obtained by Al-27 MAS NMR spectroscopy. From Si-29 MAS NMR spectra, differences in the degree of crystallinity of the samples were assessed. The results being in agreement with the diffraction data. Nitrogen physisorption runs revealed the microporous nature of the adsorbents, with a supermicropore to ultra-micropore volume ratio in good agreement, for the best crystallised samples, with the porous structure with supercages and sinusoidal channels of the ideal MCM-22 crystal. (C) 2008 Elsevier Inc. All rights reserved.

Liquid-phase thiophene adsorption on MCM-22 zeolites. Acidity, adsorption behaviour and nature of the adsorbed products

Delitala, C; Cadoni, E; Delpiano, D; Meloni, D; Alba, MD; Becerro, AI; Ferino, I
Microporous and Mesoporous Materials, **118** (2009) 11-20

The liquid-phase adsorption of thiophene from thiophene/iso-octane solutions has been investigated in batch conditions at room temperature and atmospheric pressure on MCM-22 zeolites with Si/Al in the 9-46 range. Thiophene adsorption was found to occur in two steps whatever the Si/Al ratio of the adsorbent. The presence of ferrierite besides the MCM-22 phase caused a significant loss of the adsorption performance. For pure MCM-22 samples, the Si/Al ratio influenced the adsorption performance. Based on the acid properties of the samples, investigated by adsorption microcalorimetry of ammonia, the adsorption features were interpreted by assuming that positively charged species were originated during the first step: these species underwent successive reaction with weakly adsorbed species formed in the second step, leading to heavy molecular weight organosulphur compounds. Direct evidence for the occurrence of reactive adsorption of thiophene involving its transformation into heavy molecular weight organosulphur compounds was obtained by GC/MS investigation of the nature of the adsorbed material recovered after the adsorption experiments. The peculiar structure of MCM-22 zeolites made possible the formation of long-sized organosulphur compounds. Due to the mechanism by which thiophene is transformed (i.e. progressive

addition of other thiophene molecules), the size of the resulting products was found to depend also on the concentration of the weakly adsorbed thiophene molecules able to interact with those already activated through protonation. (C) 2008 Elsevier Inc. All rights reserved.

Cutin synthesis: A slippery paradigm

Heredia, A; Heredia-Guerrero, JA; Dominguez, E; Benitez, JJ
Biointerphases, **4** (2009) P1-P3

Combined kinetic analysis of thermal degradation of polymeric materials under any thermal pathway

Sanchez-Jimenez, PE; Perez-Maqueda, LA; Perejon, A; Criado, JM
Polymer Degradation and Stability, **94** (2009) 2079-2085

Combined kinetic analysis has been applied for the first time to the thermal degradation of polymeric materials. The combined kinetic analysis allows the determination of the kinetic parameters from the simultaneous analysis of a set of experimental curves recorded under any thermal schedule. The method does not make any assumptions about the kinetic model or activation energy and allows analysis even when the process does not follow one of the ideal kinetic models already proposed in the literature. In the present paper the kinetics of the thermal degradation of both polytetrafluoroethylene (PTFE) and polyethylene (PE) have been analysed. It has been concluded, without previous assumptions on the kinetic model, that the thermal degradation of PTFE obeys a first order kinetic law, while the thermal degradation of PE follows a diffusion-controlled kinetic model. (C) 2009 Elsevier Ltd. All rights reserved.

Synthesis, Rietveld Analysis, and Solid State Nuclear Magnetic Resonance of X-2-Sc₂SiO₅

Alba, MD; Chain, P; Gonzalez-Carrascosa, T
Journal of The American Ceramic Society, **92** (2009) 487-490

Compounds containing rare earths are of increasing technological interest especially because of their unique mechanical, magnetic, electrical, and optical properties. Among them, rare earth oxyorthosilicates are attractive scintillators for gamma- and X-ray spectroscopy and detection. However, there are many structural aspects of those compounds that are not clear. In this research, the structure parameters for Sc₂Si₂O₅, X-2-polymorph, have been refined from powder X-ray diffraction (XRD) data and the Si-29 MAS NMR spectrum is reported for the first time. X-2-Sc₂SiO₅ polymorph was synthesized by the sol-gel method and characterized by XRD and Si-29 MAS NMR. The XRD pattern was indexed in a monoclinic unit cell with space group I2/c; the resulting unit cell parameters were a=9.9674(2) angstrom, b=6.4264(9) angstrom, c=12.0636(2) angstrom, and beta=103.938(1)degrees. The Si-29 MAS NMR spectrum showed a unique signal at -79.5 ppm, compatible with the unique Si crystallographic site in the unit cell. Finally, the band valence method has been applied to the calculation of a "shift parameter," which is correlated with the NMR chemical shift.

Hydrothermal Synthesis of Kalsilite: A Simple and Economical Method

Becerro, AI; Mantovani, M; Escudero, A

Journal of The American Ceramic Society, **92** (2009) 2204-2206

This study reports a simple method to synthesize pure kalsilite (KAlSiO₄) using readily available precursors, kaolinite and KOH solution, after only 12 h of hydrothermal treatment in mild conditions. A structural refinement has been carried out using the Rietveld method to obtain unit cell parameters, and the Si-29 and Al-27 magic angle spinning nuclear magnetic resonance spectra have shown the purity and complete Si/Al ordering of the kalsilite structure obtained. Finally, the morphology of the particles has been analyzed by scanning electron microscopy.

A recurrent error which needs to be resolved

Ortega, A

Thermochimica Acta, **491** (2009) 116-117

The recent paper by Jankovic et al. [B. Jankovi, B. Adnadevic, J. Jovanovic; *Thermochimica Acta* 452 (2007) 106] and other similar papers have raised a problem which needs to be resolved. These authors use the method of Kennedy and Clark [J.A. Kennedy, S.M. Clark. *Thermochimica Acta* 307 (1997) 27] which is conceptually erroneous; this is analyzed in this paper. (C) 2009 Elsevier B.V. All rights reserved.

Kinetics of the thermal decomposition of anhydrous cobalt nitrate by SCRT method

Ortega, A; Macias, M; Gotor, FJ

Journal of Thermal Analysis And Calorimetry, **98** (2009) 441-448

It has been shown the ability of the Sample Controlled Reaction Temperature (SCRT) method for both discriminate the kinetic law and calculate the activation energy of the reaction. This thermal decomposition is best described by a Johnson-Mehl-Avrami kinetic model (with $n = 2$) with an activation energy of nuclei growth which fall in the range 52-59 kJ mol⁻¹. The process is not a single-step because the initial rate of decomposition is likely to be limited by nucleation. The results reported here constitute the first attempt to use the new SCRT method to study the kinetic of the thermal decomposition of cobalt nitrate.

Duplex SiCN/DLC coating as a solution to improve fretting-corrosion resistance of steel

Pech, D; Schupp, N; Steyer, P; Hack, T; Gachon, Y; Heau, C; Loir, AS; Sanchez-Lopez, JC

Wear, **266** (2009) 832-838

Fretting corrosion damages are commonly observed when two metallic bodies, which are in contact with each other, are subjected to oscillatory motions of low amplitude. Such kind of degradation mode is often responsible for limited durability of aeronautical joints. In the present paper, a multifunctional duplex coating based on Si-C-N and diamond-like carbon (DLC) materials, combining corrosion resistance and good tribological properties is described.

Amorphous hydrogenated SiC, SiCN, SiC/DLC and SiCN/DLC were deposited on steel substrates by a plasma assisted chemical vapour deposition (PACVD) technique, using tetramethylsilane (TMS), ammonia (NH₃) or acetylene (C₂H₂) as gas precursors. Nitrogen incorporation has shown to improve the corrosion protection ability of SiC coatings. The corrosion behaviour and the tribological performance in aqueous media of SiCN/DLC coating have therefore been investigated. A test rig has been designed to validate the fretting resistance of this duplex coating for aeronautic applications. It was found that the combination of a SiCN-based PACVD sublayer with a DLC topcoat could provide an enhanced solution to withstand both fretting and corrosion. (C) 2008 Elsevier B.V. All rights reserved.

Phyllites used as waterproofing layer materials for greenhouses crops in Spain: multivariate statistical analysis applied to their classification based on X-ray fluorescence analysis

Garzon, E; Garcia-Rodriguez, IG; Ruiz-Conde, A; Sanchez-Soto, PJ
X-Ray Spectrometry, **38** (2009) 429-438

The results are presented for the chemical characterization carried out with 53 raw material samples with phyllosilicates from outcrops located between the provinces of Almeria and Granada (SE Spain) in order to use them as waterproof layers under the floors of greenhouses. For this purpose, the samples have been studied by these techniques: X-Ray Diffraction (XRD), X-Ray Fluorescence (WDXRF), Scanning Electron Microscopy (SEM), chemical analysis by energy-dispersive X-Ray detection (EDX), and thermogravimetry. To isolate groups of phyllite samples with similar chemical profiles and correlations between the samples, the WDXRF data (11 chemical elements) have been processed using the methodology of exploratory multivariate statistical analyses: cluster analysis, main-component analysis, and discriminating canon analysis. This study was performed as a screening test and as a means of finding similarities and correlations among all 53 phyllite samples, allowing the isolation of groups of phyllite samples with similar chemical profiles. The results indicate that the 53 phyllite samples can be divided into two main groups. The first group is subdivided into two subgroups (1 and 2), one of which includes most of the samples. The latter is further classified into three blocks with the same chemical composition. This allows to search for the raw material with potentially the best waterproof characteristics within the five groups. The classification is of validity as a screening test for subsequent experimental determinations concerning the physical properties of these samples. Copyright (C) 2009 John Wiley & Sons, Ltd.

Microstructural evolution characterization of Fe-Nb-B ternary systems processed by ball milling

Ipus, JJ; Blazquez, JS; Lozano-Perez, S; Conde, A
Philosophical Magazine, **89** (2009) 1415-1423

Fe-Nb-B alloys prepared by ball milling can undergo a complex microstructural evolution during milling. In order to overcome the limitations imposed by traditional X-ray bulk analysis, a comprehensive multi-technique approach was devised to systematically characterize samples with the required resolution. A combination of in situ FIB (focused ion

beam) lift-out and high-resolution ATEM (analytical transmission electron microscopy) has allowed the characterization of the phase evolution during milling. In particular, boron inclusions, not detected by X-ray diffraction, have been found to remain undissolved in the Fe matrix.

Role of iron-reducing bacteria in corrosion and protection of carbon steel

Herrera, LK; Videla, HA

International Biodeterioration & Biodegradation, **63** (2009) 891-895

The role of iron-reducing bacteria (IRB) in biocorrosion is under discussion. According to some reports, IRB are able to induce protection of carbon steel while others suggest an important enhancement of corrosion through the reduction and removal of passive films of ferric compounds on the metal surface. In this work, we review recent knowledge concerning microbial respiration, the ecology of IRB containing biofilms and the corrosive or protective effect of such biofilms on metal surfaces. (C) 2009 Elsevier Ltd. All rights reserved.

Understanding microbial inhibition of corrosion. A comprehensive overview

Videla, HA; Herrera, LK

International Biodeterioration & Biodegradation, **63** (2009) 896-900

Microorganisms are able to drastically change the electrochemical conditions at the metal/solution interface by biofilm formation. These changes can range from the induction or acceleration of corrosion to corrosion inhibition. Any inhibitory action developed by bacteria may be accomplished within the varied and complex biofilm/corrosion products interactions occurring on a biofouled metal surface. Biocorrosion and its counter process, microbial inhibition of corrosion, are rarely linked to a single mechanism or to a single species of microorganisms. Microorganisms can induce corrosion inhibition according to two general mechanisms or their combination: i) neutralizing the action of corrosive substances present in the environment; ii) forming protective films or stabilizing pre-existing protective films on a metal. Different practical cases illustrating these mechanisms are presented in this overview. It must be stressed that some times the inhibitory action of bacteria can be reversed to a corrosive action in bacterial consortia located within biofilm thickness. (C) 2009 Elsevier Ltd. All rights reserved.

High surface area alpha-alumina preparation by using urban waste

Martin-Ruiz, MM; Perez-Maqueda, LA; Cordero, T; Balek, V; Subrt, J; Murafa, N; Pascual-Cosp, J
Ceramics International, **35** (2009) 2111-2117

A new method for preparing high surface area α -alumina from urban waste is proposed. The method consists of the precipitation of a precursor that contains bohemite mixed with a linear polymer and subsequently the thermal decomposition of the precursor by heating in nitrogen and air to 1200 degrees C. The resulting α -alumina consists of nanocrystals of about 100 nm aggregated into larger particles with relatively high surface area (12 m² g⁻¹) and a significant macropore volume of 0.545 cm³ g. Methods of X-ray diffraction (XRD),

scanning electron microscopy (SEM), high-resolution transmission electron microscopy (HRTEM) and selected area electron diffraction (SAED) were used to characterize microstructure of prepared materials. Results of differential thermal analysis, thermogravimetry and emanation thermal analysis characterized the thermal behaviour of alpha-alumina precursors. (C) 2008 Elsevier Ltd and Techna Group S.r.l. All rights reserved.

Application Of Si-29 And Al-27 MAS-NMR Spectroscopy To The Study Of The Reaction Mechanism Of Kaolinite To Illite/Muscovite

Mantovani, M; Escudero, A; Becerro, AI
Clays and Clay Minerals, **57** (2009) 302-310

Understanding the mechanisms for illitization of clay minerals has important applications in reconstructing geologic histories and determining the origins of physical and chemical characteristics of buried sediments. While many studies have been carried out on this topic, few have focused on the mechanism of illite formation from kaolinite. The purpose of this study was to investigate more deeply the illitization of kaolinite in KOH solution at a high solid/liquid ratio (1000 mg/mL). X-ray diffraction (XRD) and infrared spectroscopy were used to follow the formation of new crystalline phases and the composition of the octahedral sheet, while the transformation of the Si and Al local environments was analyzed by Si-29 and Al-27 magic angle spinning nuclear magnetic resonance spectroscopy (MAS NMR). The results revealed that the first reaction stage consists of the diffusion of Al from the octahedral to the tetrahedral sheet of the kaolinite TO layers, giving rise to the precursors of the illite/muscovite nuclei. Combination of XRD with Al-27 MAS NMR measurements indicated that a minimum amount of tetrahedral Al is required in the original TO layer before condensation of a second tetrahedral sheet occurs to complete the formation of the illite/muscovite TOT layers.

Determination of nitrogen partitioning coefficients in superduplex stainless steels by NRA using a nuclear microprobe

Munoz, C; Morilla, Y; Lopez, JG; Paul, A; Odriozola, JA
Nuclear Instruments & Methods In Physics Research Section B-Beam Interactions with Materials and Atoms, **267** (2009) 2208-2211

Superduplex stainless steels (SDSSs) combine the good mechanical behavior and the high corrosion resistance of the ferrite (alpha-Fe) and austenite (gamma-Fe) phases. The SDSSs properties depend strongly on the partitioning of the elements that form the alloy. The ferrite is generally enriched in P, Si, Cr and Mo while the content of Ni, Mn, Cu and N in the austenite phase is higher. Nitrogen is known to be a strong austenite stabilizer and its presence increases the strength and the pitting corrosion resistance of the stainless steels. While the global nitrogen content in SDSSs can be readily determined using elemental analyzers, it cannot be measured at a microscopic scale. In this work, the nuclear microprobe of the Centro Nacional de Aceleradores (Sevilla) was used to obtain the quantitative distribution of nitrogen in SDSSs. A deuteron beam of 1.8 MeV was employed to determine the overall elemental concentration of the matrix by deuteron-induced X-ray emission, whereas the nitrogen partitioning coefficients were obtained by using the N-14(d, alpha(0))C-12 nuclear reaction. Mappings of

this element show that the nitrogen ratio between the ferrite and austenite phases ranges from 0.3 to 0.6 in the analyzed samples. (C) 2009 Elsevier B.V. All rights reserved.

Application of Geographic Information Systems (GIS) in the search for and characterization of raw materials of interest in ceramics and glass

Garzon, E; Garcia, IG; Ruiz-Conde, A; Sanchez-Soto, PJ

Boletín de la Sociedad Española de Cerámica y Vidrio, **48** (2009) 39-44

This work shows the application of a geographic information system (GIS) as an effective tool to undertake several phases of research on raw materials of interest in ceramics and glass, with two examples: search for and characterization of raw materials to be used as impermeable materials in addition to their potential ceramic interest in terms of quarries and the quarrying of limestone and marble. For this, three phases of work have been differentiated: the construction of a cartographic database, the combining and distilling of the databases; and finally the development of the application. From this study, it was concluded that GIS becomes a living tool in which new data can be incorporated, such as sampling points, test results, determinations made with the samples, new approaches and directions, companies that have the concession, etc., as explained with the examples described. All of this enables more rational and efficient use of the materials from the technical, environmental, and economic standpoint. The working method proposed could be clearly useful for researchers, technicians, and businessmen of this sphere that are involved in evaluating raw materials to be applied in processing materials of this sector.

Effect of the grinding mechanical treatment on the pyrophyllite textural properties

Sanchez-Soto, PJ

Boletín de la Sociedad Española de Cerámica y Vidrio, **48** (2009) 59-68

It has been investigated the effect of mechanical treatment by dry grinding, using a ball mill, on the textural properties of pyrophyllite. The nitrogen gas adsorption-desorption isotherms, obtained at -195 degrees C in the original and ground samples, have not showed pronounced hysteresis. However, it has been found that the gas adsorbed volumes increase gradually at increasing grinding time, with a maximum at 30 min. After this, these values decrease up to a situation very similar to the original unground sample. The evolution of specific surface area (S-BET), determined using the BET equation, has showed a rapid increase as increasing grinding time from a value of $2 \text{ m}^2 \times \text{g}^{-1}$ (original) up to a maximum of $60 \text{ m}^2 \times \text{g}^{-1}$ at 30 min, being $7.5 \text{ m}^2 \times \text{g}^{-1}$ at 325 min. This behaviour is explained considering the decrease of particle size of the layered silicate as influenced by grinding, but until a limit. Above this limit, the particles start to re-aggregate and agglomerate by a mechanochemical process of cold-welding, which is originated by their high surface reactivity. Consequently, the values of S-BET decrease progressively, which coincides with the greater structural degree produced in this silicate and the subsequent amorphization process. Even so, the present textural study has showed the absence of micropores in these ground materials by physisorption of nitrogen gas, concluding that this process is produced by multilayers. The pore size distribution of ground pyrophyllite samples has proved a contribution of sizes ranging between 20-50 angstrom to the increase of S-BET. Above 30 min, this contribution decreases

progressively by the re-aggregation process of the particles, with an important contribution of size pores lower than 40 angstrom.

Synthesis of Cr-doped CaTiSiO₅ ceramic pigments by spray drying

Lyubenova, TS, Matteucci, F., Costa, A.L., Donde, M., Ocaña, M, Carda, J.
Materials Research Bulletin, **44** (2009) 918-924

3.2. ARTÍCULOS PUBLICADOS EN REVISTAS NO-SCI **PAPERS IN NON-SCI JOURNALS**

Development of RefEXAFS data analysis for deeper surface structure studies

Lopez-Flores, V., Ansell, S., Ramos, S., Bowron, DT., Diaz-Moreno, S., Muñoz Páez, A.
14th International Conference on X-Ray Absorption Fine Structure (XAFS14), Proceeding, vol. 190 (2009) pp. 012110-012115

Nanoparticle based multilayers as multifunctional optical coatings

Colodrero, S., Calvo, ME., Sobrado, OS, Miguez H.
Architected multifunctional materials, vol. 1188 (2009) pp. 231-238

Release properties and acute biosecurity determination of collagen-polyvinylpyrrolidone loaded in ordered mesoporous silica

López, T., Krotzsch, E., Ortiz-Islas, E., Alvarez-Lemus, M., Balsadella, E., Martinez-Blanes, J.M., Odriozola, J.A.
Key Engineering Materials, vol. 391 (2009) pp. 169-184

Caracterización mecánica de pilares de circonio sometidos a ceramización

Velázquez Cayón, R., Bruguera Alvarez, A., Jiménez Melendo, M., Vaquero Aguilar, C., Llena Amat, J., Torres Lagares, D.
Gaceta Dental, (2009) pp. 2-6

Nacre and false nacre (fopliated aragonite) in extant monoplacophorans (Tryblidiida: molusca)

Checa González, A.G., Ramírez Rico, J.
Naturwissenschaften, (2009) pp. 111-122

La clonación de obras de arte: conflicto ético a debate en conservación restauración

Ruiz-Conde, A., González-Godoy, M.A. y Sánchez Soto, P.J.
Revista de los Museos de Andalucía Mus-A, Año VII, número 11, octubre (2009) pp. 120-122

■ 3.3. 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, sep./octubre 2009, nº 115, pp. 26-31

Editorial Capitole Press

ISSN: 1132-0346

Study of the field dependence of the magnetocaloric effect in Nd_{1.25}Fe₁₁Ti: a multiphase magnetic system

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

En: 3rd International Conference on Magnetic Refrigeration at Room Temperature, pp. 167-172

Editorial Institut International du Froid. Editor Peter.W.Egolf

ISBN: 978-2-913149-67-0

Scaling laws for the magnetocaloric effect in second order phase transitions: from physics to applications for the characterization of materials

V. Franco, A. Conde

En: 3rd International Conference on Magnetic Refrigeration at Room Temperature, pp. 207-215

Editorial Institut International du Froid. Editor Peter.W.Egolf

ISBN: 978-2-913149-67-0

Universal deltaT(T) curve-application for gadolinium and TbCo₂

Y.I. Spichkin, I. Zubkov, V. Franco and A.M. Tishin

En: 3rd International Conference on Magnetic Refrigeration at Room Temperature, pp. 217-221

Editorial Institut International du Froid. Editor Peter.W.Egolf

ISBN: 978-2-913149-67-0

■ 3.4. PATENTES / PATENTS

Estructura multicapa formada por láminas de nanopartículas con propiedades de cristal fotónico unidimensional, procedimiento para su fabricación y sus aplicaciones

Inventores: S. Colodrero, H. Míguez García, M. Ocaña

Ámbito Geográfico: Nacional.

PATENTE LICENCIADA. N. de solicitud/licencia: 200900275

Fecha Solicitud/licencia: 5/julio/2009

Entidad Gestora: CSIC

Empresa: NANOLOGICA, AB

Nanogalerías de organomicas procedimiento de obtención y su aplicación en descontaminación

Inventores: M.D. Alba, C. Pazos, E. Pavón, M.M. Orta, M.A. Castro

Ámbito Geográfico: Nacional.

PATENTE SOLICITADA. N. de solicitud: 200931250

Fecha Solicitud/Licencia: 23/diciembre/2009

Entidad Gestora: CSIC

Procedimiento hidrotérmico de obtención de la kalsilita

Inventores: A. Becerro, M. Mantovani, A. Escudero

Ámbito Geográfico: Nacional.

PATENTE SOLICITADA. N. de solicitud: 200930260

Fecha Solicitud/Licencia: 4/junio/2009

Entidad Gestora: CSIC

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

Inventores: A. Fernández Camacho, V. Fortio

Ámbito Geográfico: Nacional

PATENTE SOLICITADA. N. de solicitud: 200930085

Fecha Solicitud/Licencia: 22/abril/2009

Entidad Gestora: CSIC

Método de determinación de estado de materiales de cubierta de invernaderos

Inventores: P. Sánchez Soto, E. Garzón Garzón, I. Gador García Rodríguez, L. Morales

Ámbito Geográfico: Nacional

PATENTE SOLICITADA. N. de solicitud: 200930039

Fecha Solicitud/Licencia: 3/abril/2009

Entidad Gestora: CSIC

Procedimiento de obtención de un material cerámico de forsterita

Inventores: P. Sánchez Soto, M. Raigón Pichardo, E. Garzón Garzón, R. Bono, A. Ruiz

Ámbito Geográfico: Nacional

PATENTE SOLICITADA. N. de solicitud: 200900844

Fecha Solicitud/Licencia: 27/marzo/2009

Entidad Gestora: CSIC

Procedimiento de marcaje, encriptación, etiquetado y codificación óptica

Inventores: A. Barranco, J.L. Ocaña, J.J. García-Ballesteros, M. Morales Furio, C. Molpeceres

Alvarez, R. Casquel Delcampo, J.R. Sánchez Valencia, F.J. Aparicio Rebollo, M. Holgado Bolaños,

I. Blazczyk-Lezak, A. R. González-Elipse

Ámbito Geográfico: Nacional

PATENTE SOLICITADA. N. de solicitud: 200900310

Fecha Solicitud/Licencia: 24/febrero/2009

Entidad Gestora: CSIC

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

Inventores: H. Míguez García, M.E. Calvo Roggiani

Ámbito Geográfico: Nacional

PATENTE SOLICITADA. N. de solicitud: 200900275

Fecha Solicitud/Licencia: 30/enero/2009

Entidad Gestora: CSIC

Lente de base polimérica que comprende una capa endurecedora, una capa absorbente y multicapa interferencial y procedimiento de fabricación correspondiente

Inventores: R. Fernández Serrano, A. Vilajoana Mas, J.C. Dürsteler López, J. Gil Rostra, F. Yubero Valencia, A. R. González-Elipe

Ámbito Geográfico: Nacional

PATENTE SOLICITADA. N. de solicitud: 200900275

Fecha Solicitud/Licencia: 30/enero/2009

Solicitante: INDO INTERNACIONAL, S.A.

Procedimiento de preparación de multicapas con estructura mesoporosa ordenada, material así obtenido y utilización

Inventores: H. Míguez García, A. Soler Illia, M.C. Fuertes

Ámbito Geográfico: Nacional

PATENTE LICENCIADA. N. de solicitud: 200602405

Fecha Solicitud/Licencia: 5/julio/2009

Entidades: CSIC-CONICET

Procedimiento de fabricación de un dispositivo resistivo cerámico a partir de precursores celulósicos y producto así obtenido

Inventores: Manuel Jesús López Robledo, José Javier Quispe Cancapa

Ámbito Geográfico: Nacional

PATENTE SOLICITADA. N. de solicitud: 200900580

Fecha Solicitud/Licencia: 9/marzo/2009

Entidades: Universidad de Sevilla

The method of approximation of the magnetocaloric effect temperatura dependence by means of a Universal curve

Inventores: A.M. Tishin, Victorino Franco, Alejandro Conde, Y.I. Spichkin, I.N. Zubkov

País de Prioridad: Rusia

PATENTE SOLICITADA. N. de solicitud: 2009117924

Fecha Solicitud/Licencia: 14/mayo/2009

Entidades: AMT&C Ltd.

3.5. CONGRESOS Y REUNIONES INTERNACIONALES INTERNATIONAL CONGRESS AND MEETINGS

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

ECI Conference 2009: Advances in boundary lubrication and boundary surface films

29 marzo-3 Abril [Sevilla, España]

Juan Carlos Sánchez López [Miembro del Comité Organizador]

Third directionally solidified eutectic ceramic workshop

20-24 Abril [Sevilla, España]

Julián Martínez Fernández [Miembro del Comité Organizador]

Joaquín Ramírez Rico [Miembro del Comité Organizador]

E-MRS2009

8-12 Junio [Estrasburgo, Francia]

Juan Carlos Sánchez López [Miembro del Comité Científico]

10th International conference on atomically controlled surfaces, interfaces and nanostructures

21-25 Septiembre [Granada, España]

Agustín R. González Elipe [Miembro del Comité Organizador]

ITFPC09-Innovations on thin films. Processing and characterization

17-20 Noviembre [Nancy, Francia]

Asunción Fernández Camacho [Miembro del Comité Científico]

Shaping IV International conference on shaping of advanced ceramics

15-18 Noviembre [Madrid, España]

Antonio Ramírez de Arellano-López [Miembro del Comité Asesor Nacional]

Pedro José Sánchez Soto [Miembro del Comité Asesor Nacional]

COMUNICACIONES EN CONGRESOS Y REUNIONES / COMMUNICATIONS IN CONGRESS AND MEETINGS

3rd International Symposium “Hydrogen and Energy”

25-30 Enero [Braunwald, Suiza]

“A comparative study of the additive role in the $MgH_2-Nb_2O_5$ system vs the $MgH_2+2LiBH_4-Ti-ISO$ system materials”, E. Deprez, C. López Cartes, M.A. Muñoz, O. Friedrichs, J.C. Sánchez López, U. Bösenberg, C. Bonatto, M. Dornheim, R. Bormann, A. Fernández. Comunicación oral

“Surface analysis and oxidation state in the reactive hydride composite $2LiBH_4+MgH_2+Ti-ISO$ ”, E. Deprez, T.C. Rojas Ruiz, M.A. Muñoz Márquez, C. López Cartes, A. Fernández Camacho, C. Prestipino, F.J. Palomares, C. Bonatto, U. Bösenberg, M. Dornheim, R. Bormann. Comunicación oral

Mid Term Review Meeting, MCRTN c2c

2-7 Marzo [Sevilla, España]

“Hydrothermal transformation of kaolinite in KOH solution”, M. Mantovani, A. Escudero and A.I. Becerro. Comunicación oral

First International conference on multifunctional, hybrid and nanomaterials

15-19 Marzo [Tours, Francia]

“Light processing of nanoporous semiconducting oxides for the fabrication of optically active thin films”, J.R. Sánchez Valencia, A. Barranco, A.I. Borrás, J.P. Espinós, V. Rico Gavira, A.R. González-Elipe, S. Hamad. Poster

Nanotech Insight 2009

29 Marzo-2 Abril [Barcelona, España]

“Highly improved photocatalytic activity of TiO_2 nanoparticles by synergetic effect of sulphate promotion and platinisation”, J.A. Navío, M.C. Hidalgo, M. Maicu and G. Colón. Poster

International workshop on advanced nanostructured surfaces for industrial applications

6-7 Abril [Cambridge, Reino Unido]

“Synthesis and characterization of Thiol-and phosphine-capped gold nanoparticles”, M.A. Muñoz, E. Guerrero, T.C. Rojas Ruiz, C. López Cartes, G. Ciatto, A. Fernández Camacho. Comunicación oral

3rd International Conference on the Industrialization of DSC, DSC-IC 09

22-24 Abril [Nara, Japón]

“Integration and effect of nanoparticle-based one dimensional photonic crystals in dye sensitized solar cells”, H. Míguez García, S. Colodrero, M. Calvo, A. Mihi, M. Ocaña, G. Boschloo, L. Haggman, J.A. Anta, A. Hagfeldt. Comunicación oral

“Increasing efficiency by introducing a one dimensional photonic crystal in DSC”, S. Colodrero, A Hagfeldt, H. Míguez García. Poster

Non-destructive and Microanalytical Techniques in Art and Cultural Heritage, TECHNART 2009

27-30 Abril [Atenas, Grecia]

“Study of metallic components of historical organ pipes through synchrotron radiation X-ray microfluorescence images and grazing incidence X-ray diffraction”, L.K. Herrera, A. Justo, A. Muñoz-Páez, G. Martínez-Criado. Poster

36th International Conference on Metallurgical Coatings and Thin Films, ICMCTF 2009

27 Abril-1 Mayo [San Diego, Estados Unidos de América]

“Metal carbide/amorphous C-based nanocomposite coatings for tribological coatings”, J.C. Sánchez López, D. Martínez Martínez, M.D. Abad, A. Fernández Camacho. Conferencia Invitada

“Ti(C,O,N)-Based Coatings for Biomedical Applications: Influence of Composition and Structure in the Mechanical/Tribological and Biological Behaviour”, N. Jordao, S. Ribeiro, J.C. Sánchez López, M.D. Abad, F. Vaz, M. Henriques, R. Oliveira, R. Escobar-Galindo, S. Carvalho. Comunicación oral

“Thermal stability of SiOXNY thin films with tailored refraction index: microstructural chemical and mechanical properties”, V.C. Fortio, C. Fernández Ramos, M.C. Jiménez de Haro, M.P. Delplancke-Ogletree, A. Fernández Camacho. Comunicación oral

“Antibacterial properties and tribology of a-C: Ag coatings deposited by pulsed cathodic filter arc”, J.L. Endrino, M. Allen, J.C. Sánchez López, R. Escobar-Galindo, A. Anders, J.H. Horton, T.M. Horton, J.M. Albella. Poster

Hybrid and organic photovoltaics conference, HOPV 2009

10-13 Mayo [Benidorm, España]

“Photoconducting Bragg mirrors based on TiO₂ nanoparticle multilayers”, M. Calvo, S. Colodrero, M. Ocaña, H. Míguez García. Comunicación oral

“Increasing efficiency by introducing a one dimensional photonic crystal in DSC”, S. Colodrero, A. Hagfeldt, H. Míguez García. Comunicación oral

29th International exhibition-congress on chemical engineering, environmental protection and biotechnology, ACHEMA 2009

11-15 Mayo [Franckfurt, Alemania]

“Development of transition metal nitrides, carbides, and borides-based materials by mechanically induced self-sustaining reactions”, F.J. Gotor, J.M. Córdoba, M.A. Avilés, M.J. Sayagués and M.D. Alcalá. Comunicación oral

Thermag III

12-15 Mayo [Des Moines, Estados Unidos de América]

“Scaling laws for the magnetocaloric effect in second order phase transitions: from Physics to applications for the characterization of materials”, V. Franco and A. Conde. Conferencia

“Study of the field dependence of the magnetocaloric effect in $Nd_{1.25}Fe_{11}Ti$: a system with two main magnetic phases”, R. Caballero-Flores, V. Franco, A. Conde, W.Y. Dong and H.W. Zhang. Poster

“Universal $\Delta T(T)$ curve-application for gadolinium and $TbCO_2$ ”, Y.I. Spichkin, I. Zubkov, V. Franco and A.M. Tishin. Poster

E-MRS 2009 Spring Meeting

8-12 Junio [Estraburgo, Francia]

“Nanoparticle based multilayers as multifunctional optical coatings”, H. Míguez, M. Calvo, S. Colodrero, M. Ocaña, O. Sánchez Sobrado. Conferencia

“Nanocrystallization kinetics under instantaneous growth approximation: experiments and cellular automata simulations”, J.S. Blázquez, M. Millán, C.F. Conde and A. Conde. Conferencia

“Enhanced optical response of ordered mesoporous thin films coupled to photonic crystals”, H.R. Míguez García, N. Hidalgo, M. Calvo Roggiani. Comunicación Oral

“Characterization of Boron doped diamond like carbon films deposited by Femtosecond and nanosecond pulsed laser ablation”, A. Sikora, A. Berkesse, O. Bourgeois, J-L. Garden, C. Guerret-Piécourt, J.N. Rouzaud, J.C. Sánchez López, A.S. Loir, F. Garrelie, C. Donnet. Comunicación Oral

“N-doped TiO_2 photoactive optical thin films in the visible-light region deposited by plasma enhanced CVD”, P. Romero, A. Barranco, V. Rico, J.P. Espinós, J. Cotrino, A.R. González-Elipe. Comunicación Oral

“XPS background analysis to monitor aging processes in plasma functionalized polymers”, M.C. López Santos, F. Yubero, J. Cotrino, A. Barranco, A.R. González-Elipe. Comunicación Oral

“Oxidation resistance of (Y,Zr)-doped CrAlN coatings”, S. El Mabet, J.C. Sánchez López, M. Bri- zuela, A. García-Luis. Poster

“Wetting behavior of polycrystalline anatase films prepared by PECVD”, J.R. Sánchez Valencia, A.I. Borrás, A.R. González-Elipe. Poster

“Light processing of nanoporous semiconducting oxides for the fabrication of optically active thin films”, J.R. Sánchez Valencia, A.I. Borrás, J.P. Espinós, V. Rico Gavira, A.R. González-Elipe, A. Barranco, S. Hamad. Poster

“Luminiscent plasma nanocomposites for the fabrication of photonic sensing devices”, F.J. Aparicio, I.K. Blaszczyk, J.R. Sánchez Valencia, A.I. Borrás, A.R. González-Elipe, A. Barranco. Poster

“Influence of Mn on the magnetocaloric effect in Nanoperm-type alloys”, R. Caballero-Flores, A. Cond and L.F. Kiss. Poster

“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-Pérez. Poster

XIV Internacional Clay Conference

14-20 Junio [Castellaneta Marina, Italia]

“NA-4-Mica modified by Alkyl-ammonium ions”, C. Pazos, M.D. Alba, M.A. Castro, M.M. Orta, E. Pavón. Comunicación oral

“Acid stability of clay minerals: implications for processes in geological radioactive waste disposal”, P. Chain, M.D. Alba, M.A. Castro, M.M. Orta, E. Pavón. Poster

“Monte-Carlo simulations of inorganic cations in expandable micas”, E. Pavón, M.A. Castro, M.D. Alba, M.M. Orta, C. Pazos, M. Naranjo, N. Skipper, G. Cuello. Poster

15th International conference structures ICCS 15

15-17 Junio [Oporto, Portugal]

“Mechanochemical preparation of BaTiO₃-Ni nanocomposites with high dielectric constant”, L.A. Pérez-Maqueda, P.E. Sánchez-Jiménez, M.J. Diánez and J.M. Criado. Poster

9th Mediterranean conference on calorimetry and thermal analysis. MEDICTA 2009

15-18 Junio [Marsella, Francia]

“Simple controlled thermal analysis from milligrams to tons”, J.M. Criado, M.J. Diánez, L.A. Pérez Maqueda, A. Perejón. Comunicación oral

“A thermal study approach to roman age wall painting mortars”, A. Durán, L.A. Pérez Maqueda, J.L. Pérez-Rodríguez. Poster

“Development of a high temperature thermogravimetric system from a conventional laboratory analytical balance and a domestic microwave oven”, M.J. Diánez, L.A. Pérez Maqueda, A. Perejón and J.M. Criado. Poster

Joint meeting of the Spanish and Portuguese microscopy societies

16-19 Junio [Segovia, España]

“Microstructural characterization of Ti_xNy-Ni cermet using microscopic related techniques”, M.J. Sayagués, M.A. Avilés, J.M. Córdoba, M.D. Alcalá, F.J. Gotor. Poster

Congreso Ibérico de Tribología, IBERTRIB2009

17-18 Junio [Coimbra, Portugal]

“Raman study of the friction contact region of WC/C nanostructured coatings against various counterparts”, S. Elmrabet, M.D. Abad, J.C. Sánchez López. Poster

16th International symposium on metastable, amorphous and nanostructured materials

5-9 Julio [Beijing, China]

“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, O. Friedrichs. Conferencia

“Application of electron microscopy and spectroscopy techniques to the characterization of nanostructured TiAlSiN coatings”, V.C. Fortio, D. Philippon, T.C. Rojas, M.P. Delplanckse-Ogletree. Poster

6th World Congress on oxidation catalysis

5-10 Julio [Lille, Francia]

“Modified cryptomelane-type manganese dioxide nanomaterials for preferential oxidation of CO in presence of hydrogen”, W.Y. Hernández, M.A. Centeno, M. Montes, J.A. Odriozola. Comunicación oral

“Ce-Fe and Au/Ce-Fe catalysts for total and preferential oxidation of CO (TOX and PROX)”, O.H. Laguna, M.A. Centeno, G. Arzamendi, L. Gandía, F. Romero-Sarria, J.A. Odriozola. Comunicación oral

“Methanol oxidation over CuO-ZnO-Al₂O₃ and Pd catalysts”, G. Arzamendi, J. Echave, P. Navarro, M. Montes, M.I. Domínguez, M.A. Centeno, J.A. Odriozola, L.M. Gandía. Poster

XXIV Congress of the Spanish microscopy society and XLIV Annual meeting of the Portuguese society for microscopy

16-19 Julio [Segovia, España]

“STEM tomography characterization of nano-sized gold particles supported on heavy oxide catalysts”, J.C. González-González, J.C. Hernández Garrido, M. López Haro, E. del Río Sánchez, J.J. Delgado Jaén, A.B. Hungria, S. Trasobares, S. Bernal, P.A. Midgley, J.J. Calvino. Comunicación Oral

XXIV International Conference on Photochemistry

19-24 Julio [Toledo, España]

“Synthesis of TiO₂ by hydrolysis precipitation and hydrothermal treatment. Effect of different acids and metal impregnation”, E. Pulido Melián, O. González-Díaz, G. Colón, J.M. Doña Rodríguez, J.A. Navío and J. Pérez-Peña. Poster

International Conference on the Applications of the Mössbauer Effect (ICAME 2009)

19-24 Julio [Viena, Austria]

“Mechanical amorphization of Fe₇₅Nb₁₀B₁₅”, J.J. Ipus, J.S. Blázquez, V. Franco, A. Conde and L.F. Kiss. Poster

“Thermal stability of a supersaturated Fe-Ge-Nb solid solution produced by ball milling”, J.J. Ipus, J.S. Blázquez and A. Conde. Poster

“Magnetic and structural characterization of Mo-hitperm alloys with different Fe/Co ratio”, C.F. Conde, J.M. Borrego, J.S. Blázquez, A. Conde, P. Svec and D. Janickovic. Poster

The 5th International conference on gold science, technology and its applications, Gold 2009

26-29 Julio [Heidelberg, Alemania]

“Molecular dynamics simulation study of gold interaction modified TiO₂ surfaces”, M.A. Centeno, R.S. Avellaneda, F. Romero-Sarria, M.I. Domínguez, J. Plata, J. Fernández-Sanz, J.A. Odriozola. Poster

“Gold functionalized supported ionic liquids: a valuable catalyst for room temperature CO oxidation”, S. Ivanova, L. Bobadilla, A. Penkova, F. Romero, M.A. Centeno, J.A. Odriozola. Poster

14th International Conference on X-Ray Absorption Fine Structure (XAFS14)

26-31 Julio [Camerino, Italia]

“Study of metallic components of historical organ pipes through synchrotron radiation X-ray microfluorescence and XANES spectroscopies”, L.K. Herrera, A. Justo, A. Muñoz-Paez, J.A. Sans, G. Martínez-Criado. Comunicación Oral

International Conference on Magnetism ICM2009

26-31 Julio [Camerino, Italia]

“Breakdown of Universal behavior of the magnetic entropy change in magnetocaloric materials with first-order phase transition”, C.M. Bonilla, F. Bartolomé, L.M. García, M. Parra-Borderías, V. Franco, J. Herrero-Albillos. Comunicación Oral

19th International symposium on plasma chemistry

26-31 Julio [Bochum, Alemania]

“Formation of nitrogen functional groups on plasma treated surface polymers”, M.C. López Santos, F. Yubero, J. Cotrino, A.R. González-Elípe. Comunicación Oral

“Role of oxygen in plasma processing of materials and its control in plasma reactors”, S. Veprek, M.G.J. Veprek, A. Fernández Camacho, M. Jilek, A. Berrgmaier, F. Mirabella. Comunicación Oral

15th International conference on the strength of materials

16-21 Agosto [Dresden, Alemania]

“High temperature plastic behavior of Y:BaCeO₃ polycrystals”, C. Vaquero Aguilar, J. Martínez Fernández, M.E. Enrique Magariño. Poster

Catalysis for a Sustainable World. Europacat IX

30 Agosto-4 Septiembre [Salamanca, España]

“Catalytic microreactors for steam reforming of methanol”, F.J. Echave, M.C. Arzamendi, M.A. Centeno, L. Costa, O. Sanz, L. Gandía, J.A. Odriozola and M. Montes. Comunicación Oral

“Study of the reducibility and reactivity of lanthanum substituted perovskites in the oxidation of carbon monoxide”, J.L. Hueso, J.P. Holgado, A.R. González-Elípe and A. Caballero. Poster

“Au-Ni nanoparticles for improved CO oxidation catalysts”, F. Ternero, A. Caballero and J.P. Holgado. Poster

“Silver-based catalysts for preferential CO oxidation in hydrogen-rich gases (PROX)”, S. Todorova, A. Naydenov, J.P. Holgado, R. Pereñíguez, G. Kadinov and A. Caballero. Poster

“Supported cobalt and manganese catalysts for total *n*-hexane and ethyl acetate oxidation”, S. Todorova, A. Naydenov, J.P. Holgado, R. Pereñíguez, G. Kadinov and A. Caballero. Poster

“Redispersion of nickel metallic particles by CO treatment in Ni/ZrO₂ methane reforming catalysts”, R. Pereñíguez, V.M. González de la Cruz, A. Caballero y J.P. Holgado. Poster

“Effect of synthesis methods in the reactivity of LaNiO₃ for dry reforming”, R. Pereñíguez, V.M. González de la Cruz, A. Caballero y J.P. Holgado. Poster

“Photocatalytic degradation of phenol on immobilized TiO₂ and ZnO films”, E. Pulido-Melián, P.S.M. Dunlop, J.A. Byrne, O. González-Díaz, J.M. Doña-Rodríguez, G. Colón and J.A. Navio. Poster

“Advanced electron microscopy investigation of synthesis and OSC behavior of Ce_{0.8}Pr_{0.2}O₂/D.Al₂O₃ (D=3.5%wt SiO₂, 4% wt La₂O₃) catalysts”, M. López Haro, K. Aboussaid, J.C. González-González, J.C. Hernández Garrido, J.M. Pintado, G. Blanco Montilla, J.J. Calvino Gómez, P. Bayle-Guillemau, S. Trasobares. Poster

“Brass microreactors for catalytic applications”, L.M. Martínez T., W.Y. Hernandez, F.J. Echave, O. Laguna, O. Sanz, M.A. Centeno, M. Montes, J.A. Odriozola. Poster

“The use of microchannel reactor technology for the GTL process”, M.C. Arzamendi, M.A. Centeno, L. Costa, E. Falabella, L. Gandia, M. Montes, J.A. Odriozola. Poster

“Modification of the oxidation layer after deposition of CeO₂ and Au/CeO₂ catalysts on AISI 304 austenitic stainless steel monoliths”, L.M. Martínez T., O. Sanz, M.A. Centeno, J.A. Odriozola. Poster

“The role of solvent in the preparation of gold functionalized supported ionic liquids”, S. Ivanova, R. Avellaneda, O. Sanz, F. Romero-Sarria, M.A. Centeno, J.A. Odriozola. Poster

“Effect of different acids on the structural and photocatalytic properties of titania-silica mixed oxides”, B. Llano, G.M. Restrepo, J.M. Marín, M.C. Hidalgo, J.A. Navío. Poster

“Preparation, characterization and photocatalytic properties of TiO₂/SiO₂ films on borosilicate glass”, J.A. Navio, J.M. Marín, F. Granda, L.A. Rios, G. Restrepo, L. Galeano. Poster

“Effect of different acids on the structural and photocatalytic properties of Titania-Silica mixed oxides”, B. Llano, G. Restrepo, J.M. Marín, J.A. Navio. Poster

WTC IV Satellite Forum, Tribochemistry 2009

2-4 Septiembre [Kyoto, Japón]

“Experimental simulation of the additives tribochemical reactions in boundary lubrication regime by gas phase lubrication”, M.I. de Barros-Bouchet, D. Philippon, T. le Mogne, O. Lerasle, J.M. Martin. Comunicación Oral

EUROMAT 2009

7-10 Septiembre [Glasgow, Reino Unido]

“Electrical properties of biomimetic carbon and silicon carbide fabricated from MDF”, J.J. Quispe Cancapa, M.E. Enrique Magariño, F.M. Varela Fera, A. Ramírez de Arellano-López, M.J. López Robledo, M.A. Bautista, J. Martínez Fernández. Comunicación Oral

“Mechanical characterization of silicon carbide porous scaffolds by bending, wear and hardness tests”, C. Torres Raya, J. Ramírez Rico, F.M. Varela Fera, M.A. Bautista, J. Martínez Fernández. Comunicación Oral

“Precursor selection and properties of porous biomorphic SiC for high temperature application”, J.J. Quispe, M.A. Bautista, J. Martínez Fernández, C. Torres Raya, J. Ramírez Rico. Poster

Microscopy at the nanoscale and beyond, EMAG 2009

8-11 Septiembre [University of Sheffield, UK]

“Investigation of spatial distribution of nanoparticles on heavy metal oxide catalysts by haade-system electron tomography”, J.C. Hernández, P.A. Midgley, M. López Haro, J.C. González González, A.B. Hungria, S. Trasobares, S. Bernal M., J.J. Calvino Gámez. Comunicación Oral

ISHHC XIV International symposium on relations between homogeneous and heterogeneous catalysis

13-18 Septiembre [Estocolmo, Suecia]

“Group 10 PCP Pincer complexes as models for catalytic alcohol carboxylation”, J. Cámpora, L.M. Martínez-Prieto, C. Melero, P. Palma, E. Álvarez, C. Real. Poster

5th International Congress on the Application of Raman Spectroscopy in Art and Archeology

14-18 Septiembre [Bilbao, España]

“Raman spectroscopy characterization of charcoal in tongues and shallots of reed pipes from historical Baroque organs”, L.K. Herrera, A. Muñoz-Páez, G. Martinez-Criado, B. Sigüenza, A. Justo. Poster

“Micro-Raman and X-rays fluorescence spectroscopy as non destructive techniques for pigments and dyestuffs identification in an Arabic illuminated manuscript”, A. Durán, M.L. Franquelo, M.A. Centeno, T. Espejo, J.L. Pérez Rodríguez. Poster

E-MRS 2009 Fall Meeting

14-18 Septiembre [Varsovia, Polonia]

“Nanocrystallization kinetics under instantaneous growth approximation: experiments and

celular automática simulations”, J.S. Blázquez, M. Millán, C.F. Conde and A. Conde. Conferencia

“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-Pérez. Poster

4th International meeting UHMWPE for arthroplasty: from powder to debris and Satellite meeting – UHMWPE and medical devices: from production to the hospital

16-17 Septiembre [Turin, Italia]

“Surface functionalization of UHMWPE by plasma processes”, M.C. López Santos, F. Yubero, A.R. González-Elípe. Poster

Journées Européennes de la Photocatalyse

21-22 Septiembre [Bordeaux, Francia]

“Enhancement of photocatalytic activity of sulphated and non-sulphated TiO₂ by deposition of Pt, Au and Pd”, M. Maicu, M.C. Hidalgo, G. Colón and J.A. Navío. Poster

24th European photovoltaic solar energy

21-22 Septiembre [Hamburgo, Alemania]

“First results of the Spanish National Project *Espectro Solar*”, S. Mau, Y. Sánchez Reina, V. Rico Gavira, A. Martín, F. Rubio, J. Leloux, D. Pachon, V. Gómez, G. Juengst, T. Gerstmaier, A. Hakenjos. Comunicación Oral

10th International conference on atomically controlled surfaces, interfaces and nanostructures

21-25 Septiembre [Granada, España]

“Optically active plasma nanocomposites for the fabrication of photonic sensing devices”, F.J. Aparicio, I.K. Blaszczyk, A.I. Borrás, M. Holgado, J.R. Sánchez Valencia, A. Griol, H. Sohlstrom, A.R. González-Elípe, A. Barranco. Comunicación Oral

“Photo-luminescence property of ZnO thin films prepared by PECVD”, P. Romero, J. Toudert, J.R. Sánchez Valencia, A. Barranco, A.R. González-Elípe. Comunicación Oral

7th International workshop on microwave discharge fundamentals and applications

23-27 Septiembre [Hamamatsu, Japón]

“Remote microwaves plasmas for the synthesis of active optical thin films for photonic applications”, A. Barranco, F.J. Aparicio, I.K. Blaszczyk, A.I. Borrás, M. Holgado, J.R. Sánchez Valencia,

A. Griol, H. Sohlstrom, A.R. González-Elipe. Conferencia

Nanomechanical testing in materials research and development

11-16 Octubre [Toscana, Italia]

“Scratching behavior of nanostructured TiAlN and TiAlSiN protective coatings”, P. Nagy, V.C. Fortio, D. Philippon, M.P. DelPlancke-Ogletree, A. Fernández Camacho. Poster

International congress of modern bone regeneration, BONE-TEC 2009

8-11 Octubre [Hannover, Alemania]

“Potential use of mesoporous silica based materials for bone repair”, L. Santos-Ruiz, D. Amat, A. Díaz-Cuenca and J. Becerra. Poster

3rd International Meeting on Architectural of the Mediterranean, RIPAM 2009

15-17 Octubre [Lisboa, Portugal]

“Mortars in medieval mural paintings of Carinthia and its influence on Slovenia”, A. Kriznar, A. Ruiz-Conde and P.J. Sánchez Soto. Poster

13th European Conference on applications of surface and interface analysis. ECASIA '09

18-23 Octubre [Antalya, Turquía]

“Nitrogen plasmas functionalization of polymers and DLC materials”, M.C. López Santos, F. Yubero, J. Cotrino, A. Barranco. Comunicación oral

“Hydrogen vs deuterium at the surface of H₂O and D₂O ice by REELS”, F. Yubero, K. Tokesi. Comunicación oral

“Study of the morphology of NiO nanostructures grown on HOPG by Tougaard Method and AFM; a comparative study”, L. Soriano, I. Preda, A. Gutiérrez, J. Méndez, L. Alvarez, F. Yubero, J.M. Sanz. Comunicación oral

“Silica based mixed oxide thin films to be applied in ophthalmic colored glasses”, J. Gil Rostra, F. Yubero, A.R. González-Elipe, R. Fernández, T. Vilajoana, P. Artús, J.C. Dürsteler. Poster

“Surface characterization of CrO₂ thin films”, C. Aguilera, F. Yubero, J.P. Espinós, A.R. González-Elipe. Poster

9º Congreso Internacional de metalurgia y materiales

19-23 Octubre [Buenos Aires, Argentina]

“Un Nuevo método de control del espesor del recubrimiento de TiN sobre Titanio. Análisis térmico a velocidad constante (ATVC)”, J.M. Criado, M.J. Diáñez, L.A. Pérez Maqueda, A. Pe-rejón y E. Donoso. Comunicación oral

“Evaluaciones microcalorimétricas del proceso de precipitación en aleaciones de Cu-Ti-Co”, E. Donoso, M.J. Diáñez y J.M. Criado. Poster

62nd Annual gaseous electronics conference

20-23 Octubre [Norfolk, Virginia, Estados Unidos de América]

“Line intensities in nitrogen low-pressure microwave discharges”, L.P. Lemos Alves, M.C. López Santos, J. Cotrino. Poster

International workshop synthesis and commercialization of advanced nano-structured materials and coatings

22 Octubre [Moscú, Rusia]

“Multifunctional bioactive nanostructured films for metallic implants”, I.A. Bashkova, N.A. Gloushankova, PH.V. Kiryukhantsev-Korneev, A.N. Sheveiko, A.S. Grigoryan, B.N. Mavrin, A. Fernández Camacho, E.A. Levashov. Comunicación oral

“Hard nanostructured coatings produced by magnetron sputtering of Max-phase $Ti_{2-x}Cr_xAl$ targets”, PH.V. Kiryukhantsev-Korneev, A.N. Sheveiko, T.C. Rojas Ruiz, A. Fernández Camacho, B.N. Mavrin, E.A. Levashov, D.V. Shtansky. Poster

10º Congreso Interamericano de microscopía electrónica, CIASEM 2009

25-28 Octubre [Rosario, Argentina]

“Síntesis de hidroxiapatita en silica mesoporosa: un estudio por microscopía electrónica de alta resolución”, D.R. Acosta Najarro and A. Díaz-Cuenca. Comunicación oral

Materials Science & Technology 2009

25-29 Octubre [Pittsburgh, Estados Unidos de América]

“Magnetic anisotropy in nanocrystalline alloys: influence of temperatura and interactions”, V. Franco and A. Conde. Conferencia

Contaminated site management in Europe

27-29 Octubre [Gent, Bélgica]

“Characterization and selection of materials for the In Situ remediation of a metal contaminated soil”, R. Glez-Núñez, M.D. Alba, M.M. Orta, M.A. Castro, M. Vidal, A. Rigol. Comunicación oral

AVS 56th International Symposium.

8-13 Noviembre [San José, California, Estados Unidos de América]

“Study of the influence of ballistic and diffusive deposition particles on the evolution of the surface morphology of thin films”, R. Alvarez, P. Romero-Gomez, J. Gil Rostra, A. Palmero, J. Cotrino, F. Yubero, A.R. González-Elipe. Comunicación oral

“Hydrogen quantification at surfaces by electron spectroscopy”, F. Yubero. Comunicación oral

“Direct measurement of porosity in glancing angle deposited thin films”, J.R. Sánchez-Valencia, F. Yubero, A.R. González-Elipe. Comunicación oral

Directionally solidified eutectic ceramic workshop

10-13 Noviembre [Sevilla, España]

“Microstructure, creep and residual stresses of directionally solidified Al₂O₃-based eutectics”, J. Ramírez-Rico, J. Martínez-Fernández, A.R. de Arellano-López, P.B. Oliete, J.I. Peña, V. Orera, J.L. Routbort and D. Singh. Comunicación oral

“Nanoscale study of the subcritical to mirror transition in single-crystal sapphire fibers”, J.L. López-Cepero, J.J. Quispe, J. Martínez-Fernández, A.R. de Arellano-López. Comunicación oral

“Three directional fractography of sapphire: a context view”, J.L. López-Cepero, J.J. Quispe-Cancapa, J. Martínez-Fernández and A.R. de Arellano-López. Comunicación oral

“Microstructural and mechanical evaluation of porous silicon carbide for high temperature applications”, J.L. López-Cepero, J.J. Quispe-Cancapa, J. Martínez-Fernández and A.R. de Arellano-López. Comunicación oral

“Room temperature mechanical properties of biomimetic silicon carbide for medical applications”, C. Torres Raya, M.A. Bautista, F. Gutiérrez Mora, J. Martínez Fernández, J. Ramírez Rico, F.M. Varela Feria. Poster

“Temperature dependence of the electrical behavior of silicon carbidebased composites fabricated from cellulose precursors”, J.J. Quispe Cancapa, J. Martínez Fernández, D. Hernández Maldonado, M.E. Enrique Magariño, T.S. Orlova. Poster

“Microstructural and mechanical evaluation of Cu-Based active brazing alloy and refractory metal interlayers to joint silicon nitride to Ni-base superalloy”, R. Asthana, J. Martínez Fernández, F.M. Varela Feria, M. Singh. Poster

“Fabrication and high temperature plasticity of directionally solidified and polycrystalline photon-conducting perovskite oxides”, M.J. López Robledo, M.E. Enrique Magariño, M. Jiménez Melendo, C. Vaquero Aguilar, J. Martínez Fernández, J.I. Peña. Poster

“Compressive strength degradation in ZrB₂-based ultra high temperature composites”, J. Ramírez Rico, J. Martínez Fernández, M.A. Bautista, M. Singh. Poster

Shaping IV International conference on shaping of advanced ceramics

15-18 Noviembre [Madrid, España]

“Thermal behavior of kaolinite powders: multistep dehydroxylation and high-temperature phases”, F.J. Gotor, M. Macías, A. Ortega, P.J. Sánchez Soto. Comunicación oral

“Structural model of layer silicates as influenced by dry grinding”, P.J. Sánchez Soto, A. Ruiz Conde and E. Garzón Garzón. Poster

Innovations in thin film processing and characterisation, ITFPC2009

17-20 Noviembre [Nancy, Francia]

“Characterization of T_{1-x}Al_xN coatings with selective IR reflectivity”, V.C. Fortio, D. Philippon, T.C. Rojas, N.N. Novikova, E.A. Vinogradov, A. Fernández. Comunicación oral

“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. Poster

IX Congreso iberoamericano de energía mecánica, CIBIM 9

17-20 Noviembre [Las Palmas de Gran Canaria, España]

“Diseño de un dilatómetro de alta resolución para estudios de cinética de sinterización y cambios de fase en aluminosilicatos en atmósfera controlada en el rango de temperaturas de 25 a 1500°C”, J.M. Criado, M.J. Diánez, L.A. Pérez-Maqueda y E. Donoso. Comunicación oral

10th Annual conference on laser ablation

22-27 Noviembre [Singapur]

“Study of Boron doped diamond like carbon films elaborated by femtosecond and nanosecond pulsed laser ablation”, A. Sikora, A.S. Loir, F. Garrelie, C. Donnet, R. Stoian, O. Bourgeois, J.L. Garden, J.N. Rouzaud, J.C. Sánchez López, T.C. Rojas Ruiz. Poster

American Geosciences Union Fall Meeting

14 Diciembre [San Francisco, Estados Unidos de América]

“Kaolinite illitization at 300 °C and 1000 bars with increasing time”, M. Mantovani, A. Escudero, A.I. Becerro. Poster

3.6. CONGRESOS Y REUNIONES NACIONALES NATIONAL CONGRESSES AND MEETINGS

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

VI Simposio Colombiano de Catálisis, VI SICCAT
28-30 Octubre [Medellin, Colombia]
Miguel Angel Centeno Gallego [Miembro del Comité Científico]

1st Spanish national conference on advances in materials recycling and eco
12-13 Noviembre [Madrid, España]
Pedro José Sánchez Soto [Miembro del Comité Científico]

Sociedad Española de la Arcillas, Jornada Científica conmemorativa 50 Aniversario
19 Noviembre [Madrid, España]
Pedro José Sánchez Soto [Miembro del Comité Organizador]

COMUNICACIONES EN CONGRESOS Y REUNIONES COMMUNICATIONS IN CONGRESS AND MEETINGS

1er Congreso Nacional de Nanotecnología
24-26 Mayo [Valparaiso, Chile]

“Crecimiento de cristalitas nanométricas en aleaciones base cobre”, R. Palma, A. Sepúlveda, E. Donoso, A. Zúñiga, J.M. Criado y M.J. Diánez. Comunicación oral

SECAT'09
29 Junio-1 Julio [Ciudad Real, España]

“Redispersión de níquel mediante tratamiento con CO en catalizadores Ni/ZrO₂ para el reformado de metano”, V.M. González de la Cruz, R. Pereñíguez, J.P. Holgado, A. Caballero. Comunicación oral

“Estudio de la oxidación selectiva de H₂S mediante XAS y Raman en condiciones de reacción”, M.D. Soriano, J.P. Holgado, J. Jiménez-Jiménez, P. Concepción, A. Caballero, E. Rodríguez-Castellón, J.M. López-Nieto. Comunicación oral

“LaNiO₃ para el reformado seco de metano. Influencia del método de síntesis”, R. Pereñíguez, V.M. González de la Cruz, A. Caballero, J.P. Holgado. Comunicación oral

“Catalizadores de Au soportado sobre óxidos mixtos Ce-Zr para la oxidación total de CO”, O.H. Laguna, F. Romero-Sarria, M.A. Centeno, J.A. Odriozola. Comunicación oral

“Preparación de líquidos iónicos soportados y su funcionalización con oro”, S. Ivanova, R. Avelaneda, O. Sanz, F. Romero-Sarria, M.A. Centeno, J.A. Odriozola. Comunicación oral

“Nanopartículas de Au-Ni para la mejora de la oxidación catalítica del CO”, F. Ternero, A. Caballero y J.P. Holgado. Poster

“Estudio de la actividad fotocatalítica de sistemas Pd-TiO₂ en la degradación del fenol: Efecto de la sulfatación previa del semiconductor y de la concentración del metal”, M. Maicu, M.C. Hidalgo, G. Colón y J.A. Navío. Poster

“Efecto de la modificación con tierras raras y metales de transición sobre soportes tipo CeO₂, y su aplicación en la oxidación catalítica de CO”, W.Y. Hernández, M.A. Centeno, F. Romero-Sarria y J.A. Odriozola. Poster

“Catalizadores bimetálicos Ni-Sn/Al₂O₃-MgO para reformado con vapor de metanol: efecto del contenido de Mg del soporte”, A. Penkova, L. Bobadilla, S. Ivanova, F. Romero-Sarria, M.A. Centeno, J.A. Odriozola, A.C. Roger, A. Kiennemann. Poster

“Monolitos oro/bentonita/fecralloy para la oxidación catalítica de CO y fenol”, M.I. Domínguez L.M. Martínez, T.N. Sanabria, S. Moreno, R. Molina, J.A. Odriozola, M.A. Centeno. Poster

“Oxidación de CO sobre óxidos de manganeso”, M.A. Peluso, L. Falco, W.Y. Hernández, M.A. Centeno, J.E. Sambeth, H. Thomas. Poster

“CuO-CeO₂ soportado sobre micromonolitos de latón para la reacción de CO_{prox}”, O. Sanz, L.M. Martínez T., W.Y. Hernández, F.J. Echave, O.H. Laguna, L. Costa, M.A. Centeno, M. Montes, J.A. Odriozola. Poster

“Reformado de metanol con vapor sobre Pd/ZnO”, B. Arhoun, F.J. Echave, O. Sanz, M.A. Centeno, J.A. Odriozola, M. Montes. Poster

“Estudio DRIFTS-MS de la influencia de la atmósfera de activación en catalizadores Au/CeO₂”, S.A. Cruz, M. Martínez T., F. Romero-Sarria, M.A. Centeno, J.A. Odriozola. Poster

XXXII Reunión Bienal de la Real Sociedad Española de Física

7-11 Septiembre [Ciudad Real, España]

“Estudio del efecto magnetocalórico: influencias de la geometría y heterogeneidades de las muestras magnéticas”, R. Caballero-Flores, V. Franco y A. Conde. Poster

“Dependencia de la coercitividad en polvos metálicos basados en Fe y obtenidos por molien-
da”, J.J. Ipus, J.S. Blázquez, F. Franco, A. Conde y S. Lozano-Pérez. Poster

Congreso Nacional de la Sociedad Española de Cirugía Bucal

17-19 Septiembre [Almería, España]

“Caracterización microestructural y mecánica de sistemas implantoprotésicos sometidos a
ceramización”, C. Vaquero Aguilar, A. Brugera Alvarez, J. Llena Amat, J.L. Gutiérrez Pérez, R.
Velázquez Cayón, O. Llena Amat, M. Jiménez Melendo. Comunicación oral

IV Reunión de la Asociación de Usuarios de Sincrotrón de España

15-18 Septiembre [Barcelona, España]

“Strong metal-support interaction (SMSI) observed by ambient pressure photoemission spec-
troscopy (APPES) in a Ni/CeO₂ system”, V.M. González de la Cruz, J.P. Holgado, T. Herranz, M.
Salmeron y A. Caballero. Poster

“Ambient pressure photoemission spectroscopy (APPES) characterization of Au-Ni nanopar-
ticles deposited in Ceria”, F. Ternero, A. Caballero y J.P. Holgado. Poster

“Estudio de catalizadores de vanadio para la oxidación selectiva de H₂S mediante XAS y Raman
en condiciones de reacción”, M.D. Soriano, J.P. Holgado, J. Jiménez-Jiménez, P. Concepción, A.
Caballero, E. Rodríguez-Castellón y J.M. López-Nieto. Poster

“Study of cultural heritage materials pieces of the andalusian baroque period with synchrotron
radiation based techniques”, A. Muñoz-Páez, L.K. Herrera, G. Martínez-Criado, J.A. Sans, A.
Justo. Poster

“Análisis GISAXS de capas delgadas columnares de TiO₂ preparadas por evaporación en ángulo
rasante (GAPVD)”, L. González García, A. Barranco, A. Muñoz Páez, A.R. González-Elipe, M.C.
García Gutiérrez, J. Hernández, D. Rueda, T. Ezquerro. Poster

XLIX Congreso de la Sociedad Española de Cerámica y Vidrio

28-30 Octubre [Jaén, España]

“Caracterización de soportes vítreos constituyentes de placas fotográficas (s. XX)”, G. Durán
Domínguez, M. Arjonilla Alvarez, A. Ruiz Conde, P.J. Sánchez Soto. Comunicación oral

“Síntesis reactiva de carbonitruro de vanadio”, M.A. Roldán, M.D. Alcalá, C. Real. Poster

“Caracterización química y mineralógica de filitas del SE de la península ibérica con interés
potencial como materias primas cerámicas: aplicación del análisis estadístico multivariante
para su clasificación”, L. Morales Hernández, E. Garzón Garzón, I. Gador García Rodríguez, A.
Ruiz Conde, P.J. Sánchez Soto. Poster

“Caracterización y catalogación de un plato de loza dorada malagueña”, S. Fernández de Miguel, A. Díez Monsalve, P.J. Sánchez Soto, J. Pascual Cosp. Poster

“Fabricación de soportes cerámicos a partir de diferentes residuos industriales”, J. Pascual Cosp, P.J. Sánchez Soto, J.A. Zapatero Arenzana, A.J. Ramírez del Valle. Poster

“La clonación artística en la conservación-restauración del patrimonio histórico-artístico cerámico y vítreo”, M.A. González Godoy, A. Ruiz Conde, P.J. Sánchez Soto. Poster

1st Spanish national conference on advances in materials recycling and eco
12-13 Noviembre [Madrid, España]

“Processing of mullite-based ceramic composites from metal wastes and by-products of mining”, E. Garzón Garzón, J. Pascual Cosp, A. Ruiz Conde, L. Morales Hernández, P.J. Sánchez Soto. Comunicación oral

Sociedad Española de la Arcillas, Jornada Científica conmemorativa 50 Aniversario
19 Noviembre [Madrid, España]

“Influencia del proceso de biomineralización en las propiedades hidráulicas de dos tipos de suelos”, L. Morales Hernández, E. Garzón Garzón, P.J. Sánchez Soto. Comunicación oral

“Análisis estadístico multivariante de filitas para su aplicación como material ecoeficiente para impermeabilización”, L. Morales Hernández, E. Garzón Garzón, A. Ruiz Conde, P.J. Sánchez Soto. Poster

3.7. CURSOS / COURSES

CURSOS DE POSTGRADO / POSTGRADUATE COURSES

MÉTODOS FÍSICOS DE ANÁLISIS DE CAPAS FINAS Y SUPERFICIES DE SÓLIDOS



Organizado por el Instituto de Ciencia de Materiales de Sevilla

Directores: Dr. Guillermo Munuera y Dr. Juan Pedro Espinós

Fecha de Celebración: 22 al 26 de junio de 2009

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 | Dra. Asunción Fernández

Espectroscopía de Fotoemisión de Rayos X: Composición Superficial | Dr. Guillermo Munuera

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 Manzorro
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
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
Retrodispersión Rutherford | Dr. Javier García
Microscopía de Fuerzas Atómicas | Dr. Carmen López Santos

APLICACIÓN DE LA RADIACIÓN SINCROTRÓN A LA CARACTERIZACIÓN DE MATERIALES



Organizado por el Instituto de Ciencia de Materiales de Sevilla

Directores: Dra. Adela Muñoz Páez

Fecha de Celebración: 30 de septiembre al 2 de octubre de 2009

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** | Dra. Adela Muñoz Páez
- Difracción de Rayos X con Radiación Sincrotrón** | Dr. Carlos Frontera, ICMB, Barcelona
- Espectroscopía de Absorción de Rayos X** | Dr. Jesús Chaboy Nalda, Zaragoza
- Demostración práctica de los métodos de Análisis de Espectroscopía EXAFS** | Dr. Juan Pedro Holgado
- Espectroscopía de Fotoelectrones: Fotoemisión** | Dr. Juan Pedro Holgado Vázquez
- Fotoemisión a Altas Presiones** | Dr. Alfonso Caballero Martínez
- La Línea Española Spline del ESRF. Fotoemisión a Altas Energías** | Dr. Germán Castro, ESRF, Grenoble, Francia
- 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 Estrasburgo, Bélgica
- Microscopía de Rayos X: Principios y Aplicaciones** | Dra. Gema Martínez Criado, ESRF, Grenoble, Francia
- La línea BM16 del ESRF, Una estación multidisciplinar para la Comunidad Española** | Dra. A. Labrador, ESRF, Grenoble, Francia
- La Fuente de Luz Sincrotrón "ALBA". Estado de la Fuente y Líneas en Construcción** | Dra. Virginia Pérez Dieste, ALBA, Barcelona

DETERMINACIÓN DE ESTRUCTURAS EN SÓLIDOS REALES: TÉCNICA DE RESONANCIA MAGNÉTICA NUCLEAR



Organizado por el Instituto de Ciencia de Materiales de Sevilla

Directores: Dra. María Dolores Alba Carranza

Fecha de Celebración: 7 al 11 de septiembre de 2009

Horas lectivas: 15 horas teórica + 15 horas prácticas

Dirigido a: Licenciados o alumnos de los últimos cursos

Este curso pretende suministrar los conocimientos básicos para el estudio de los sólidos reales a través de una técnica que informa acerca del orden local de los átomos de la red. Para ello, se hará una breve introducción teórica de los sólidos reales, haciendo hincapié en aquellos aspectos estructurales que demandan el empleo de técnicas instrumentales que aporten información a corto alcance.

Además, se darán los principios básicos en los que se basa la resonancia magnética nuclear que irán acompañados de una colección de problemas. Por último, se plantearán las dificultades mostradas por esta técnica en su aplicación al estado sólido en función de la naturaleza del núcleo a estudiar. Las secciones prácticas incluirán el uso del equipo para resolver casos prácticos sencillos y el empleo del paquete informático apropiado para el procesado y tratamiento matemático de los espectros.

Introducción | Dra. María Dolores Alba Carranza
Conceptos Básicos | Dr. 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 $\frac{1}{2}$ Abundantes | Dr. Miguel Angel Castro Arroyo
RMN de Sólido de Núcleos con Espín $\frac{1}{2}$ Poco Abundantes | Dr. Jesús Sanz
RMN de Sólido de Núcleos con Espín mayor de $\frac{1}{2}$ | Dra. Teresa Blasco
RMN de Sólido de Núcleos con Espín $\frac{1}{2}$ 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. M^a 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. María 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



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

Física 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 Caba-llero | 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 Ga-llardo 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

OTROS / OTHER

XRD non-ambient & DIFFRAC^{PLUS} at Institutos y Servicios de Investigación CITIUS

Director: Dr. Miguel Angel Castro Arroyo

Profesores: Dra. María Dolores Alba, Dra. Ana Isabel Becero Nieto, Ldo. Pablo Chain, Ldo. Juan Isidro Corredor, Dr. Alberto Escudero, Lda. Esperanza Pavón

Fecha de Celebración: 30 marzo – 1 abril 2009

Organizado por la Universidad de Sevilla

Curso de Postgrado Interuniversitario “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

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)

■ 3.8. CONFERENCIAS INVITADAS IMPARTIDAS POR PERSONAL DEL ICMS INVITED CONFERENCES BY PERSONNEL OF THE ICMS

- 20 de enero **Modelling the dipolar interactions between superparamagnetic nanoparticles in nanocrystalline alloys**
Victorino Franco
Lugar: Nanyang Technological University, Singapur, República de Singapur
- 24 de enero **Field dependence of the magnetocaloric effect in second order phase transition: from Physics to applications for the characterization of materials**
Victorino Franco
Lugar: Nanyang Technological University, Singapur, República de Singapur
- 6 de febrero **Magnetic anisotropy in soft magnetic nanocrystalline alloys**
Victorino Franco
Lugar: Nanyang Technological University, Singapur, República de Singapur
- 14 de mayo **Synthesis and characterization of $Ce_{1-x}Eu_xO_{2-x/2}$ mixed oxides and their catalytic**
Willinton Yesid Hernández Enciso
Lugar: Université Catholique de Louvain. Louvain-la-Neuve, Bélgica
- 21 de mayo **Síntesis y propiedades ópticas de nanopartículas luminiscentes uniformes basadas en fluoruros de tierras raras**
Manuel Ocaña Jurado
Lugar: Facultad de Ciencias, Universidad Autónoma de Madrid
- 27 de mayo **Gold catalysts based on modified CeO_2 employing transition metals (Zr, Zn, Fe) for CO oxidation reactions (WGS-PROX)**
Oscar Hernando Laguna
Lugar: Chemical Engineering and Technology. Estocolmo, Suecia
- 4 de septiembre **The magnetocaloric effect of soft magnetic alloys: can we predict the response of a material?**
Victorino Franco
Lugar: University of South Florida. Tampa, Estados Unidos de América
- 22 de octubre **Diseño de instrumentación con control inteligente de temperatura por la propia muestra: Aplicaciones a la síntesis y sinterización de materiales**
José Manuel Criado Luque
Lugar: University de Chile, Santiago, Chile

- 9 de noviembre **Tribological behaviour of titanium carbide/amorphous carbon nano-composite coatings**
 Juan Carlos Sánchez López
 Lugar: Ecole Centrale de Lyon, Francia
- 10 de noviembre **Nanostructured materials or how to control material properties? A microstructural-chemical and functional approach**
 Juan Carlos Sánchez López
 Lugar: INSA, Lyon, Francia
- 19 de noviembre **The magnetocaloric effect of soft magnetic alloys: can we predict the response of a material?**
 Victorino Franco
 Lugar: Carnegie Mellon University. Pittsburgh, Estados Unidos de América
- 19 de noviembre **Espectroscopía DRIFTS: consideraciones teórico-prácticas**
 Miguel Angel Centeno Gallego
 Lugar: Universidad Nacional de Colombia. Santa Fé de Bogotá, Colombia
- 20 de noviembre **Synthesis and characterization of Au/doped ceria catalysts for the total oxidation of CO: the case of Au/Ce_{1-x}Eu_xO_{2-x/2}**
 Willinton Yesid Hernández Enciso
 Lugar: Institut für Oberflächenchemie und Katalyse. Ulm, Alemania

■ 3.9. CONFERENCIAS IMPARTIDAS EN EL ICMS CONFERENCES IN THE ICMS

■ CICLO DE CONFERENCIAS / CONFERENCES

10 de junio | **Procesos de oxidación selectiva de metano y etano para la producción de hidrógeno y/o olefinas**

José Manuel López Nieto
Instituto de Tecnología Química (CSIC-UPV)

16 de septiembre | **Acumulación de hidrógeno en sólidos. Desde volumen a lámina delgada**

José Ramón Ares Fernández
Laboratorio de Materiales de Interés en Energías Renovables (MIRE). Departamento de Física de Materiales C-IV. Universidad Autónoma de Madrid

9 de octubre | **Panorama Nacional e Internacional en la Gestión de los Residuos Radioactivos**

Julio Estudillo Pastor
Jefe del Departamento de Coordinación de Proyectos e I+D ENRESA

22 de octubre | **Producción de Energía: Alternativas y Estrategias Catalíticas**

Luis J. Alemany Arrebola
Departamento de Ingeniería Química. Universidad de Málaga

19 de noviembre | **Nanotecnología de Materiales Poliméricos**

José María Kenny
Instituto de Ciencia y Tecnología de Polímeros de Madrid

27 de noviembre | **Nuevos Materiales Fotocatalíticamente Activos**

Marcos Fernández García
Instituto de Catálisis y Petroleoquímica

■ SEMINARIOS / SEMINARS

29 de enero | **Aplicación de materiales porosos en adsorción y catálisis**

Celio Cavalcante Jr.
Vicedirector del Centro de Tecnología de la Universidad Federal de Ceará. Fortaleza, Brasil

13 de abril | **Surface functionalization of materials using Direct Laser Interference Patterning (DLIP) with nanosecond and femtosecond lasers**

Andrés Lasagni

Fraunhofer Institute for Material and Beam Technology. Dresden, Alemania

12 de mayo | **Superhard Nanocomposites: Origin of hardness enhancement, properties and applications**

Stan Veprek

Department of Chemistry. Technical University Munich, Alemania

26 de mayo | **Novel Materials for Energy Efficient Technologies**

Oliver Gutfleisch

Institute for Metallic Materials, IFW Dresden, Alemania

24 de septiembre | **Espectroscopía de Masas**

Empresa TECNOVAC, Tecnología de Vacío, S.L.

30 de octubre | **Applications of nanocomposite metal-containing amorphous carbon films**

José Luis Endrino Armenteros

Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC)

3.10. TESIS DOCTORALES/ DOCTOR DEGREE THESIS

Título: Physico-Chemical research of Cultural Heritage materials using microanalytical methods

Autor: Liz Karen Herrera Quintero

Directores: Angel Justo Erbez y José Luis Pérez Rodríguez

Calificación: Sobresaliente "Cum Laude"

Centro: Universidad de Sevilla

Título: Síntesis y caracterización de materiales cerámicos binarios y ternarios de vanadio en el sistema (V, Ti, C, N)

Autor: Manuel Alberto Roldán

Directores: Concepción Real Pérez y Andrés Ortega Romero

Calificación: Sobresaliente "Cum Laude"

Centro: Universidad de Sevilla

Título: Intercalación y estabilidad de butilamonio y compuestos inorgánicos en el espacio interlamina de vermiculitas

Autor: María del Carmen Jiménez de Haro

Directores: José Luis Pérez Rodríguez

Calificación: Sobresaliente "Cum Laude"

Centro: Universidad de Sevilla

Título: Intercalation of redox active species in Spanish vermiculites
Autor: Verónica Ramírez del Valle
Directores: José Luis Pérez Rodríguez y Anton Lerf
Calificación: Sobresaliente “Cum Laude”
Centro: Universidad de Sevilla

Título: Plasmas de nitrógeno y funcionalización superficial de materiales poliméricos y recubrimientos tipo diamante con aplicaciones biomédicas
Autor: María del Carmen López Santos
Directores: José Cotrino Bautista y Agustín R. González-Elipe
Calificación: Sobresaliente “Cum Laude”
Centro: Universidad de Sevilla

Título: Microestructura y comportamiento termomagnético de aleaciones (FeCo)(NbZr)(GeB) obtenidas por molienda
Autor: Jhon J. Ipus Bados
Directores: Alejandro Conde Amiano y Javier S. Blázquez Gámez
Calificación: Sobresaliente “Cum Laude”
Centro: Universidad de Sevilla

■ 3.11. PREMIOS Y RECONOCIMIENTOS/PRIZES AND ACKNOWLEDGEMENTS

Premio Extraordinario de doctorado 2008 de la Universidad de Sevilla a Leidy Marcela Martínez Tejada.

Premio a Investigadores Noveles en el Área de Física Experimental 2008 de la Real Sociedad Española de Física y Fundación BBVA a Javier S. Blázquez Gámez

Premio a Investigadores Jóvenes de la Real Academia Sevillana de Ciencias y Real Maestranza de Caballería de Sevilla 2009 a Javier S. Blázquez Gámez

COOPERACIÓN CIENTÍFICA SCIENTIFIC COOPERATION

- 4.1.** Cooperación Internacional y otros
International cooperation and others
- 4.2.** Unidades Asociadas
Associated units
- 4.3.** Estancias de personal del ICMS en otros
centros
Personnel of the ICMS in
other laboratories
- 4.4.** Estancias de investigadores en el ICMS
Personnel of other laboratories in the
ICMS



■ 4.1. COOPERACIÓN INTERNACIONAL Y OTROS INTERNATIONAL COOPERATION AND OTHERS

Bulgaria/Bulgary

Spectroscopic and catalytic characterization of supported gold catalysts: mechanistic investigation of the Nature of the active sites | M.A. Centeno

Código: 2007BG0010
Organismo Financiador: CSIC – Academia de Ciencias Búlgara
Periodo: 2008-2009

Estados Unidos de América

Third directionally solidified eutectic ceramics workshop | J. Martínez Fernández

Código: FA2386-09-1-1037
Organismo Financiador: Air Force Office of Aerospace R&D
Periodo: 2009-2010

Portugal

New multifunctional coatings for load-bearing biomedical applications | J.C. Sánchez López, M.D. Abad, S. El Mrabet, V. Godinho, C. Lopez-Cartes

Código: 2007PT0043
Organismo Financiador: CSIC – FCT
Periodo: 2008-2009

Reino Unido / United Kingdom

Tribological properties of carbon-based nanostructures | J.C. Sánchez López, M.D. Abad, E. Guerrero, T.C. Rojas, A. Fernández

Código: 2007GB0014
Organismo Financiador: CSIC – Royal Society
Periodo: 2008-2009

4.2. UNIDADES ASOCIADAS / ASSOCIATED UNITS

LABORATORIO DE MATERIALES Y SUPERFICIES / LABORATORY OF MATERIALS AND SURFACES

La Junta de Gobierno del CSIC, en su reunión de fecha 28 de marzo de 2000, aprobó la propuesta de reconocimiento de la Unidad Asociada denominada **“Laboratorio de materiales y superficies”** de los Departamentos de Física Aplicada I (Facultad de Ciencias) e Ingeniería Civil de Materiales y Fabricación (E.T.S.I.I.) de la Universidad de Málaga a través del Instituto de Ciencia de Materiales de Sevilla.

El responsable de esta Unidad Asociada, por parte de la Universidad de Málaga es el Dr. José Pascual Cosp, Profesor Titular de la Universidad de Málaga, y por parte del C.S.I.C. en el Instituto, es el Dr. Luis A. Pérez Maqueda.

Las dos líneas principales de actuación son:

“Desarrollo de sistemas de fabricación de láminas delgadas de circonia por spray pirólisis, termoproyección y spray-plasma”

“Fabricación de materiales cerámicos compuestos a base de mullita-alúmina y/o de aluminato de calcio por reciclaje de residuos procedentes de la actividad minero-metalúrgica”

Las acciones propuestas destacan por su carácter multidisciplinar dentro del área de Ciencias de Materiales. En ella es necesario la participación de físicos, químicos especialistas en síntesis y en diversas técnicas experimentales de caracterización de las propiedades de superficie y de transporte de las capas formadas, así como de ingenieros para el estudio del comportamiento mecánico y termomecánico.

The CSIC’s Board of Governors, in its meeting from the 28th March 2000, passed the proposal to recognize the Associated Unit titled **“Laboratory of materials and surfaces”**, of the University of Malaga’s Departments of Applied Physics I (Faculty of Sciences) and Civil Engineering of Materials and their Production (E.T.S.I.I.), through the Material Science Institute of Sevilla.

The person in charge of this Associated Unit is Dr. José Pascual Cosp from the University of Malaga and Dr. Luis A. Pérez Maqueda from the CSIC’s Institute.

Its two main lines of working are:

“Development of systems for making zirconia thin films by spray pyrolysis, thermoprojection and plasma-spray”

“Making of ceramic materials composed by mullite-alumina and/or calcium aluminate recycling residues coming from mining-metallurgical activity”

The proposed actions are outstanding for its multidisciplinary character in the area of Materials Science. In this area it’s necessary the participation of Physics, Chemists specialised in synthesis and in different characterization experimental techniques of the surface and transport properties of formed films, as well as of Engineers for the study of mechanical and thermomechanical behaviour.

GRUPO DE FOTOCATÁLISIS Y ELECTROQUÍMICA APLICADA AL MEDIO AMBIENTE **LABORATORY OF PHOTOCATALYSIS AND ELECTROCHEMISTRY APPLIED TO THE ENVIRONMENT**

La Junta de Gobierno del CSIC, en su reunión de fecha 22 de diciembre de 2004, aprobó la propuesta de reconocimiento de la Unidad Asociada denominada **“Grupo de Fotocatálisis y Electroquímica aplicada al Medio Ambiente”** de la Universidad de Palmas de Gran Canaria a través del Instituto de Ciencia de Materiales de Sevilla.

El responsable de esta Unidad Asociada, por parte de la Universidad de Las Palmas de Gran Canaria es el Prof. Jesús Pérez Peña, Catedrático de la Universidad de las Palmas de Gran Canaria, y por parte del C.S.I.C en el Instituto, es el Dr. José Antonio Navío Santos, Catedrático de la Universidad de Sevilla.

Las líneas principales de actuación son:

- “Fotocatálisis en procesos ambientales”**
- “Espectro-electroquímica aplicada al medio ambiente”**
- “Materiales para tratamientos de aguas residuales”**

Entre las acciones propuestas destacar los objetivos de preparación de nuevos materiales fotocatalizadores, así como la caracterización de los mismos y su estudio en aplicaciones de fotocatalisis solar para descontaminación y tratamiento de aguas residuales.

The CSIC’s Board of Governors, in its meeting from the 22nd December 2004, passed the proposal to recognize the Associated Unit titled **“Laboratory of Photocatalysis and Electrochemistry Applied to the Environment”**, of the University of Las Palmas de Gran Canaria through the Material Science Institute of Seville.

The person in charge of this Associated Unit is Prof. Dr. Jesús Pérez Peña from the University of Las Palmas de Gran Canaria and Dr. José Antonio Navío Santos from the CSIC’s Institute.

The main research lines of working are:

- “Photocatalysis for environmental processes”**
- “Spectroscopical-electrochemistry applied to environment”**
- “Natural processes for the treatment of waste water”**

Among the proposed actions we may emphasize the objectives of preparation of new photocatalysts materials, their characterisation and the study of their applications in solar photocatalysis and treatment of waste water.

4.3. ESTANCIAS DE PERSONAL DEL ICMS EN OTROS CENTROS PERSONNEL OF THE ICMS IN OTHER LABORATORIES

Servicios Centrales de la Universidad de Cádiz		
Purto Real, Cádiz, España	Dra. T. Cristina Rojas Ruiz	[2 días]
Institut für Oberflächenchemie und Katalyse, Universität Ulm		
Ulm, Alemania	Ldo. Willinton Yesid Hernández	[2 días]
Instituto de Ciencia de Materiales de Madrid		
Madrid, España	Lda. Emilie Deprez	[1 semana]
	Dr. Miguel Ángel Márquez	[1 semana]
Institute of General and Inorganic Chemistry. Bulgarian Academy of Sciences		
Sofia, Bulgaria	Dr. Miguel Angel Centeno Gallego	[1 semana]
	Dra. Francisca Romero Sarriá	[1 semana]
GKSS Forschungszentrum		
Geetshacht, Alemania	Lda. Emilie Deprez	[1 semana]
Centro de Ingeniería de Superficies, AIN		
Pamplona, España	Dr. David Philippon	[1 semana]
Universidad Nacional		
Bogotá, Colombia	Dr. Miguel Angel Centeno Gallego	[1 semana]
University of Colorado at Boulder		
Colorado, Estados Unidos de América	Dr. Luis A. Pérez Maqueda	[2 semanas]
	Dr. Pedro Enrique Sánchez Jiménez	[12 meses]
Instituto de Química del Estado Sólido. Academia de Ciencias Checa		
Rez, República Checa	Dr. Luis A. Pérez Maqueda	[2 semanas]
	Ldo. Antonio Perejón Pazo	[3 meses]
Universidad de Chile		
Santiago de Chile, Chile	Dr. José Manuel Criado Luque	[2 semanas]
	Dra. María Jesús Diánez Millán	[2 semanas]
CATA, Universidad Católica de Lovaina		
Lovain-la-Neuve, Bélgica	Ldo. Willinton Yesid Hernández	[1 mes]
Nanyang Technological University		
Singapur, República de Singapur	Dr. Victorino Franco	[1 mes]
Research Centre Arcelor-Mital		
Liège, Bélgica	Dr. David Philippon	[7 semanas]

NASA Glenn Research Center Ohio, Estados Unidos de América	Dr. Julián Martínez Fernández	[10 semanas]
University of South Florida Tampa, Estados Unidos de América	Dr. Victorino Franco	[2 meses]
Kungliga Tekniska Högskolan (KTH) Chemical Science and Engineering Teknikringe Estocolmo, Suecia	Ldo. Oscar Hernando Laguna Espitia	[2 meses]
Instituto de Tecnología Química Valencia, España	Ldo. Luis Bobadilla Baladrón	[3 meses]

■ 4.4. ESTANCIAS DE INVESTIGADORES EN EL ICMS PERSONNEL OF THE OTHER LABORATORIES IN THE ICMS

University of Cambridge Cambridge, Reino Unido	Andrew E.H. Wheatley	[3 días]
Technische Universität München, TUM Munich, Alemania	Stan Veprek	[3 días]
Institute for Metallic Materials Dresden, Alemania	Oliver Gutfleisch Carine Rongeat	[3 días] [10 días]
Ames Laboratory. Iowa State University Iowa, Estados Unidos de América	V.K. Pecharsky	[1 semana]
Institute of General and Inorganic Chemistry, Bulgarian Academy of Sciences Sofia, Bulgaria	Mihail Mihaylov Elena Ivanova	[10 días] [10 días]
A.F. Ioffe Physico-Technical Institute. Russian Academy of Sciences Rusia	Tatiana S. Orlova	[2 semanas]
NASA Glenn Research Center Ohio, Estados Unidos de América	Mrityunjay Singh	[2 semanas]
Universidades do Minho Guimaraes, Portugal	Sofía Lima Ribeiro	[2 semanas]
INSA-Lyon Lyon, Francia	Philippe Steyer	[2 semanas]

Instituto de Ciencia de Materiales de Madrid Madrid, España	José Luis Endrino Armenteros	[2 semanas]
Instituto de Química Inorgánica Rez, República Checa	Jan Subrt	[2 semanas]
Universidad de Pardubice Pardubice, República Checa	Jiri Malek	[2 semanas]
Bulgarian Academy of Sciences Sofia, Bulgaria	Tatiana Tabakova Vasco Idiakev	[2 semanas] [2 semanas]
UNESP-BOTUCAPU-SP Brasil	Rafael Innocenti Vieira Da Silva Margarida Juri Saeki	[1 mes] [1 mes]
Instituto de Investigaciones en Catálisis y Petroquímica, INCAPE Santa Fé, Argentina	Viviana Guadalupe Milt Mill	[2 meses]
Universidad Nacional de la Plata La Plata, Argentina	Miguel Andrés Peluso	[2 meses]
Universidad Nacional de Antioquia Medellin, Colombia	Biviana Llano Agudelo	[2 meses]

OTRAS ACTIVIDADES OTHER ACTIVITIES



5.1. Actividades de Divulgación Científica Activities for Dissemination of Science



5.1. ACTIVIDADES DE DIVULGACIÓN CIENTÍFICA ACTIVITIES FOR DISSEMINATION OF SCIENCE

Feria de la Ciencia / Fair of Science



La VII Feria de la Ciencia (14, 15 y 16 de mayo de 2009, 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:

“Sol, Agua, Hidrógeno y Energía”

The VII Fair of Science (14, 15, and 16 May 2009, in Seville) constituted a meeting point where many activities for spreading of science and technology were carried out. Demonstrations and experiments were presented to facilitate the understanding of scientific aspects. The Materials Science Institute of Seville presented the activity:

“Sun, Water, Hydrogen and Energy”

Coordinador/Coordinator: Dr. Gerardo Colón Ibáñez

Semana de la Ciencia y la Tecnología Science and Technology Week



Jornadas de puertas abiertas (Semana del 9 al 12 de Noviembre de 2009, 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 (9-12 November 2009). 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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