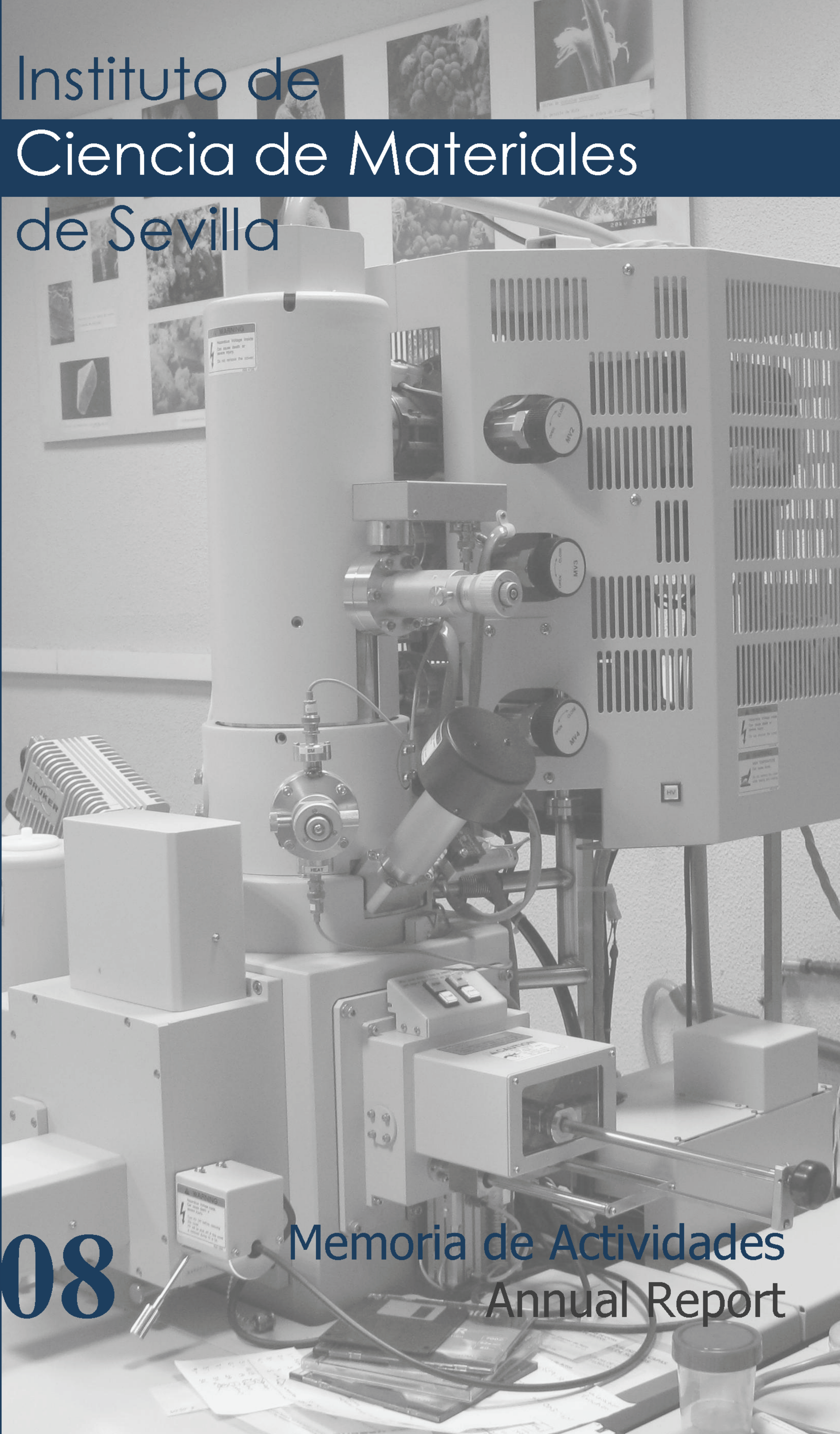
Instituto de Ciencia de Materiales de Sevilla



Consejo
Superior de
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Universidad
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Junta de
Andalucía

2008

Memoria de Actividades
Annual Report

Consejo Superior de Investigaciones Científicas
Universidad de Sevilla
Junta de Andalucía

INSTITUTO DE CIENCIA DE MATERIALES DE SEVILLA

Memoria de Actividades
Annual Report
2008

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DISEÑO
José Carlos Rivero Cabello

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DEPÓSITO LEGAL

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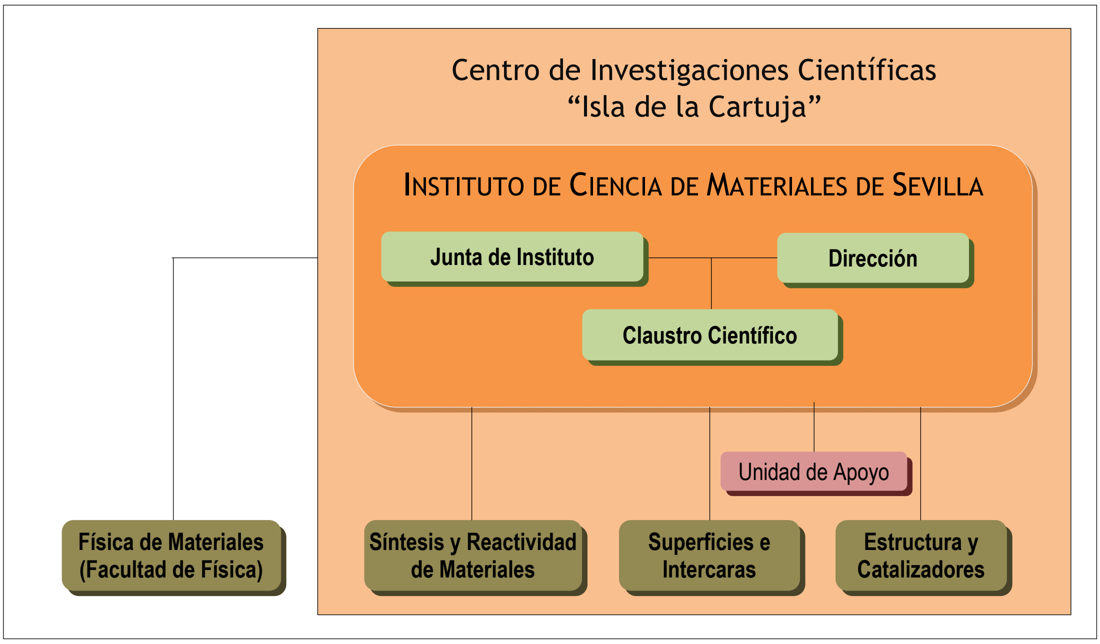

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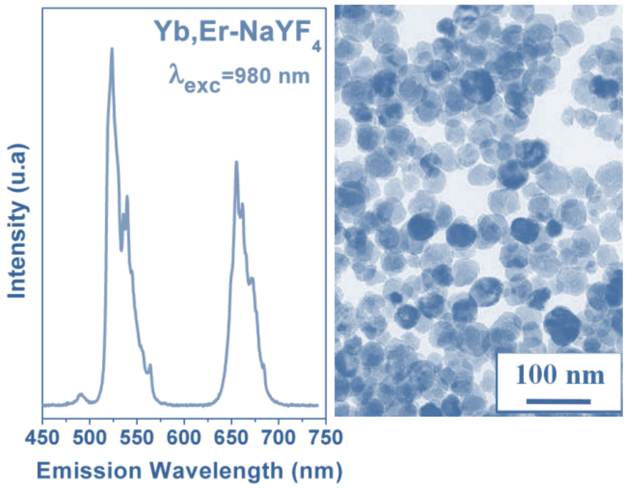

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2.1. Resumen de Actividad Científica Relevante / Highlights

Síntesis de nanopartículas esféricas basadas en $NaYF_4$, con tamaño controlado y luminiscencia “up-conversion”, en medio líquido sin surfactantes ni otros aditivos orgánicos / Synthesis of spherical up-conversion $NaYF_4$-based nanophosphors with tunable size in liquid media without surfactants or capping additives

Es bien conocido que cuando se dopan sólidos de distinta composición con ciertos cationes de tierras raras resultan materiales luminiscentes con importantes aplicaciones en los campos de la biotecnología y optoelectrónica. Entre los sistemas más investigados destacan aquellos basados en NaYF4 porque cuando esta matriz es codopada con cationes erbio e iterbio, se obtiene uno de los más eficientes sistemas con luminiscencia tipo “up-conversion” (UC; emisión de luz visible con longitud de onda menor que la de la radiación de excitación, generalmente infrarroja) conocidos hasta ahora. Debido a esta propiedad, se han sugerido importantes aplicaciones para este tipo de material tales como su uso para láseres de estado sólido, monitores de pantalla plana, biosensores, etc. Esta última aplicación es especialmente interesante pues la radicación de excitación de estos sistemas (infrarroja), es débilmente absorbida por el tejido biológico no causando daños al mismo, lo cual representa una importante ventaja frente a otros sistemas luminiscentes que se excitan generalmente con radiación ultravioleta.

Para la mayor parte de estas aplicaciones se requieren nanopartículas uniformes con tamaño y forma controlados y altamente dispersas. Para obtener estos materiales se han desarrollado diversos procedimientos, la mayor parte de los cuales tienen lugar a alta temperatura (200-300ºC) y conllevan el uso de disolventes orgánicos tóxicos (trioctilfosfina óxido) o de alto punto de ebullición (octadeceno, octilamina), agentes complejantes y surfactantes.

El grupo de Nanomateriales Ópticos del ICMSE ha desarrollado un método muy simple que posibilita la síntesis de nanopartículas esféricas uniformes de ⍰-NaYF4 codopadas con Yb3+ y Er3+ que presentan luminiscencia UC. El procedimiento se basa en reacciones de precipitación homogénea a temperatura baja (60-120ºC) a partir de disoluciones de fluoruro sódico y precursores adecuados de los iones lantánidos usando mezclas etilenglicol/agua como disolvente, sin adicionar otros agentes complejantes o surfactantes. Esta ruta de síntesis permite controlar el tamaño de partícula en el rango 45-155 nm a través del ajuste de los parámetros de reacción (temperatura y relación etilenglicol/agua). En la micrografía TEM de la Figura 1 se presenta un ejemplo representativo de este material junto con su espectro de luminiscencia obtenido con excitación infrarroja (longitud de onda = 980 nm), en el que se observan bandas de emisión en las regiones verde (525 nm) y roja (655 nm).

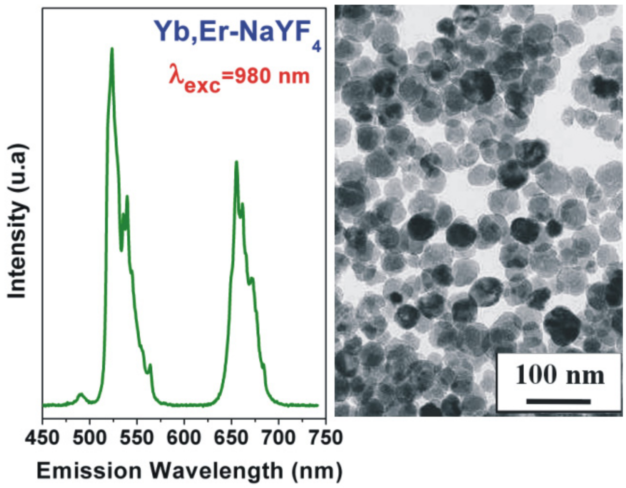
Estos resultados han sido publicados en la revista “European Journal of Inorganic Chemistry” (N.O. Nuñez, et al (2008) 4517) cuyo comité editorial resaltó nuestro trabajo y lo eligió para ilustrar la portada del número en el que fue publicado (Figura 2).

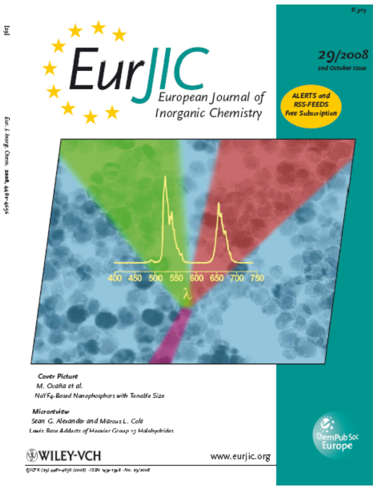
It is well known that when different solids are doped with lanthanide (Ln) ions, interesting luminescent materials are obtained with important applications in the fields of optoelectronic and biotechnology. Among the investigated systems, those based on sodium yttrium fluoride (NaYF4) have been recently the subject of a tremendous attention because this matrix can be co-doped with ytterbium and erbium cations becoming the more efficient up-conversion (UC) phosphor (emission of light with lower wavelength than that of the excitation radiation) known up today. Owing to this property, many promising uses have been suggested for these systems such as solid-sate lasers, flat-panel displays and biological labelling, to mention a few. Particularly advantageous is the use of the NaYF4-based UC nanophosphors as bioprobes mainly because the low energy IR light is weakly absorbed by the biological tissue causing no damage in biological samples.

For many of these applications the availability of uniform nanoparticles with controlled size, shape and good dispersiblity is highly desirable. To obtain these materials, several rather sophisticated approaches have been developed most of which involve the use of very toxic (trioctylphosphine oxide) and/or high boiling point (octadecene, octylamine) organic solvents, complexing agents and surfactants and/or high reaction temperatures (200-300ºC).

The group of Optical Nanomaterials of the ICMSE has developed an alternative and very simple route for the synthesis of spherical UC β-NaYF4-based nanophosphors based on a precipitation reaction at rather low temperature (60-120ºC) from solutions containing sodium fluoride and appropriated Ln precursors in a common solvent (ethylene glycol/water mixtures), without the use of any other additive (complexing agent or surfactant). The method also permits to control the size of the precipitated particles in the 45-155 nm range through the adjustment of the reaction parameters (temperature and ethylene glycol/water ratio). An example of these up-converting materials is shown in the TEM picture of Fig. 1 along with its corresponding emission spectrum obtained with IR (980 nm) excitation, which shows bands centred at the green (525 nm) and red (655 nm) regions.

These results have been published in European Journal of Inorganic Chemistry (N.O. Nuñez, et al (2008) 4517). The editorial office of this journal has highlighted our paper as a featured article which was chosen to illustrate the cover of the issue in which it was published (figure 2).





COMPORTAMIENTO TRIBOLÓGICO DE RECUBRIMIENTOS NANOCOMPOSITE DE CARBURO DE TITANIO CON CARBONO AMORFO (TiC/a-C) / TRIBOLOGICAL BEHAVIOR OF TITANIUM CARBIDE/AMORPHOUS CARBON NANOCOMPOSITES COATINGS (TiC/a-C)

El comportamiento tribologico de recubrimientos en forma de nanocomposites de carburo de titanio y carbono amorfo (TiC/a-C) preparado por técnicas de PVD y CVD resulta muy dependiente de la técnica de deposición, las condiciones de síntesis y del test empleadas. A ello ha de sumársele la dificultad existente para comparar entre los resultados publicados debido al diferente modo de describir las propiedades de fricción con respecto a la composición química.

Este trabajo se dedicó al estudio de los factores influyentes en el comportamiento tribológico de nanocomposites TiC/a-C usando una serie de capas finas preparadas por la técnica de magnetron sputtering variando la potencia aplicada a cada blanco (Ti o grafito) [1]. La microestructura evoluciona desde TiC cuasi-policristalino a un nanocomposite formado por nanocristales de TiC dispersos en una matriz de carbón amorfo [2]. El contenido de a-C, que cumple la función de fase lubricante, aparece como un parámetro crucial para controlar las propiedades tribológicas y su cuantificación fue realizada mediante espectroscopia de pérdida de energía de electrones (EELS). Un cambio significativo en el comportamiento tribológico es observado para nanocomposites con un contenido de a-C superior al 60-65 %. El coeficiente de fricción desciende desde 0.6 a 0.1 y las velocidades de desgaste de las capas por un factor 10. El examen de las zonas desgastadas (bola y recubrimiento) por microscopia confocal Raman puso de manifiesto la presencia de óxidos metálicos y compuestos carbonáceos como responsables del comportamiento observado en la fricción (véase tabla resumen en Fig.2). Tres regímenes de fricción diferentes fueron señalados de acuerdo con la modificación química superficial inducida por los tests de fricción: 1) Lubricación por a-C (a-C%>60–65): 2) No lubricante (TiC) y 3) No lubricante (Ti/TiC). Esta explicación fue posteriormente validada por comparación con los numerosos datos reportados en la literatura tras expresarlos en function de las fracciones de fases nanocristalinas y amorfa que eliminaba la aparente dispersión de resultados tribológicos. La determinación de este umbral de a-C% resulta muy util para el diseño a medida de nanocomposites auto-lubricantes y puede servirnos para anticipar el comportamiento tribológico de este tipo de recubrimientos en aplicaciones prácticas dadas.

The tribological behaviour of nanocomposite coatings made of nanocrystalline metal carbides and amorphous carbon (a-C) prepared by PVD/CVD techniques is found to be very dependant on the film deposition technique, synthesis conditions and testing parameters. Moreover, the comparison among literature data results often complicated due to the different way used by the author to report the variation of the friction properties in respect to the chemical composition.

This work was devoted to an assessment of the factors governing the tribological performance of TiC/a-C nanocomposites using a series of films prepared by magnetron sputtering technique varying the power applied to each target (titanium or graphite) [1]. The film microstructure evolved from a quasi-polycrystalline TiC to a nanocomposite formed by nanocrystals of TiC embedded in an amorphous carbon matrix [2]. The content of amorphous carbon, that plays the role of lubricant phase, appeared as a crucial parameter to control the tribological properties and its quantification was assessed by electron energy-loss spectroscopy (EELS). A significant change in the tribological performance is observed for nanocomposites with amorphous carbon phase contents above 60-65 %. The friction coefficient decreases from 0.6 to 0.1 and the film wear rates by a factor of 10. Examination of the wear scars on ball and film surfaces by Raman confocal microscopy allowed to determine the presence of metallic oxides and carbonaceous compounds responsible of the observed friction behaviors (cf. summary table in Fig.2). Three different friction regimes were highlighted according to the surdface-modified composition: 1) a-C lubricated (a-C contents>60–65%): 2) Unlubricated (TiC) and 3) Unlubricated (Ti/TiC). This explanation was later validated by comparing with various data reported in the literature that were revised in terms of nanocrystalline/amorphous fractions allowing to understand the apparent dispersion in the tribological performance. This a-C fraction threshold can be very useful for tailored design of self-lubricant nanocomposites and might anticipate the tribological response in practical applications.

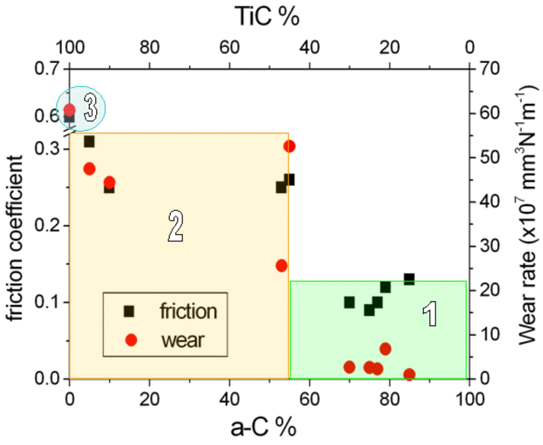
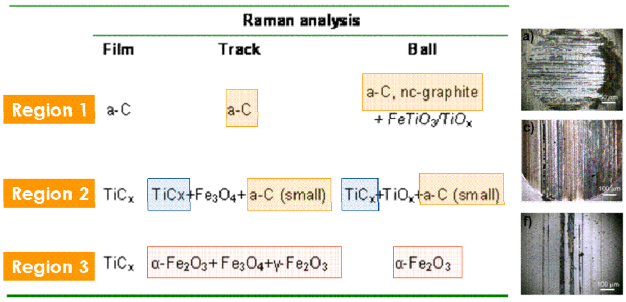


Fig. 1. Variación del coeficiente de fricción y de la resistencia al desgaste en función de la fracciones de carburo y fase amorfa.
Dependence of the friction coefficient and wear rates as a function of the carbide and amorphous fractions.



	Raman analysis		
	Film	Track	Ball
Region 1	a-C	a-C	a-C, nc-graphite + $FeTiO_3/TiO_x$
Region 2	TiC_x	$TiCx+Fe_3O_4+$a-C (small)	TiC_x+TiO_x+a-C (small)
Region 3	TiC_x	α-$Fe_2O_3+Fe_3O_4+\gamma$-Fe_2O_3	α-Fe_2O_3

Fig. 2. Tabla resumen del análisis Raman llevado a cabo en tres huellas de desgaste representativas de cada uno de los regímenes de fricción observados.
Summary table of the Raman analysis carried out on three wear scars representative of each tribological regime.

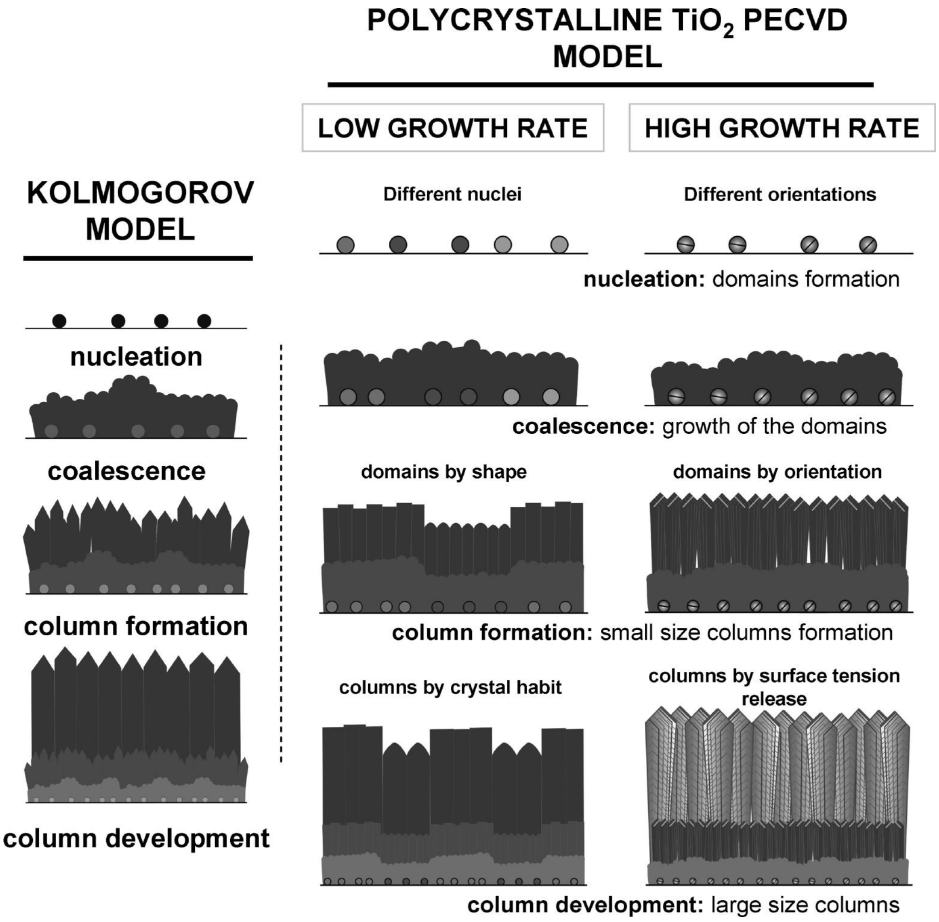
Referencias / References

[1] J.C. Sánchez-López, D. Martínez-Martínez, C. López-Cartes, A. Fernández, Surf. Coat. Technol. 202, 4011-4018 (2008).
[2] D. Martínez-Martínez, C. López-Cartes, A. Fernández, J.C. Sánchez-López. Thin Solid Films 517, 1662–1671 (2009).

GROWTH OF CRYSTALLINE TiO_2 BY PLASMA ENHANCED CHEMICAL VAPOR DEPOSITION (PECVD) / CRECIMIENTO DE TiO_2 CRISTALINO POR MEDIO DE DEPOSICIÓN DESDE FASE VAPOR ASISTIDO POR PLASMA (PECVD)

PECVD es un método fuera del equilibrio y baja temperatura para la preparación de capas delgadas que consiste en la descomposición controlada de un precursor volátil con un plasma. De esta forma se pueden preparar capas delgadas de polímeros, óxidos, nitruros, etc. seleccionando convenientemente el precursor volátil adecuado y las condiciones del plasma. Generalmente, debido a la baja temperatura del proceso, las láminas delgadas que se preparan suelen ser amorfas, pudiendo cristalizar por calentamiento moderado del sustrato. Así, se han obtenido capas delgadas de TiO_2 en su forma cristalina de anatasa por calentamiento a temperaturas de 250 ºC. En el presente trabajo se ha estudiado el crecimiento de capas de anatasa preparadas mediante PECVD, encontrándose que el proceso de crecimiento sigue el modelo de Kolmogorov [1,2], desarrollado para describir la evolución de capas cristalinas a partir de medios homogéneos saturados. Además de describir las distintas etapas del crecimiento cristalino, se ha encontrado que las capas cristalinas de TiO_2 presentan aspectos específicos en función de la velocidad de crecimiento. A bajas velocidades de crecimiento, la capa se forma a través del desarrollo de hábitos cristalinos diferentes cuya formación está controlada por el suministro de material desde el plasma. Para altas velocidades de crecimiento, este no es el factor limitante y se desarrollan facetas que sirven para relajar la tensión superficial del sistema. En el transcurso de esta investigación se ha puesto también de manifiesto que el crecimiento de dominios cristalinos está probablemente controlado por las primeras etapas de nucleación. De acuerdo a nuestro conocimiento esta es la primera vez que se referencia el crecimiento de dominios cristalinos en capas delgadas. La formación de estos dominios puede ser de gran relevancia para diferentes aplicaciones de capas finas de anatasa, por ejemplo, para su uso como superficies autolimpiables o como fotocatalizador, donde la estructura, textura y rugosidad de la superficie son factores primordiales para la actividad de las capas.

PECVD is a non-equilibrium low-temperature method of preparation of thin films consisting of the controlled decomposition of a volatile precursor with a plasma. In this way, thin films of polymers, oxides, nitrides, etc. can be prepared by selecting the appropriate volatile precursor(s) and plasma conditions. Due to the low temperature of preparation, amorphous thin films are usually obtained. Crystallization can occur by heating the substrate during the deposition, being found that the required temperature by PECVD is generally smaller than by other methods of preparation of the thin films. Thus, anatase thin films of TiO_2 can be obtained at temperatures as low as 250 ºC. In the present work we have studied the crystallization of the anatase thin films prepared by PECVD and found that the growth process follows the Kolmogorov's model[1,2] developed to describe the evolution of crystalline films from a saturated homogeneous medium. Besides describing the different stages of crystalline growth, we have found that the formation crystalline films of TiO_2 present some specific features depending on the growing rate of the films. At low growing rates film formation occurs through the development of different crystal habits controlled by the supply of material from the plasma. At high growing rates, this is not the limited step of thin film growth and facets develop in the crystal to release the surface tension. In the course of this investigation, it has been also shown that the growth of microstructural domains is likely controlled by the nucleation stage. As far as we know this is the first time that formation of microstructural domains in thin films is reported. The formation of these domains may be of great relevance for different application of anatase thin films. For instance, by their use as self-cleaning surfaces or as photocatalysts, where the structure, texture, and roughness of the surface are major factors for the performance of the films.



Referencias / References

[1] Kolmogorov, A. N. Dokl. Acad. Nauk SSSR 1949, 65, 681.
[2] Thompson, C. V. Annu. ReV. Mater. Sci. 2000, 30, 159.

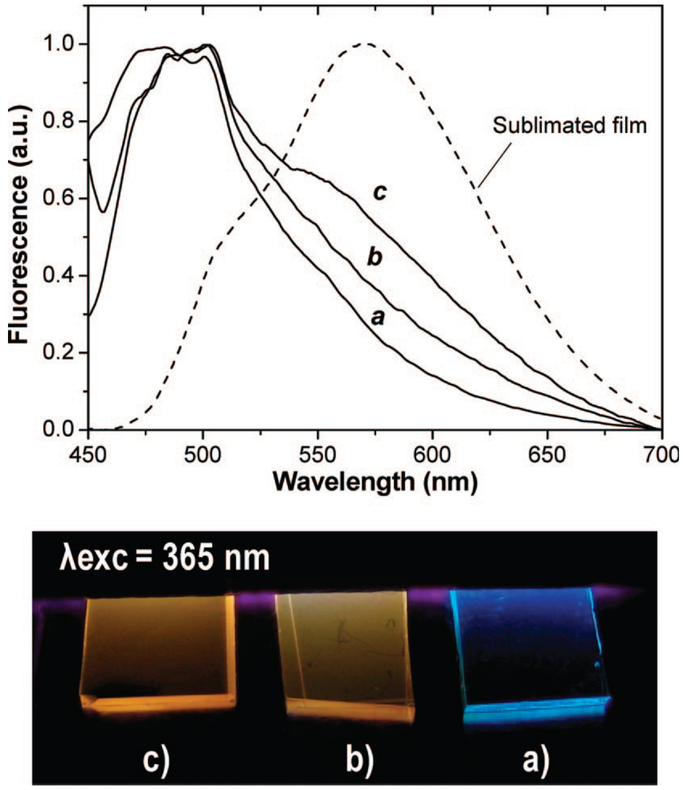
Láminas Delgadas Ópticamente Activas y Luminiscentes Preparadas mediante Polimerización con Plasmas / Optically Active Luminescent Thin Films Deposited by Plasma Polymerization

Se ha desarrollado un nuevo método de preparación de capas delgadas fluoresences que combina la evaporación de moléculas de colorante con su polimerización parcial con la ayuda de un plasma de Ar. Las capas obtenidas son planas, químicamente estables y no dispersan la luz. Dado este conjunto de propiedades, este tipo de capas delgadas son extraordinariamente apropiadas para su integración en dispositivos fotónicos. Un ejemplo de las posibilidades del método se refiere a la preparación de capas delgadas poliméricas de perileno con un espesor de 30-150 nm, su caracterización mediante diferentes métodos y el análisis de sus propiedades ópticas. Estas capas son extraordinariamente absorbentes y muy planas, con una rugosidad cuadras media (rms) en el rango de 0.3-0.4 nm. En comparación con capas obtenidas por sublimación de perileno que presentan una gran dispersión de la luz, las cpaas polimerizadas presentan bandas de absorción bien definidas en el rango de 400-450 nm y el típico espectro de emisión del perileno en torno a 475 nm. Las capas están formadas por una matriz constituida a partir de fragmentos de la molécula de perileno y moléculas intactas que son las que confieren las propiedades ópticas a este material. Las extraordinarias propiedades ópticas y micorestructurales de este material y la posibilidad de crecerlas usando técnicas litográficas las hacen especialmente apropiadas para su integración en componentes fotónicos para diversas aplicaciones. Un estudio preliminar del uso de estas capas como sensores ópticos de NO_2 es una de las posibilidades de usos contempladas.

Otro conjunto de capas fluorescentes de otras moléculas de colorantes se están estudiando en la actualidad.

A new method of preparation of fluorescent thin films has been developed. It combines the evaporation of the dye molecules with their partial polymerization with the aid of an Ar plasma. The films are flat, chemically stable and do not scatter the light. Because of these properties they are suitable for integration into photonic devices. One example of the possibilities of the method refers to the preparation of plasma polymerized thin films of perylene with thicknesses 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. 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 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 NO_2 is also presented.

Other examples of fluorescent thin films of other dye molecules, alone or embedded in a matrix, are under study.



DEPOSICIÓN DE NANOPARTÍCULAS DE AU EN TiO_2 SULFATADO CON MEJORA SUSTANCIAL DE SUS PROPIEDADES FOTOCATALÍTICAS / DEPOSITION OF AU NANOPARTICLES ON SULPHATED TiO_2 WITH SUBSTANTIAL IMPROVEMENT OF THE PHOTOCATALYTIC PROPERTIES

Los procesos de Catálisis Heterogénea realizados sobre nanopartículas de oro soportadas en materiales oxídicos han sido muy estudiados en los últimos años para diferentes aplicaciones, tales como oxidación catalítica a baja temperatura de CO o propeno, reacciones de “water gas shift”, o el incremento de la actividad fotocatalítica del TiO_2. En general, se acepta que las propiedades catalíticas de los sistemas Au/óxido dependen en gran medida del tamaño y distribución de las nanopartículas de oro y de su interacción con el soporte.

En cuanto a las aplicaciones fotocatalíticas de ese sistema, la adición de las nanopartículas de oro se ha venido realizando con la intención de incrementar la fotoactividad del TiO_2, objetivo todavía muy importante en el campo de la fotocatálisis. Las nanopartículas de oro u otros metales nobles depositadas en la superficie del TiO_2 pueden incrementar la eficiencia del proceso fotocatalítico al actuar como colectores de electrones y disminuir la recombinación de electrones y huecos fotogenerados. Por otro lado, el pretratamiento con ácido sulfúrico del TiO_2 estabiliza el área superficial de este óxido previniendo la sinterización y estabilizando la fase anatasa hasta altas temperaturas y generando al mismo tiempo materiales con un alto número de defectos debido a la deshidroxilación durante la calcinación del exceso de protones adsorbidos.

En este trabajo, se ha estudiado la influencia del tratamiento previo de sulfatación del TiO_2 en la estructura, morfología y dispersión del oro depositado en su superficie, así como en las propiedades fotocatalíticas de este sistema. Se evaluaron dos métodos de deposición: fotodeposición y reducción química por citrato. El método citrato produjo partículas de oro más homogéneas y de menor tamaño con una mejor dispersión que el método de fotodeposición (Figura 1), llevando a una mayor mejora de la actividad fotocatalítica para la degradación de fenol tanto en muestras sulfatadas como en no-sulfatadas.

Para ambos métodos de deposición, se alcanzó un mayor incremento de la actividad fotocatalítica por adición de oro en muestras previamente sulfatadas y calcinadas a temperaturas relativamente altas (Figura 2). La dispersión y el tamaño medio de partícula de oro no se vieron influenciados por este tratamiento de sulfatación previa del TiO_2. El incremento de la mejora de la actividad en las muestras sulfatadas con respecto a las no sulfatadas se puede justificar entonces por la mayor fuerza de adsorción y una superior comunicación electrónica entre las partículas de Au y el TiO_2 que se produce en superficies con gran número de defectos y vacantes de oxígeno como son las superficies sulfatadas después de ser calcinadas a 700ºC.

En este estudio, se ha mostrado que la combinación de tratamiento con sulfatos del TiO_2 y la deposición de Au por el método citrato es un magnífico procedimiento para obtener partículas de oro de tamaño homogéneo y gran dispersión con una fuerte adsorción e interacción con el soporte. Este sistema posee unas magníficas propiedades fotocatalíticas pero igualmente podría ser un excelente sistema extendido a otras áreas de la catálisis realizada con oro soportado.

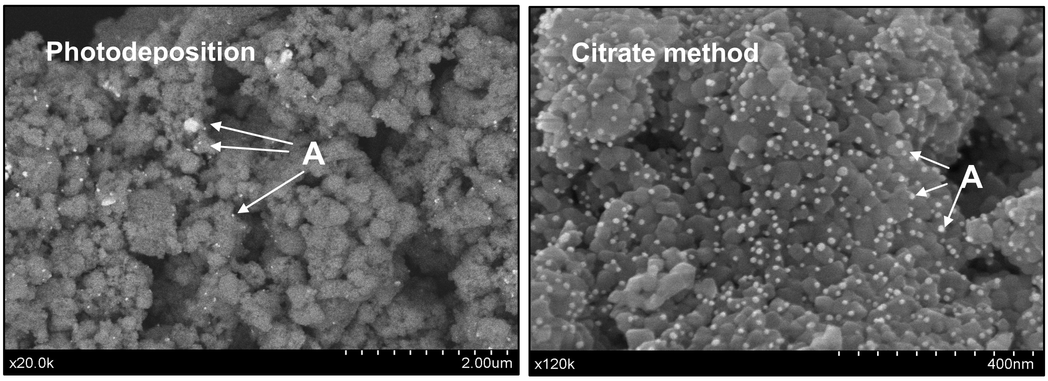


Fig. 1

Heterogeneous catalysis performed by gold nanoparticles supported on oxidic materials has been widely studied in the last years for many different applications; such as low temperature catalytic oxidation of CO or propene, water gas shift reactions or promotion of the photocatalytic activity of TiO_2. In general, it is accepted that the catalytic properties of Au/oxide catalysts depend highly on the size and distribution of gold nanoparticles and on the interaction between the metal and the support.

Regarding photocatalytic applications, the addition of gold nanoparticles has been studied with the intention of increasing the photoactivity of TiO_2, which continues to be an important objective of research in the field of photocatalysis. Gold nanoparticles and other noble metals deposited on the TiO_2 surface have been reported to increase the efficiency of the photocatalytic process by acting as electron sinks and decreasing the recombination rate of the photogenerated charges. On the other hand, sulphuric acid pre-treatment of TiO_2 stabilises TiO_2 surface area against sintering and anatase crystalline phase until calcination temperatures as high as 700ºC generating at the same time highly defective materials through the dehydroxylation process of the excess of adsorbed protons during calcination.

In this work, the influence of sulphated pre-treatment of TiO_2 on the structure, morphology and dispersion of gold as well as on the photocatalytic properties of Au/TiO_2 was studied. Two different methods for gold deposition were evaluated, photodeposition and chemical reduction by citrate. The citrate method showed more homogeneous and smaller gold particles with a better dispersion than photodeposition (Figure 1), leading to a higher improvement of the photocatalytic activity for phenol degradation for both series, sulphated and not sulphated.

For both deposition methods, a high promotion of the photocatalytic activity of TiO_2 was reached by addition of gold and a previous sulphate treatment followed by calcination at relatively high temperature (Figure 2). Gold particle average size and dispersion were not influenced by the sulphated pre-treatment of the TiO_2. The much higher improvement in the activity of pre-sulphated samples compared to non-sulphated ones is ascribed to the stronger bonding and superior electronic communication between the gold particles and the TiO_2 surface on highly defective surfaces as sulphated surfaces are after calcination at 700ºC.

In this study, it has been shown that the combination of sulphate pre-treatment of TiO_2 and gold deposition by the citrate method is a good procedure for obtaining gold particles of homogenous size and dispersion with a strong bonding and interaction between the gold particles and the TiO_2 surface. This system appears to have very good properties for photocatalytic applications; but likewise it could result as an excellent system extended to other areas of catalysis by supported gold.

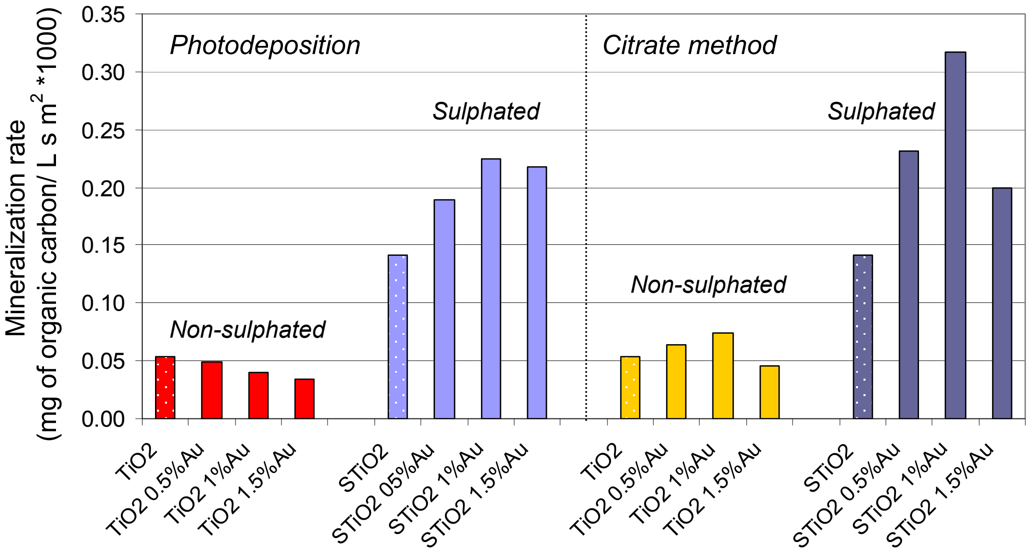


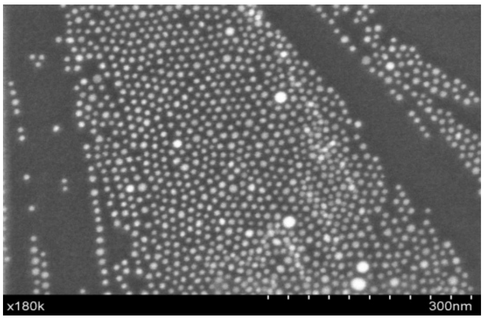
Fig. 2

CARACTERIZACION MEDIANTE ESPECTROSCOPIA DE FOTOEMISION A PRESION AMBIENTAL (APPES) DE NANOPARTICULAS DE Au-Ni DEPOSITADAS EN CERIA

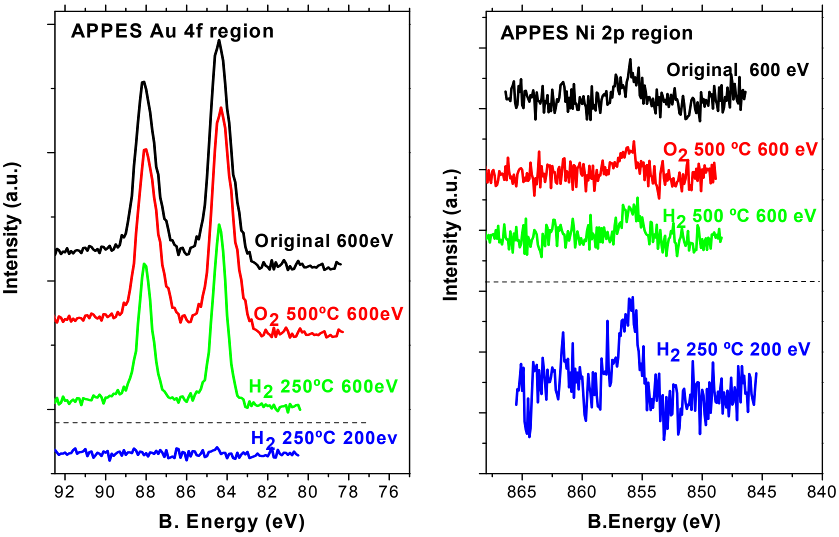
AMBIENT PRESSURE PHOTOEMISSION SPECTROSCOPY (APPES) CHARACTERIZATION OF Au-Ni NANOPARTICLES DEPOSITED IN CERIA

En este trabajo se han preparado una serie de nanoparticulas (NPs) de Au, Ni y Au-Ni siguinedo un procedimiento descrito previamente en la bibliografía. Estas NPs se han depositado en un soporte de CeO_2 (contenido metálico total del 2% atomico).

Los resultados obtenidos en la reacción de oxidación catalítica de CO muestran que, como era de esperar, el sistema Au/CeO_2 presenta unas mejores prestaciones catalíticas que el monometílico de Ni/CeO_2. Sin embargo, el sistema catalítico bimetálico $Au\text{-}Ni/CeO_2$ presenta una actividad superior, lo cual es una indicación d ela existencia de algún tipo de interacción (electrónica o estructural) entre ambos metales.



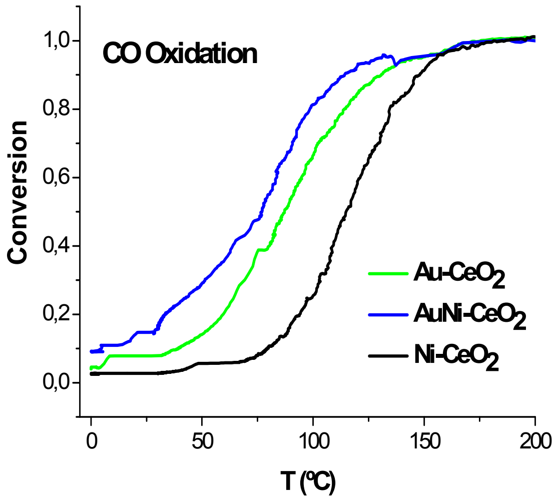
Los resultados obtenidos mediante espectroscopia de fotoemisión a presión ambiental (APPES) muestran sin lugar a dudas que el oro y el niquel se encuentan asociados, formando partículas bimetálicas. El uso de dos valores diferentes para la energía de los fotoelectrones generados durante el proceso de fotoemisión (200 y 600 eV) nos ha permitido analizar las muestras con diferentes resoluciones en profundidad. Asi, mientras la señal Ni 2p es similar en ambos casos, la region Au 4f depende drásticamente de la energía de excitación utilizada. Como se observa en la figura, cuando se utilizan fotoelectrones de 200eV no se detecta la presencia de oro en la muestra, lo que es una indicación de que este metal no se encuentra expuesto en la superficie, y es por tanto una evidencia de que las nanoparticulas presentan una estructura “core-shell”, con el oro en el centro de las mismas y el niquel expuesto en la superficie.



De acuerdo con los resultados en la reacción de oxidación de CO, el catalizador Au-Ni/CeO2 presenta la mayor actividad. Dado que la superficie de las NPs están enriquecidas en niquel, el oro del interior de estas partículas debe estar modificando electronicamente estos átomos de niquel, dando lugar a partículas más activas que las correspondientes monometálicas.

Nanoparticles (NPs) of Au, Ni and Au-Ni have been prepared according to a method previously described in the bibliography, and deposited on a CeO2 powder support (total content of metal of 2 atomic %).

The catalytic data for the CO oxidation reveals that, as expected, the Au/CeO2 system has a better performance than the monometallic Ni/CeO2 catalyst. However, the bimetallic Au-Ni/CeO2 system shows a higher activity, which must be taken as an indication of some kind of interaction (electronic or structural) between both metals.



The results obtained by in situ APPES spectroscopy have shown as gold and nickel are associated forming bimetallic entities. The use of two different values for the photoelectrons generated by the photoemission process (200 and 600 eV) allows us to analyze the samples at different deepness. So, while the Ni 2p signal is similar in both cases, the Au 4f region changes dramatically when the photoelectrons energy changes from 600 to 200 eV. As no gold can be detected at 200 eV, this result is a clear evidence of a Au(core)-Ni(shell) structure of the NPs.

According to the catalytic performances results in the CO oxidation reaction, the catalyst presents the higher activity, even better than the gold monometallic one. As the bimetallic particles are nickel-enriched at the surface, this clearly shows that the core-located gold modifies electronically the nickel at the surface of the NPs. As a result, the catalytic performance of this surface nickel is better than both monometallic.

Referencias / References

- Yin, Y.; Alivisatos, A.P. Nature 2005. 437, 664-670.
- M. Haruta, T. Kobayashi, H. Sano, N. Yamada, Chem. Lett. 2 (1987) 405.
- D. Astruc, F. lu, and J.R. Aranzaes, Angew. Chem. Int. Ed. 44 (2005) 7852-7872.
- H. Winnischofer, T. C. R. Rocha, et al. ACS Nano, 2008, 2(6), 1313-1319
- VM.Gonzalez-DelaCruz, J.P.Holgado, R.Pereñiguez, A.Caballero; J. Catal. 257, 2008, 307-314

CATALIZADORES DE ORO SOPORTADO EN DIÓXIDO DE TITANIO: COMPARACIÓN ENTRE LA OXIDACIÓN FOTOQUÍMICA DE FENOL Y LA OXIDACIÓN DE CO EN FASE GAS / TITANIA-SUPPORTED GOLD CATALYSTS: COMPARISON BETWEEN THE PHOTOCHEMICAL PHENOL OXIDATION AND GASEOUS CO OXIDATION

En los últimos años, el número de contribuciones cinéticas centradas en los estudios de catalizadores conteniendo oro, ha crecido considerablemente debido, fundamentalmente, a su alta actividad y relativa baja temperatura en un gran número de diferentes reacciones catalíticas, en particular de oxidaciones. Aunque la mayoría de las reacciones referenciadas son procesos en fase gas, el empleo de catalizadores de oro en oxidaciones en fase líquida es sin embargo mucho más reciente. Dentro del amplio número de catalizadores estudiados, aquellos que usan el TiO2 como soporte son los más numerosos. De otra parte, como foto-catalizadores heterogéneos, el sistema Au/TiO2, ha sido, recientemente, objeto de interés, como una vía para incrementar la actividad foto-catalítica del TiO2.

Dentro de este contexto, se ha preparado, por el método de deposición-precipitación, una serie de muestras de Au/TiO2 con contenidos nominales de oro comprendidos en el intervalo 0.11%-1.26%. Las muestras preparadas han sido caracterizadas por diferentes técnicas como XRD, SBET, XRF, TEM, XPS y DR UV–Vis y su actividad catalítica ha sido estudiada en dos procesos diferentes: la oxidación en fase gas de CO y la degradación foto-catalítica de fenol en agua. Los resultados de estos estudios para cada una de las reacciones referidas, ha mostrado que la actividad catalítica de los sólidos depende del contenido nominal de oro (Fig. 1). Además de este hecho, el tamaño de partícula juega un papel determinante en la actividad catalítica para la reacción de oxidación de CO pero, aparentemente, no parece influir considerablemente en el proceso foto-catalítico para la reacción de degradación de fenol. De otra parte, las propiedades electrónicas de los sólidos estudiados, evaluadas por los valores estimados de energías de los “band-gap”, indican que éste si parece ser un parámetro fundamental en la actividad foto-catalítica (Fig.2) no ejerciendo, sin embargo, una clara influencia en la reacción de oxidación de CO.

En resumen (ref.1) se puede decir que para la oxidación en fase gas de CO, la actividad catalítica es una función del tamaño de partícula y del contenido nominal de oro, siendo el efecto del tamaño de partícula más importante para bajos contenidos de oro. Sin embargo, para la reacción de oxidación foto-catalítica de fenol, el incremento considerable que ejerce el oro sobre la actividad parece producirse principalmente por contribución de las partículas más pequeñas (<3 nm) depositadas en la superficie del TiO2. En este caso, la actividad foto-catalítica depende de los valores de los “band-gap”, y en particular del contenido de oro.

In the latest years the number of works focussed on gold-containing catalysts has increased exceptionally, due to their very high activity at low temperature in a large number of different catalytic reactions, in particular, oxidation ones. Althought most of the catalytic reactions reported are gaseous ones the use of gold catalysts in catalytic liquid phase oxidations is more recent. Among the large number of gold catalysts tested, those using TiO2 as support are majority. Additionally, as heterogeneous photocatalysts, gold supported on titania, has been subject of a recent interest as an efficient way to enhance the photocatalytic activity of TiO2.

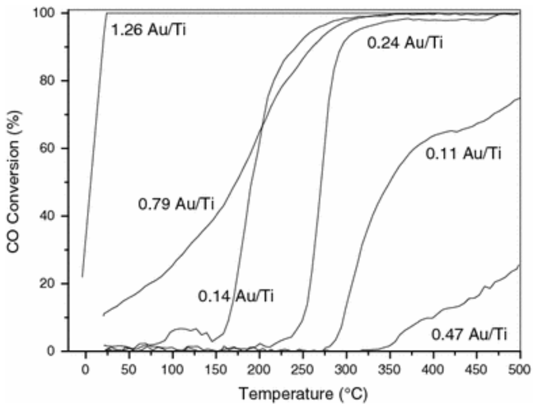


Fig. 1. CO conversion versus temperature for the studied catalysts

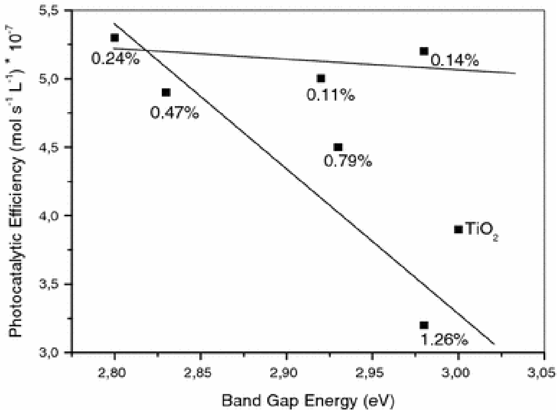


Fig. 2 Phenol photodegradation rate as a function of the band gap of the studied solids

With this in mind a series of Au/TiO2 samples with gold loadings ranging from 0.11% to 1.26% have been prepared by deposition–precipitation, characterised by means of XRD, SBET, XRF, TEM, XPS and DR UV–Vis techniques and tested in the gaseous CO oxidation and photocatalytic degradation of phenol in aqueous media. The catalytic performances of the solids on both reactions depend on the gold content (Fig.1). Besides this, the gold particle size plays a determinant role in the catalytic activity for the CO reaction, but apparently its influence on the photocatalytic activity appears to be negligible and only very small gold particles seem to participate on the photocatalytic process. On the other hand, the electronic properties of the solids, measured by its band gap energy, are a key factor in the photochemical activity (Fig.2) but do not have a clear influence in the CO oxidation reaction.

In summary (ref. 1) for the CO oxidation reaction, the catalysts activity is a function of the gold particle size and gold content, being the effect of the particle size more important at low gold coverage. However, for the photochemical phenol oxidation, the enhancement effect of gold seems to be produced mainly by the small gold particles (<3 nm) deposited on the surface of titania with independence of the size of bigger particles. The photocatalytic activity is then depending on the band gap value of the solid and especially on the gold loading.

Referencias / References

- M. A. Centeno, M. C. Hidalgo, M. I. Domínguez, J. A. Navío, J. A. Odriozola, Catalysis Letters 123 (3-4), pp. 198-206

Aplicación de las Espectroscopías de RMN de ^{29}Si y ^{27}Al al estudio del Mecanismo de transformación de Caolinita en Illita/Moscovita

Application of ^{29}Si y ^{27}Al MAS NMR spectroscopy to the Study of the Reaction Mechanism of Kaolinite to Illite/Muscovite

El grado de transformación de los minerales de la arcilla a illita se emplea frecuentemente como un geotermómetro que permite reconstruir la hitoria termal y tectónica de sedimentos y sistemas hidrotermales activos y fósiles. Con el objetivo de adquirir una visión más completa de la illitización de caolinita en disolución de KOH, se ha realizado un conjunto de experimentos empleando una elevada relación sólido/líquido (1000 mg/mL) mucho más cercana a la esperada en sistemas naturales que la empleada en la bibliografía relacionada. Se ha puesto especial énfasis en los primeros estadíos de la reacción, cuando se están formando los núcleos de illita. La metodología consistió en el tratamiento hidrotermal de caolinita en disolución de KOH a 300ºC y 500 bares de presión externa, empleando diferentes tiempos de reacción. Los experimentos se llevaron a cabo en la Laboratorio hidrotermal instalado en el Bayerisches Geoinstitut (Alemania). La transformación de los entornos de Si y Al se siguió mediante RMN de ^{29}Si y ^{27}AL, respectivamente, que permiten detectar la formación de núcleos incipientes de illita cuando los diagramas de difracción y los espectros de IR sólo muestran láminas de caolinita.

Los diagramas de difracción (XRD) de la Figura 1 indican que sólo tras 13 horas de reacción se forman cristales de illita con tamaño de dominios lo suficientemente grandes como para ser detectados por difracción. Tiempos de reacción inferiores sólo dan lugar a productos con XRD y espectros de IR idénticos a los de la caolinita inicial. No ocurre lo mismo, sin embargo, con los espectros de MAS-NMR, que muestran cambios apreciables tras sólo una hora de tratamiento. Así, el espectro de MAS-NMR de ^{29}Si muestra una nueva contribución a frecuencias superiores a la de la caolinita cuya intensidad aumenta con el tiempo de reacción y cuya posición coincide con la de los entornos Q3(1Al), Q3(2Al), y Q3(3Al). Por lo tanto, tras una hora de reacción, ya hay signos de la presencia de Al en la capa tetraédrica de las láminas de caolinita. La asignación de las nuevas señales que aparecen en los espectros de MAS-NMR de 27Al (Fig. 2) no es tan directa. La señal a 68.8 ppm que se observa en las muestras tratadas durante 13 y 24 horas puede asignarse a Al tetraédrico en las láminas de illita, detectadas mediante XRD. Sin embargo, la asignación de la resonancia a 60 ppm no es tan simple. Una explicación razonable puede encontrarse del hecho observado del desplazamiento a frecuencias más altas de la señal de Al tetraédrico cuando aumenta la sustitución de Si por Al en la capa tetraédrica de las arcillas. Así, la reacción hidrotermal debe inducir la difusión de Al desde la capa octaédrica a la tetraédrica de la caolinita, de manera que a cortos tiempos de reacción habrá difundido una pequeña cantidad de Al cuya señal aparece a 60 ppm, y cuando el tiempo de reacción aumenta la cantidad de Al que sustituye al Si aumenta y la señal del Al se desplaza a frecuencias mayores (68,8 ppm). Estas observaciones indicarían que la primera etapa en la illitización de caolinita implica la difusión de Al desde la capa octaédrica a la tetraédrica. Una explicación alternativa es la formación, concomitante con la illita, de otro silicoaluminato sódico, como la zeolita F (KAlSiO4 hidratado), que presenta una resonancia de Al tetraédrico a esa misma frecuencia. Finalmente, con el fin de formar láminas TOT, debe producirse la condensación de una segunda capa tetraédrica en la lámina TO precursora. Los diagramas de XRD sólo muestra la reflexión de 10.2 Å característica de las láminas TOT de illita tras 13 horas de reacción, tiempo al que se observa una cambio en la relación de intensidades de los picos a 68,8 ppm / 60,0 ppm en el espectro de MAS-NMR de 27Al. Estos hechos parecen indicar que la condensación de una segunda capa tetraédrica requiere un contenido mínimo de Al tetraédrico en la lámina precursora.

The degree of reaction of clay minerals to illite is frequently used as a geothermometer to allow reconstructions of the thermal and tectonic history of sedimentary basins and active and fossil hydrothermal systems. In order to get a more complete overview of the kaolinite illitization, a set of experiments have been carried out in the present study using a high solid/liquid ratio (1000 mg/mL), closer to the natural systems than those used in the related literature. Special emphasis has been put on the first reaction stages, when incipient illite/muscovite nuclei are being formed from kaolinite layers. The methodology followed has consisted of the hydrothermal treatment, at 300ºC and 500 bars external pressure (carried out at the hydrothermal laboratory, Bayerisches Geoinstitut, Germany), of a powdered kaolinite in KOH solution during different times. The transformation of the Si and Al environments has been followed by ^{29}Si and 27Al MAS NMR spectroscopy, respectively, which allow detecting and studying the illite/muscovite nuclei formed at the first reaction stages, when the XRD and IR patterns only show kaolinite layers.

The XRD patterns of Fig.1 indicate that illite/muscovite crystals with domain size big enough as to be detected by diffraction are formed only after 13 hours reaction. At shorter reaction times, the XRD patterns only show reflections of kaolinite. Similar conclusions are obtained from the IR spectra. This is not the case, however, of the ^{29}Si and ^{27}Al MAS NMR spectra, which show appreciable changes even after only 1 hour reaction. Thus, the ^{29}Si MAS NMR spectra show a new broad contribution on the high frequency side of the main kaolinite resonance, whose intensity increases with increasing reaction time, and whose position coincides with that of the Q3(1Al), Q3(2Al), and Q3(3Al) environments. Therefore, after only one hour reaction, there are signs of the presence of Al in the tetrahedral sheet of some kaolinite layers. The assignation of the new signals observed in the ^{27}Al MAS NMR spectra (Fig. 2) at 60.0 and 68.8 ppm is not straightforward. The high frequency ^{27}Al NMR resonance in the spectra of the samples treated for 13 and 24 hours can be assigned to Al in the tetrahedral sheet of the illite/muscovite phase formed as a consequence of the reaction. However, the assignation of the resonance at 60 ppm observed in the spectra of all treated samples is not that simple. A reasonable explanation is obtained from the observed tendency for deshielding at tetrahedrally coordinated Al with increasing substitution of Al for Si in the tetrahedral sheet of layered aluminosilicates. The hydrothermal treatment of kaolinite must induce a diffusion of Al from the octahedral to the tetrahedral sheet of the layers. At short reaction times, the amount of Al that has diffused is expected to be low, and those tetrahedral Al nuclei produce the signal at 60.0 ppm observed in the ^{27}Al NMR spectra of the samples treated during short periods of times (1, 4, and 7 hours); when increasing reaction time, the amount of Al in the tetrahedral sheet increases and the ^{27}Al NMR signal shifts towards higher frequency values. These observations indicate that the first stage in the illitization of kaolinite in the conditions of the present experiments is the diffusion of Al from the octahedral to the tetrahedral sheet of the kaolinite layers. The Al diffusion gives rise to partially transformed kaolinite layers which must be the precursors of the illite/muscovite nuclei. An alternative explanation is the formation of a collateral product, previous to the formation of illite, like zeolite F, (hydrated $KAlSiO_4$), which shows a tetrahedral Al resonance at exactly 60.0 ppm. In order to go from a TO layer, characteristic of kaolinite, to a TOT one, typical of the illite/muscovite structure, a second tetrahedral sheet must be connected to the pre-existing TO layer. The XRD patterns only show a 10.2 Å peak characteristic of TOT illite/muscovite layers after 13 hours treatment. These facts seem to indicate that the condensation of a second tetrahedral sheet requires a minimum content of tetrahedral Al to be produced.

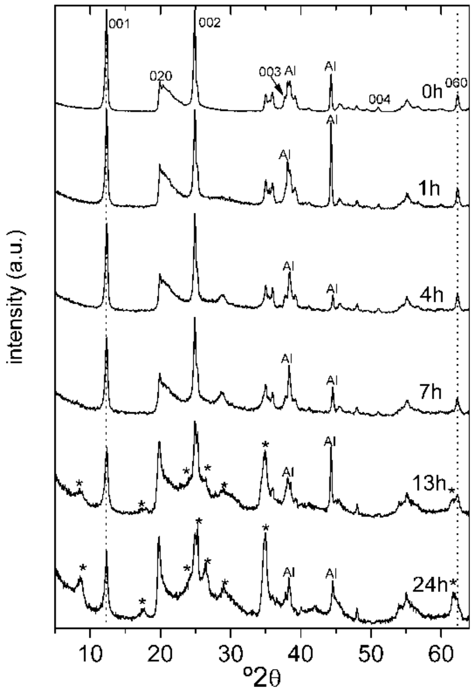


Fig. 1. Diagramas de difracción de rayos X de la caolinita antes y después de su reacción hidrotermal en disolución de KOH durantes diferentes tiempos.

XRD patterns of kaolinite before and after hydrothermal treatment in KOH solution at increasing reaction times. *: Reflections from muscovite/illite. Al: Al from the sample holder.

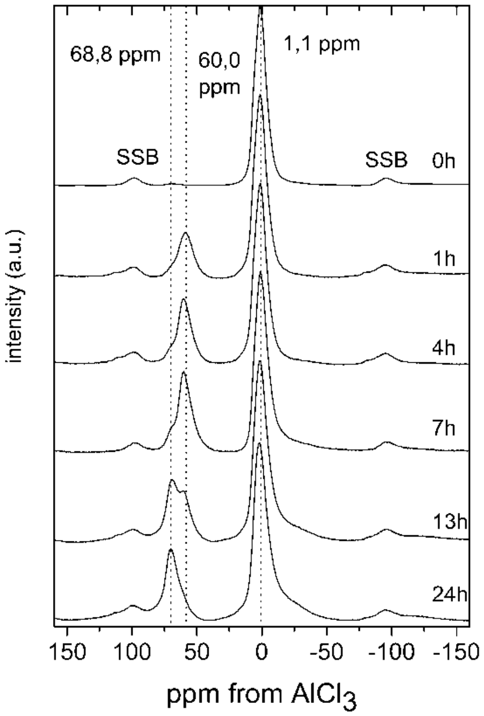


Fig. 2. Espectros de ^{27}Al MAS NMR de la caolinita antes y después de su reacción hidrotermal en disolución de KOH durantes diferentes tiempos.

^{27}Al MAS NMR spectra of kaolinite before and after hydrothermal treatment in KOH solution at increasing reaction times.

ORDENAMIENTO DE CATIONES INTERLAMINARES EN MICAS DE ALTA CARGA

INTERLAYER CATIONS ARRANGEMENT ON HIGH CHARGED MICA

La estructura de la región interlaminar de micas de alta carga expansibles, Mica-n (n=2,3 y 4) es uno de los problemas fundamentales en mineralogía. Los estudios de 1H MAS NMR sugieren que el agua interlaminar muestra un comportamiento similar al agua líquida, sin embargo, aún no hay un conocimiento preciso de ello. Mediante el uso de difracción de neutrones con un método diferencial aproximado, utilizando las micas deshidratadas como sistema de referencia, se puede conseguir aislar la difracción correspondiente al agua líquida respecto al del agua interlaminar y de esta manera, obtener las funciones de distribución radiales normalizadas.

El objetivo de esta investigación ha sido, por tanto, estudiar las muestras Li-Mica-n hidratadas mediante difracción de neutrones utilizando el método de sustitución isotópica de H/D y 6Li/natLi en la interlámina. La sustitución isotópica de hidrógeno ofrece la posibilidad de estudiar detalladamente la estructura del agua. Por otro lado, la sustitución isomórfica del Litio se usa para estudiar el entorno de coordinación de este ión: si los picos Li-O y Li-H o Li-D de la primera esfera de coordinación se pueden resolver, la integración de estos picos se puede usar como una prueba de la presencia de complejos de esfera interna de Li+ con la superficie de la mica, esto es, de un enlace directo del ión con la superficie del silicato.

Se han usado como materiales de partida Na-Micas-n (n=2, 3 y 4) preparadas a través de una metodología desarrollada por nuestro grupo de investigación (Chem. Mater. 2006, 18, 2867). Las muestras Li-n-Micas se prepararon de acuerdo con el método descrito por Powell et al. (J.Phys.Chem.B 1998, 102, 10899); cada muestra se preparó en la forma 6Li y natLi (92,5% 7Li and 7,5% 6Li). La hidratación de las Li-Micas-n se llevo a cabo mediante la saturación de las muestras en D_2O o H_2O. Cada muestra equilibrada fue sellada en un contenedor de plástico hermético y transportada hasta el Institute Laue Langevin, ILL, en Grenoble.

Las medidas de difracción de neutrones se llevaron a cabo en el difractómetro D4 de la fuente de neutrones del ILL. La longitud de onda incidente fue 0,5024 Å, medida usando Ni en polvo como referencia. Las muestras se introdujeron en unos contenedores cilíndricos de vanadio de radio interior 6,7 mm y exterior 7,0 mm, selladas con un anillo metálico. El portamuestra, una vez lleno, fue pesado antes y después de cada medida, para verificar que no hubiera pérdida de agua durante la medida. Se registraron a temperatura ambiente los difractogramas del portamuestra vacío, el fondo del instrumento y un cilindro de Vanadio de 6,08 mm de diámetro. A los datos se le han sustraído el fondo, la señal del portamuestra vacío y la dispersión múltiple se ha normalizado respecto a la dispersión del cilindro de vanadio y grabados en intervalos de k de 0,05 Å-1, donde k es el módulo del vector de dispersión.

En el estudio de la sustitución H/D, los picos de Bragg se eliminan y genera un diagrama que correlaciona los protones del agua con los de la mica. En la figura 1 izquierda se muestran estas funciones, ΔIHm(k), para la 6Li-Mica-2 y natLi-Mica-2. Los picos de Bragg residuales de las dos funciones son muy pequeños: el hecho de que estén invertidos en la muestra natLi-Mica-2 sugieren que son el resultado de errores experimentales más que de una periodicidad real en las correlaciones H-Mica. En esta figura, se muestran, a su vez, las funciones semiempíricas usadas para corregir las componentes de la dispersión propia (líneas discontínuas).

La función diferencia de primer orden en el espacio real GH(r) se obtiene tras la substracción de la función semiempírica ajustada de ΔIHm(k) y realizando la transformada de Fourier del resultado. En la figura 1 derecha se muestra la función GH(r) para 6Li y natLi-mica-2. Estas funciones están dominadas por el pico del OH intramolecular a 0,97 Å para la 6Li-Mica-2 y 0,95 Å para natLi-Mica-2, resultados que están de acuerdo con lo descrito en la bibliografía (Powell et all, J. Phys Chem B, 102, 52, 1998). La integración sobre estos primeros picos da lugar al número de coordinación hidrógeno-oxígeno. Los valores obtenidos son nHO=0,587 ± 0,004 y 0,635 ± 0,004 para 6Li-Mica-2 y natLi-Mica-2, respectivamente. Estos resultados muestran una discrepancia con análisis previos realizados en silicatos similares.

The structure of the interlayer region of swelling high-charged micas, Mica-n (n=2, 3 and 4) is one of the fundamental problems of clay science. 1H MAS NMR studies suggest that the interlayer water is liquid-like. Thus, it is possible by the combination of neutron diffraction and an approximate difference method, using the dehydrated mica as reference system, to isolate this liquid type diffraction and hence obtain normalized radial distribution functions.

The aim of this research was the study of hydrated Li-Mica-n using both H/D and 6Li/natLi isotopic substitution in the interlayer space. The hydrogen isotopic substitution offers the possibility of studying the detailed water structure. The lithium isotopic substitution can be used to study the lithium coordination environment: if the Li-O and Li-H or Li-D peaks in the first coordination shell are resolvable, the ratio of the integrals of these peaks could be used as a test for the presence of innersphere complexes of Li+ with the mica surface, i.e., of direct bonding of Li+ to the mica surface.

Na-Micas-n (n=2,3,4) prepared as reported by our research group were used as starting materials (Chem. Mater. 2006, 18, 2867). Li-Micas-n were prepared in accordance with the method described by Powell et al. (J.Phys.Chem.B 1998, 102, 10899), each sample being synthesized in the 6Li and natLi (92,5% 7Li and 7,5% 6Li) forms and hydrated both with H_2O and D_2O. A total of twelve samples were obtained. Hydration of Li-n-Micas was carried out by saturation of the samples in D_2O or H_2O. Each equilibrated sample was sealed in an airtight plastic container and transported to the Institut Laue Langevin, ILL.

The neutron diffraction measurements were performed on the D4 diffractometer on the steady-state neutron source of the ILL. The incident wavelength was 0.5024 Å, measured using a Ni powder reference. The samples were contained in a 6.7 mm i.d., 7.0 mm o.d. cylindrical vanadium container sealed with a metallic O-ring. The loaded sample container was weighed before and after each measurement to verify that no dehydration had occurred due to inadequate sealing of the container. Diffraction patterns the empty sample container, the instrument background and a 6.08 mm diameter Vanadium rod were recordered at ambient temperature. The data were corrected for background, empty container, and multiple scattering normalized to the scattering from a vanadium rod and recordered into k intervals of 0.05 Å-1, where the modulus of the scattering vector.

For H/D substitution the Bragg scattering will be eliminated and will produce a diffuse pattern related to the H-water and H-mica correlations. The measured ΔIHm(k)for the 6Li and natLi samples are shown in Figure 1 left. The residual Bragg peaks in the two functions are very small: the fact that they are inverted in the natLi-Mica-2 data suggests that they are the results of experimental errors rather than of any real periodicity in the H-mica correlations. In this figure the semiempirical function used to correct the self-scattering component of the diffraction is also shown (dashed line).

The real-space first order difference function GH(r) is obtained after the subtraction of the fitted semiempirical function from the ΔIHm(k) and the Fourier transformation of the resulting functions.The GH(r) for the 6Li- and natLi-mica-2 are shown in Figure 1 right. The GH(r) plots are dominated by the intramolecular OH peak at 0.97 Å for 6Li-Mica-2 and 0.95 for natLi-Mica-2, which is in a good agreement with the literature (Powell et all, J. Phys Chem B, 102, 52, 1998). The integration over the first peak gives the hydrogen-oxygen coordination number, the values obtain are nHO=0.587 ± 0.004 and 0.635 ± 0.004 for 6Li-Mica-2 and natLi-Mica-2 respectively. These results show a discrepancy with previous analysis with similar silicates.

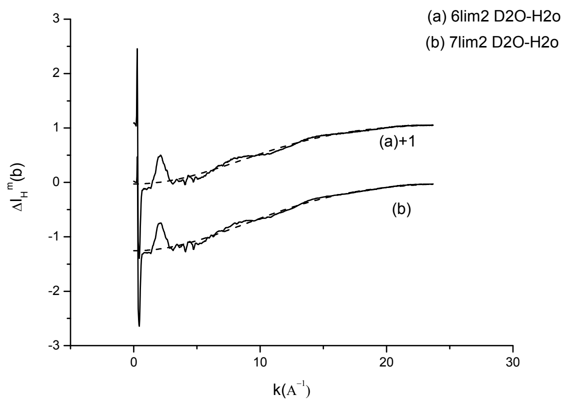


Fig. 1 izquierda: Las funciones diferencia, ΔIHm(k) (línea continua) para (a) 6Li-2-Mica y (b) natLi-2-Mica con la función de ajuste semiempírica de la dispersión propia (líneas discontinúas).

Left: The difference function, ΔIHm(k) for (a) 6Li-Mica-2 and (b) natLi-Mica-2 with fitted self scattering background (dashed lines) and background plus molecular form factor (solid lines).

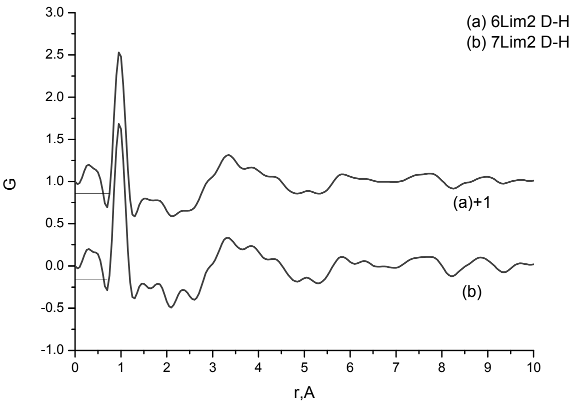


Fig. 1 derecha: Las funciones diferencia de primer orden en el espacio real GH(r) para (a) 6Li-2-Mica y (b) natLi-2-Mica obtenidas mediante la transformada de Fourier de las ΔIHm(k) corregidas por las dispersión propia.

Right: The real-space first-order difference functions, GH(r) for (a) 6Li-Mica-2 and (b)natLi-Mica-2 obtained by Fourier transformations of the unsmoothed data.

2.2. 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 Difractometer 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 equiped with detector sensible to position
- Espectrómetro de Fluorescencia de Rayos X Siemens SRS3000 X-Ray Fluorescence Spectrometer (Siemens SRS3000)
- Prensa hidraúlica 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 MICROSCOPÍA ELECTRÓNICA DE BARRIDO
SCANNING ELECTRONIC MICROSCOPY SERVICE

La microsocopía 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 tecnique 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 Metalyzer
- Laboratorio Fotográfico
  Photographic laboratory

SERVICIO DE MICROSCOPÍA ELECTRÓNICA DE TRANSMISIÓN
TRANSMISSION ELECTRONIC MICROSCOPY SERVICE

La microsocopía 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.

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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 ESPECTROSCOPÍA 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.

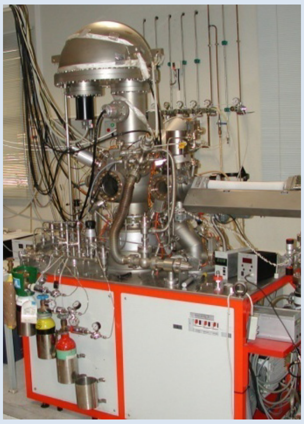
La característica más importante de la Espectroscopía de Fotoelectrones (XPS/ESCA) es el permitir diferenciar distintos estados de oxidación y/o situaciones del entorno (coordinación) de los átomos en las muestras sólidas analizadas así como el estudio de perfiles de composición combinando la técnica 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 dirime 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.

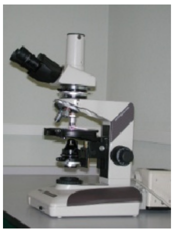
H																	He
Li	**Be**											**B**	**C**	**N**	**O**	F	Ne
Na	Mg											**Al**	**Si**	**P**	**S**	Cl	**Ar**
K	Ca	Sc	**Ti**	**V**	**Cr**	**Mn**	**Fe**	**Co**	**Ni**	**Cu**	**Zn**	Ga	Ge	**As**	Se	Br	Kr
Rb	Sr	**Y**	**Zr**	**Nb**	**Mo**	Tc	Ru	Rh	Pd	**Ag**	**Cd**	In	**Sn**	**Sb**	Te	I	Xe
Cs	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 spectific 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 equiped 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 piroélectrico de monocristales y cerámicas dieléctricas Equipment for measurement of resistivity, dielectric constant and piroelectric coefficient of single cyrstals and ceramics
- Espectrofotómetro de descarga luminiscente (GDS 750A LECO INST.) Flow discharge spectrofotometer (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 accesory (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 espectrometer (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 µp 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 TOPOME-TRIX 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-Heraus 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)

2.3. FINANCIACIÓN / FUNDS

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

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

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

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

RESUMEN / ABSTRACT

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

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

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 standars (NANOINDENT)

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

RESUMEN / ABSTRACT

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

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

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 / 30-09-2009
Organismo Financiador/Financial source: Unión Europea
Importe total/Total amount: 2.200.000 € (360.000 €)
Investigador responsable/Research head: Barranco, A. (Coord.)
Componentes/Research group: Glez-Elipe, A.R., Cotrino, J., Espinós, J.P., Yubero, F.

RESUMEN / ABSTRACT

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

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

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

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

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

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

Fenómenos de absorción y emisión ópticas en cristales fotónicos coloidales Optical absorption and emission phenomena in colloidal photonic crystals

Código/Code:	MAT2005-03028 (Plan Nacional)
Periodo/Period:	31-12-2005 / 31-12-2008
Organismo Financiador/Financial source:	Ministerio de Ciencia y Tecnología
Importe total/Total amount:	107.100 €
Investigador responsable/Research head:	Míguez García, H.
Componentes/Research group:	Ocaña, M., Mihi, A., Colodrero, S.

RESUMEN / ABSTRACT

Este proyecto pretende estudiar las modificaciones que tienen lugar tanto en la absorción como en la emisión ópticas de distintos compuestos cromóforos y colorantes 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 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 estudio se emplearán, por un lado, cristales fotónicos coloidales como matrices en los que se infiltrarán los distintos colorantes tanto orgánicos como inorgánicos cuya absorción y emisión serán analizadas. Por otro, se desarrollaran nuevas estructuras coloidales en las que los elementos cromóforos o activos formen parte de un dopante del cristal fotónico, que se comportará como un cristal extrínseco desde el punto de vista óptico.

The aim of this project is to study the modification of the optical absorption and emission of chromophores as a result of being part of a photonic crystal structure. This analysis will be done both from the applied and fundamental point of view, focusing on materials of interest for current optics or pigment industry. The main motivation of our research regarding its possible applications is the possibility to vary these optical phenomena in a controled manner, so they can be amplified or inhibited to will. In its fundamental aspects, our proposal seeks a deep understanding of the interaction between light and matter in which there exists a modulation of the dielectric constant and strong dispersity effects, and in which photons can travel at very low speeds. For this analysis, we will fabricate colloidal photonic crystals as matrices in which we will infiltrate the different organic and inorganic dyes or chromophores whose absorption and emission will be studied. Also, new photonic crystal structures in which these active compounds will be included as part of an optical dopant will be fabricated. The optical behaviour of these extrinsic photonic crystals will be analysed.

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

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

RESUMEN / ABSTRACT

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

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

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.El principal

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.

Intercalación de arcillas con ultrasonidos y reacciones de transferencia de electrones. Producción de arcillas funcionarizadas con estructura complejas jerarquizadas en el espacio interlaminar Intercalation of clay minerals by means of ultrasound treatment and electron transfer reactions: producing funsionalised clays with complex hierarchical structures in the interlayer space

Código/Code: MAT2005-04838 (Plan Nacional)
Periodo/Period: 31-12-2005 / 31-12-2008
Organismo Financiador/Financial source: Ministerio de Ciencia y Tecnología
Importe total/Total amount: 103.530 €
Investigador responsable/Research head: Pérez Rodríguez, J.L.

RESUMEN / ABSTRACT

El objetivo principal de este proyecto es aprovechar el efecto de los tratamientos con ultrasonidos y las propiedades rédox de algunos silicatos laminares para diseñar y sintetizar a partir de estos, mediante la intercalación, composites con propiedades conductoras. Con la sonicación se pretende obtener una máxima deslaminación y reducción de las partículas, sin modificar su estructura, para facilitar la intercalación o dispersión sin perder las propiedades de estos silicatos. Se prestará atención a la razón Fe2+/Fe3+ de las vermiculitas (oxidadas y reducidas), ya que estas al actuar como sistema rédox pueden ejercer un papel fundamental en la intercalación, y en las propiedades conductoras. La técnica de ultrasonidos facilitará además la intercalación, prestándose una atención especial a que el huésped se sitúe en el espacio interlaminar. Con todo lo expuesto, se pretende obtener composites de vermiculitas con nuevas o mejores propiedades que los actualmente preparados utilizando esmectitas. A efectos comparativos se prepararán composites con caolinitas, intercalando los mismos huéspedes que en las vermiculitas. A los composites preparados se les medirán sus propiedades térmicas, termomecánicas, eléctricas y electromecánicas y se evaluará la posibilidad de utilizarlos en la fabricación de recubrimientos de protección catódica contra la corrosión.

The main objective of this project is to make use of the combined effect of sonication and redox properties of some layer silicates to prepare conductive composites in intercalated management. By sonication we intend to delaminate and reduce the particle size without modifying the clay structure (and properties) while enhancing intercalation and dispersion. Special attention will be paid to the ratio Fe2+/Fe3+ in oxidized ad reduced vermiculites because its redox behaviour may play an important role in intercalation and conductive properties. Sonication will be also used to promote intercalation. Thus, it is intended to obtain vermiculite composites with new and enhanced properties as compared with the smectites composites. Kaolinite composites will be also prepared for comparison. All the composites will be characterized in terms of their thermal, thermo mechanical, electrical and electromechanical properties. Additionally their use as corrosion protection coatings will be evaluated.

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:	Cotrino Bautista, J.
Componentes/Research group:	González-Elipe, A.R., Espinós, J.P., Yubero, F., Barranco, A.

RESUMEN / ABSTRACT

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

This project aims at the development of a new family of oxide thin films optically active that are able to develop a series of properties useful for several photo-functional applications in fields like optics, solar energy recovery or sensors. Oxide thin films (TiO2, SiO2, ZnO) with very well controlled microstructure will be prepared by different methods (PVD, PECVD and atmospheric pressure plasmas) and modified by infiltration with optically active components (dyes and metal particles) or, for TiO2 and ZnO, by doping with some anions (i.e., nitrogen, fluor or carbon) suitable to make these oxide semiconductors active to the visible light of the electromagnetic spectrum. The photo-functional properties of the prepared thin film materials will be tested for their applications as photochromic coatings, optical gas sensors, plasmon resonant behavior, films with light-controlled wetting properties and photoelectrochemical cells. A strict control of the micro and nano-structure of the thin films will be achieved by using specific strategies for their growth. Analysis of the growing mechanisms leading to the different micro/nano-structures by means of the concepts of the Dynamic Scale Theory will permit a tailored synthesis of the host thin films. Similarly, the plasma conditions will be conveniently monitored and modeled to get a full description of the growing mechanisms and, in its case, be able to modify it if required for the desired applications.

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 centrando 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.

Nanopartículas magnéticas de metales nobles con funcionalización y microestructura controladas Magnetic nanoparticles of noble metals with controlled microstructure and functionalisation

Código/Code:	NAN2004-09125-C07-04
Periodo/Period:	31-12-2005/ 31-12-2008
Organismo Financiador/Financial source:	Ministerio de Ciencia y Tecnología
Importe total/Total amount:	199.140 €
Investigador responsable/Research head:	Fernández, A.
Componentes/Research group:	Sánchez-López, J.C., Friedrichs, O., Martínez Martínez, D., López Cartes, C., Rojas, T.C., Guerrero, E., Muñoz-Márquez, M.A.

RESUMEN / ABSTRACT

En esta propuesta se establece una colaboración multidisciplinar para desarrollar investigación, nuevas técnicas experimentales y aplicaciones biomédicas sobre la base de las extraordinarias propiedades y procedimientos originales de fabricación de un nuevo tipo de nanopartículas magnéticas biofuncionales. Partiendo de una serie de resultados obtenidos en trabajos previos de colaboración entre algunos de los grupos participantes, se pretende ahora utilizar la plataforma que ofrece la Acción Estratégica de Nanociencia y Nanotecnología para abordar extensamente y en profundidad aspectos fundamentales y aplicaciones biomédicas. Por una parte, se propone una investigación coordinada dirigida a comprender las causas del magnetismo permanente observado en estas nanopartículas y esclarecer los factores que gobiernan tan singular comportamiento. Por otra, investigar su potencialidad en el estudio de interacciones biomoleculares y explorar su utilización en nuevos tipos de biosensores y su aplicación como agentes de contraste en resonancia magnética de imagen (MRI) y en el marcaje de células troncales murinas.

The main aim of this proposal is to establish a multidisciplinary approach to carry out research and to develop experimental techniques and biomedical applications on the extraordinary properties and the original preparation procedure of a new type of biofunctional magnetic nanoparticles. On the basis of results from previous collaborations we now intend to profit from the Acción Estratégica de Nanociencia y Nanotecnología to perform extensive studies on fundamental aspects and biomedical applications of these magnetic nanoclusters. On one hand, a co-ordinated investigation aiming at understanding the causes of the permanent magnetism observed in these nanoparticles is put forward. On the other, a series of studies are proposed on their use for the comprehension of specific biomolecular interactions and for the development of new types of biosensors. Their potentiality as new contrast agents in magnetic resonance imaging and for murine stem cell labelling will be extensively investigated as well.

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

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

Código/Code:	ENE2007-67926-C02-01
Periodo/Period:	1-12-2007/30-11-20108
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., Pereñiguez, 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 ultimo es la mejora de la reacción de reformado de hidrocarburos para producción de H2(+CO), principalmente metano y propano, al ser esta una reacción dependiente de la estructura, y por tanto sensible al tamaño de partícula.

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

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

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

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

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

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

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

Capas absorbentes y de puntos cuánticos y estructuras nanofotónicas para el desarrollo y optimización de dispositivos ópticos Absorbent and quantum dots layers and nanophotonic structures for the development and optimization of optical devices

Código/Code: NAN2004-09317-C04-01
Periodo/Period: 31-12-2005/ 31-12-2008
Organismo Financiador/Financial source: Ministerio de Ciencia y Tecnología
Importe total/Total amount: 103.500 €
Investigador responsable/Research head: González-Elipe, A.R.
Componentes/Research group: Caballero, A., Cotrino, J., Espinós, J.P., Yubero, F., Holgado, J.P., Barranco, A.

RESUMEN / ABSTRACT

Con este proyecto se propone el desarrollo de estructuras y materiales nanotecnológicos que, al ser integrados sobre elementos fotónicos, formen dispositivos cuya respuesta dependa de la longitud de onda de la luz (λ) con la que interaccionen. Su ámbito de actuación se circunscribirá al visible y al infrarrojo próximo. Para lograr respuestas selectivas a la λ se trabajará tanto con materiales absorbentes, basados en nanopartículas (puntos cuánticos) y colorantes encapsulados en matrices transparentes (mediante técnicas de plasma y de sol-gel), así como con estructuras fotónicas bidimensionales. La investigación se centrará en sintetizar capas delgadas de matrices orgánicas e inorgánicas con microestructura nanométrica controlada que, por un lado incorporen colorantes (i.e. Rhodaminas, phtalocyaninas y porfirinas), y por el otro puntos cuánticos comerciales. Los elementos fotónicos con los que se integrarán estos materiales y estructuras serán fotodiodos de silicio, fibras ópticas convencionales, fibras de cristal fotónico, así como otras estructuras fotónicas (anillos resonadores, cavidades resonantes) que resultarán de esta investigación. Los dispositivos a conseguir con este proyecto son de dos clases: detectores insensibles al ángulo de detección (para comunicaciones ópticas difusas multiplexadas en λ), y sensores de fibra óptica basados en nuevas técnicas de transducción. El carácter innovador del proyecto se centra en el desarrollo de nuevos procedimientos para la preparación de materiales y estructuras nanométricas muy superiores en prestaciones a los materiales clásicos actualmente existentes. Ello permitirá su integración de dispositivos ópticos dotándoles de prestaciones muy optimizadas y superiores respecto a las de elementos equivalentes del mercado.

This project proposes the development of nanotechnological structures and materials that, by their integration onto photonic elements, give rise to devices with a wavelength (λ) dependent response. The scope of action of these devices will be the visible and near infrared ranges. To get selectivity in the response according to λ, work will be carried out to obtain absorbent materials, based in nanoparticles (i.e. quantum dots) and dyes encapsulated in transparent matrices prepared by plasma and sol/gel techniques, as well as bidimensional photonic structures. The research will be focussed in the synthesis of organic and inorganic matrices with a well controlled nanometric microstructure that, on the one side incorporate dyes (i.e. Rhodamine, phtalocyanines y porphirins) and, on the other, commercial quantum dots. The photonic elements with which these materials and structures will be integrated will consist of Si photodiodes, conventional optical fibres, photonic crystal fibres, as well as other photonic structures (resonator rings, resonant cavities) that will come out from this investigation. The devices to be developed in the project will be of two kinds: detectors insensitive to the angle of detection (for diffuse optical communications multiplexed in λ) and optical fibre sensors based in new transduction techniques. The innovative character of the project is centred in the development of new procedures for the preparation of nanometric materials and structures which are superior in performance to the classical materials available at present. This will enable their integration in optical devices for an optimised and superior function with respect to the equivalent ones available in the market.

Adsorción y autoensamblado de aminas y ácidos carboxílicos alifáticos en soportes modelo como surfactantes en los procesos de flotación y recuperación de minerales. Estudio por técnicas de SPM Adsorption and self-assembly of linear fatty amines and carboxylic acids on model supports acting as surfactants in mineral flotation

Código/Code:	CTQ2005-00998
Periodo/Period:	31-12-2005/ 31-12-2008
Organismo Financiador/Financial source:	Ministerio de Educación y Ciencia
Importe total/Total amount:	47.600 €
Investigador responsable/Research head:	Benítez, J.J.
Componentes/Research group:	Sánchez-Soto, P.J., Garzón, E., Stanislaw, J.

RESUMEN / ABSTRACT

La modificación de las características superficiales de un sólido por adsorción de surfactantes es un fenómeno físico-químico fundamental que constituye la base importantes procesos industriales tales como el diseño de recubrimientos (pinturas, etc…) o la flotación de minerales. En este último caso se emplean tanto surfactantes de tipo catiónico, aniónico o neutros. Un caso de particular importancia económica e industrial lo constituye la separación de silvita (KCl) y halita (NaCl) en las plantas de flotación de potasas con vistas a proporcionar una fuente de potasio de uso agrícola. El surfactante de mayor aplicación en este sentido lo constituyen las aminas alifáticas primarias lineales de cadena larga (C12-C18). El presente proyecto de investigación tiene como objetivo el estudio de la adsorción y autoensamblado de surfactantes tipo (catiónicos: aminas alifáticas y aniónicos: ácidos carboxílicos) en distintas condiciones y soportes modelo empleando diferentes técnicas analíticas, pero con especial contribución de la microscopía de fuerzas atómicas (AFM). La información obtenida a nivel fundamental constituirá una plataforma para la interpretación de los fenómenos que concurren en los procesos de flotación industrial, con especial interés en el caso de la silvita. Se abordará también dos aspectos adicionales de gran repercusión en la eficacia de la flotación del KCl como son la adición de co-surfactantes neutros (cierto tipo de alcoholes) y el efecto perjudicial de la presencia de silicatos en las fuentes naturales de potasas. La información obtenida será de gran valor desde la perspectiva de la aplicación a corto/medio plazo en el proceso industrial real. Así se deriva de la participación de una importante corporación industrial del sector como ente interesado en el desarrollo del proyecto.

Surface modification of solids with surfactants is a basic concept with important industrial applications such as paints and mineral flotation. In this later case, cationic, anionic and non-ionic surfactants are employed. A particular case, with great economic and industrial importance, is sylvite (KCl) separation from halite (NaCl) in potash flotation. KCl is employed in the formulation of fertilizers. In this process, long chain linear fatty amines (C12-C18) are employed as surfactants. The objective of this project is to study the adsorption and self-assembly of both cationic (fatty amines) and anionic (fatty acids) on model supports and under variable experimental conditions. Several analysis techniques will be used, but the contribution from atomic force microscopy (AFM) will be very important. Obtained results at the fundamental level will be the base for the interpretation of processes involved in flotation with specific interest on the case of sylvite. Other important issues such as the influence of neutral additives (alcohols) acting as frothers and the perturbing effect of silicates in KCl flotation will be addressed. This information is of a great value and potential industrial application in a short/mid term, as revealed from the interest in the development of this research project shown by the main potash manufacturer in the world.

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

The study of soft magnetic materials obtained by rapid quenching and milling/mechanical alloying (amorphous and nanocrystalline alloys and nanopowders) is proposed. Concerning the milling technique, we will try to improve the knowledge of the influence of different experimental parameters (involved in the preparation and processing of the powder) on the microstructure and magnetic properties of the material. In the nanocrystalline alloys it is proposed to analyse the influence of different composition changes of the alloys on the microstructure of the nanocrystal-intergranular phase system and its correlation with the magnetic properties of the material, as a way to optimize them. The interactions responsible for the grain coupling and their modelisation, to explain the temperature dependence of the magnetic behaviour of these materials, will be also a subject of our study. In the multicomponent amorphous alloys, the objetives are focused on the optimization of their magnetic properties and the viability to develop nanostructures improving their magnetic properties. In view of its current interest, due to their potential technological applications, we will study the magnetocaloric response of the different materials, trying to optimize its refrigeration capacity and the optimal operational temperature, and we will analyse changes in the magnetocaloric response in the presence of nanocrystals.

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 Feria, 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 implementa 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.

Influencia del campo eléctrico, deuteración y dopaje con l-alanina sobre la transición de fase tricrítica del cristal ferroeléctrico TGSe y estudio de situaciones estacionarias Influence of the electric field, deuteration and doping with L-alanine on tricritical phase transition in ferroelectric crystal TGSe and study of steady state through conduction calorimetry.

Código/Code:	FIS2005-02444
Periodo/Period:	31-12-2005 / 31- 12- 2008
Organismo Financiador/Financial source:	Ministerio de Ciencia y Tecnología
Importe total/Total amount:	10.710 €
Investigador responsable/Research head:	Del Cerro, J.
Componentes/Research group:	Zamora, M., Ramos, S., Gallardo, M.C., Rey, A., Jiménez, J., Martín Olalla, J.M., Romero Landa, F.J.

RESUMEN / ABSTRACT

Mediante la técnica calorimétrica “Square Modulate Thermal Analysis” (SMTDA) desarrollada por el Grupo se estudiará la influencia del campo eléctrico y la tensión mecánica uniaxial moderada sobre el calor específico y el calor latente en la transición ferro-paraeléctrica de la familia de cristales DTGSe, en procesos de calentamiento y enfriamiento. Se pretende estudiar la influencia de la deuteración sobre los coeficientes del potencial de Landau que describe la transición tricrítica del TGSe puro. En el caso del DTGSe, transición discontinua, se estudiará el efecto del campo eléctrico sobre el calor latente y la cinética de la transición de fase. Se realizarán medidas dieléctricas para comprobar la consistencia de los resultados anteriores y obtener información sobre la figura de mérito piroeléctrica de esos cristales.

The square modulated thermal analysis (SMTDA) ---a technique developed by our group--- will be used to study the influence of the electric field and uniaxial mechanical stress on the specific heat and latent heat of ferroelectric-paraelectric phase transition in DTGSe during heating and cooling process.

We will study the influence of deuteration on the coefficients of the Landau potential describing the tricritical phase transition of pure TGSe. For DTGSe, a discontinuous transition, the influence of the electric field on the latent heat and kinetic phase transition will be studied. Dielectric measurement will be carried out to show the consistency of previous results and to look for the piroelectric figure of merit in these crystals.

Materials World Network: Ceramic Composites from Natural and Synthetic Scaffolds 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 auna nueva clase de materiales compuestos. A diferencia de 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 vias 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. Petersburgo.

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., Diánez, M.J., Criado, J.M., Alcalá, M.D., Poyato, J., Pérez Rodríguez, J.L., Sánchez Jiménez, P.E.

RESUMEN / ABSTRACT

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

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

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.

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

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

RESUMEN / ABSTRACT

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

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

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- 2012
Organismo Financiador/Financial source:	Junta de Andalucía
Importe total/Total amount:	96.200 €
Investigador responsable/Research head:	Cotrino Bautista, J.
Componentes/Research group:	Gónzalez-Elipe, A.R., Yubero, F.

RESUMEN / ABSTRACT

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

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

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

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

RESUMEN / ABSTRACT

El proyecto de investigación consiste en el análisis de las interacciones a nivel molecular de los monómeros constituyentes del biopolímero natural cutina con vistas al diseño de rutas de síntesis y reconstrucción "botton-up" de materiales biomiméticos artificiales no tóxicos y biodegradables con aplicaciones como material de envasado y de encapsulado y liberación controlada de fármacos.

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

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

Ayuda complementaria al proyecto “Superar la fragmentación de la investigación europea en películas delgadas multifuncionales”

Complementary support to the Project “To overcome the fragmentation of European research in multifunctional thin films”

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

RESUMEN / ABSTRACT

El proyecto está dedicado a promover la investigación europea en capas finas “nanoestructuradas” y “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); Universitá Politecnica delle Marche (UPM, Italia); University of Nottingham (UNIN, UK); Free University of Brussels (ULB, Bélgica); Technological University for Steel and Alloys (MSISA, Rusia); Institute for Spectroscopy RAN (ISP, Rusia); SH SISTEMI s.r.l. (SHS, Italia); Technion (TEC, Israel); Instituto de Ciencia de Materiales de Sevilla (ICMSE, España); Johann Wolfgang Goethe University (GU, Alemania); CRC HAS Chemical Research Center of the Hungarian Academy of Sciences (CRC, Hungría); Cambridge University (CU, UK); INNO Group (INNO, France); Eurogroup Consulting (EURG, Bélgica).

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

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

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

RESUMEN / ABSTRACT

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

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

Producción de H_2. Reactores de microcanales H_2 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 centrando 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 Inmobilization of toxic and radioactive wastes by silicates

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

RESUMEN / ABSTRACT

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

In The present Project tries to use high-charged silicates, which are designed under procedures that allow controling the quantity and distribution of the tetrahedral active centers. They will be submitted to a set of chemical soft treatments in order to inmobilize toxic elements. This project will be carried out in collaboration with BEFESA and ENRESA companies. Firstly, the effect that the experimental variables involved in the procedure of synthesis exert on the distribution of the active centers of the materials will be analyzed. In the second stage, the synthetic silicates will be treated under soft hydrothermal conditions with solutions containing carefully selected toxic and radioactive elements. Finally, the degree of retention of these elements in the new obtained phases will be estimated. The Research Team (R.T.) will

incorporate an experimental methodology developed by itself that includes the combined employment of Nuclear Magnetic Resonance of Solids, X-ray Diffraction, X-rays Fluorescence and Microfluorescence, which will give information of the long range order and the local environment of the active centers of the residues, responsible of it dangerousness. It will have to give direct and not yet available information of the final mechanism of fixation, which is the main objective of this Project. The expected Results will bring basic useful information about the mechanisms of interaction of metallic ions with the framework of expansible aluminosilicates and its relation with the local arrangement of their atoms. Moreover, it will bring a useful knowledge allowing to develop new suitable procedures for immobilization of industrial waste, in collaboration with the companies of the sector, which marks the innovative character of the Project.

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

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

RESUMEN / ABSTRACT

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

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

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

Código/Code: P07-FQM-02520 (Proyecto de Excelencia)
Periodo/Period: 01-02-2008 / 31-01- 2012
Organismo Financiador/Financial source: Junta de Andalucía
Importe total/Total amount: 241.668 €
Investigador responsable/Research head: Holgado Vázquez, J.P.

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

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

RESUMEN / ABSTRACT

El objetivo principal del proyecto ART-DECO es el desarrollo de nuevos procesos de recubrimiento decorativo, de cerámicas, vidrios, metales y polímeros, de aplicación en sectores de escala como construcción, automoción o electrodomésticos, mediante tecnologías avanzadas, que permitan una rápida implementación industrial. Estos procesos deben ser 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 antialergénicos.
- Recubrimientos decorativos de alta resistencia al desgaste y a la erosión.

Como objetivo secundario, la ejecución del proyecto ART-DECO permitirá la creación de un polo de competencia en tratamientos y tecnologías avanzadas de superficies, donde los

socios del proyecto, apoyados por los organismos de investigación, ejerzan un liderazgo a nivel mundial en el desarrollo y utilización de los nuevos procesos de recubrimiento.

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

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

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

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

OTROS PROYECTOS / OTHER PROJECTS

Peliculas nanocompuestas con propiedades luminiscentes para la síntesis de estructuras fotónicas

Periodo/Period:	2008
Organismo Financiador/Financial source:	CSIC
Importe total/Total amount:	30.000 €
Investigador responsable/Research head:	Angel Barranco Quero

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

Tratamiento de emisiones gaseosas industriales de disolventes para la protección ambiental

Código/Code:	305P10269

Periodo/Period: 2005 / 2008
Organismo Financiador/Financial source: Proyecto CYTED (Programa Iberoamericano de Ciencia y Tecnología para el desarrollo). Área 3 Promoción del desarrollo industrial
Importe total/Total amount: 150.000 € (Todos los grupos)
Investigador responsable/Research head: Mario Montes (Coord.), José A. Odriozola

Ultra high temperature ceramics for aerospace use

Código/Code: FA8655-07-1-3087
Periodo/Period: 01-08-2007 / 01-08- 2008
Organismo Financiador/Financial source: European Office of Aerospace R&D
Importe total/Total amount: 45.000 €
Investigador responsable/Research head: Julián Martínez Fernández

Absorberdores volumétricos avanzados para tecnología de alta concentración solar

Código/Code: CIT-120000-2005-49
Periodo/Period: 14-12-2005 / 30-06-2008
Organismo Financiador/Financial source: Ministerio de Industria Ministerio de Educación y Ciencia – PROFIT
Importe total/Total amount: 115.000 €
Investigador responsable/Research head: Antonio Ramírez de Arellano-López

AYUDAS DE LA JUNTA DE ANDALUCÍA A LOS GRUPOS DE INVESTIGACIÓN
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	20.281,76 €
FQM123	Sólidos Cristalinos	Criado Vega, Alberto	8.709,08 €
FQM130	Propiedades Térmicas y Dieléctricas de Sólidos	Del Cerro González, Jaime	7.562,39 €
FQM163	Propiedades Mecánicas de Sólidos	Domínguez Rodríguez, Arturo	20.281,76 €
FQM181	Fotocatálisis Heterogénea: Aplicaciones	Navío Santos, José Antonio	6.728,18 €
FQM187	Nuevos Materiales a Partir de Silicatos Naturales	Pérez Rodríguez, José Luis	10.945,34 €
FQM196	Superficies, Interfaces y Capas Finas	Rodríguez González-Elipe, Agustín	27.276,37 €
FQM212	Química del Estado Sólido	Castro Arroyo, Miguel Angel	6.527,66 €
FQM342	Materiales Biomiméticos y Multifuncionales	Martínez Fernández, Julián	12.178,56 €
FQM356	Nanomateriales Ópticos	Ocaña Jurado, Manuel	13.929,48 €

TECNOLOGÍA DE LA PRODUCCIÓN / TECNOLOGY OF THE PRODUCTION

Código	Denominación	Responsable	Financiación
TEP106	Química de Superficies y Catálisis	Odriozola Gordón, José Antonio	11.597,01 €
TEP110	Reactividad de Sólidos	Criado Luque, José Manuel	6.213,74 €
TEP204	Materiales Avanzados	Sánchez Soto, Pedro José	4.681,86 €
TEP217	Materiales Nanoestructurados y Microestructura	Fernández Camacho, Asunción	11.585,02 €

CONVENIOS Y CONTRATOS / CONTRACTS AND AGREEMENTS

Investigación y desarrollo de aplicaciones nanotecnológicas en aglomerados de piedra

Periodo/Period: 30-04-2007 / 01-05-2008
Organismo Financiador/Financial source: Consentino, S.A.
Importe total/Total amount: 100.224 €
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 fotovoltáicas

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

Metalización decorativa y funcional

Periodo/Period:	10-05-2007 / 11-07-2008
Organismo Financiador/Financial source:	Valeo Iluminación, S.A.
Importe total/Total amount:	50.000 €
Investigador responsable/Research head:	Juan Pedro Espinós
Componentes/Research group:	Agustín R. González-Elipe, José Cotrino, Francisco Yubero, Angel Barranco

Investigación de nuevas reacciones y procesos industriales de descomposición de CO_2, 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:	15-02-2007 / 15-04-2008
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 sistemas electrónicos de olfato para la evaluación de calidad del aceite de oliva

Periodo/Period:	25-7-2007 / 31-12-2008
Organismo Financiador/Financial source:	Sos Güetarra, S.A.
Importe total/Total amount:	12.506 €
Investigador responsable/Research head:	José Cotrino Bautista

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

Remediación de suelos contaminados a partir de residuos no peligrosos y otros subproductos

Periodo/Period: 21-12-2007 / 21-8-2008
Organismo Financiador/Financial source: BEFESA Gestión de Residuos Industriales
Importe total/Total amount: 14.870 €
Investigador responsable/Research head: María Dolores Alba
Componentes/Research group: Ana Isabel Becerro, Miguel Angel Castro

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

Microrreactores catalíticos para el reformado de gas y reacción de Fischer-Tropsch

Periodo/Period: 01-01-2008 / 31-12-2008
Organismo Financiador/Financial source: Petróleo Brasileiro, S.A. (CEMPES-PETROBRAS)
Importe total/Total amount: 105.318 €
Investigador responsable/Research head: José Antonio Odriozola
Componentes/Research group: Miguel Angel Centeno, Dirk Hufschmidt

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

Testing of the deposition conditions of nanofilms for infrared reflectivity applications

Periodo/Period: 20-04-2008 / 19-09-2008
Organismo Financiador/Financial source: Virtual Institute of Nano Films
Importe total/Total amount: 5.540,52 €
Investigador responsable/Research head: Fernández Camacho, Asunción

Informe acerca del estado de la mercancía transportada por el buque “Sea Doll” desde el puerto de Mersin (Turquia) al de Sevilla

Periodo/Period: 1-1-2008 / 29-2-2008
Organismo Financiador/Financial source: Lorenzo Loximet, S.L.
Importe total/Total amount: 7.500 €
Investigador responsable/Research head: José Antonio Odriozola Gordón

Infiltration of polycarbonate in silica particle films to achive transparent porous self-standing

Periodo/Period:	1-9-2008 / 1-12-2008
Organismo Financiador/Financial source:	Nanologica, AB
Importe total/Total amount:	2.922,94 €
Investigador responsable/Research head:	Hernán Ruy Míguez García
Componentes/Research group:	Mauricio Calvo Roggiani, Silvia Colodrero Pérez

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

Periodo/Period:	3-3-2008 / 3-3-2010
Organismo Financiador/Financial source:	Abengoa Solar New Tecnologies, S.A.
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 / 31-12-2008
Organismo Financiador/Financial source:	Consentino, S.A.
Importe total/Total amount:	32.248 €
Investigador responsable/Research head:	Francisco Yubero Valencia
Componentes/Research group:	Agustín R. González-Elipe, Juan Pedro Espinós Manzorro, José Cotrino Bautista, Angel Barranco Quero

Investigación del comportamiento a alta temperatura de los aceros inox idables ferríticos

Periodo/Period:	1-3-2008 / 31-3-2008
Organismo Financiador/Financial source:	Acerinox, S.A.
Importe total/Total amount:	39.900 €
Investigador responsable/Research head:	José Antonio Odriozola Gordón

Informes técnicos relativos a barras corrugadas de acero de calidad B500SD almacenadas en las instalaciones de “Carbón Puerto Operaciones Portuarias, S.A.” y transportadas por los Buques Tsarin y Evin

Periodo/Period: 10-1-2008 / 25-1-2008
Organismo Financiador/Financial source: Mac Rolling Mill, S.L.U.
Importe total/Total amount: 8.700 €
Investigador responsable/Research head: José Antonio Odriozola Gordón

Caracterización estructural de materiales del patrimonio histórico

Periodo/Period: 2-5-2008 / 31-12-2008
Organismo Financiador/Financial source: Consejeria de Cultura. Junta de Andalucia
Importe total/Total amount: 3.620,69 €
Investigador responsable/Research head: José Luis Pérez Rodríguez
Componentes/Research group: Angel Justo Erbez, M. Luisa Franquelo Zoffmann, M. Belinda Sigüenza Carballo

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

XAS Study of Ti and V based catalysts added to reactive hydride composite materials for H_2 storage applications

Asunción Fernández Camacho, Emilie Deprez
ESRF (European Synchrotron Radiation Facilities), Grenoble, Francia

PRODUCCIÓN CIENTÍFICA
SCIENTIFIC PRODUCTION

3

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

Influence of amine template on the photoactivity of TiO_2 nanoparticles obtained by hydrothermal treatment
Colon, G; Hidalgo, MC; Navio, JA; Melian, EP; Diaz, OG; Dona, JM
Applied Catalysis B-Environmental, **78** (2008) 176-182

TiO_2 nanoparticles have been prepared by amine template-assisted sol-gel precipitation and further hydrothermal treatment. We have investigated the effect of different amines (hydrazine and triethylamine) in the final surface and structural properties. It has been stated that the different amounts of amine could act as an interesting template upon hydrothermal treatment. Further thermal treatment also leads to a significant improvement in the photocatalytic properties of the studied systems. Surface and morphological features notably differ from TiO_2 prepared using different synthetic routes. Wide surface and structural characterization of the samples have been carried out, and correlations with precipitation pH are pointed out from this characterization. In all cases, amine template TiO_2 obtained exhibit high conversion values for phenol photo-oxidation reaction. Further calcination treatment of all the studied systems clearly leads to photocatalytic conversions higher than that exhibited by TiO_2 Degussa P25. (C) 2007 Elsevier B.V. All rights reserved.

Modification of the photocatalytic activity of Pd/TiO_2 and Zn/TiO_2 systems through different oxidative and reductive calcination treatments
Aramendia, MA; Borau, V; Colmenares, JC; Marinas, A; Marinas, JM; Navio, JA; Urbano, FJ
Applied Catalysis B-Environmental, **80** (2008) 88-97

Two different solids consisting of Pd or Zn-containing titania systems (metal/titanium nominal ratio of 1%) were submitted to diverse oxidative and reductive calcination treatments and tested for gas-phase selective photooxidation of 2-propanol. As regards the Pd system, reduction at low temperature (<= 500 degrees) resulted in a gradual increase in catalytic activity which was ascribed to the gradual reduction of bulk palladium to Pd-0. Thermal treatment of the system at high temperature (850 degrees C) in static air, air flow or hydrogen flow led to a decrease in activity as the result of the sharp decrease in surface area. Nevertheless, those systems containing Pd-0 only were more active than the one consisting of Pd + PdO. Finally, Pd-system overcame I'd migration to the surface on reduction at 850 degrees C which resulted in a significant increase in selectivity to acetone up to 97% for a time on stream of 5 h. As regards the Zn-containing system, none of the applied treatments resulted in improvement in photocatalytic activity. It seems that the most favourable situation for photocatalysis is that on which Zn atoms are substituting titanium ones in the lattice, whereas segregation of Zn to form small ZnO clusters is especially detrimental to activity. (C) 2007 Elsevier B.V. All rights reserved.

Study of the synergic effect of sulphate pre-treatment and platinisation on the highly improved photocatalytic activity of TiO_2

Hidalgo, MC; Maicu, M; Navio, JA; Colon, G

Applied Catalysis B-Environmental, **81** (2008) 49-55

An important improvement of the photocatalytic activity of sol-gel prepared TiO_2 has been achieved by sulphate pre-treatment, calcination at high temperature and further platinisation of the samples. The presence of sulphuric acid clearly stabilised TiO_2 surface area against sintering, maintaining at the same time anatase phase until higher calcination temperatures than in non-sulphated samples. Platinisation of the samples with different nominal amounts of platinum (from 0.5 to 2.5 wt%) was performed and the influence of sulphate treatment on the dispersion and deposit size of platinum on the TiO_2 surface was studied. Characterisation results and photocatalytic activity of these catalysts were compared with those of unmodified TiO_2. Simultaneously sulphated and platinised TiO_2 samples were highly active for phenol degradation, used as model reaction for the photocatalytic studies, having higher activities than only platinised or only sulphated samples. The activity of these samples were several orders of magnitude higher than that of the commercial TiO_2 Degussa P25 (platinised or unmodified) as well, with independence of the nominal amount of platinum of the samples. A wide characterisation of the samples was performed and correlations between characterisation results and activity properties are reported. (C) 2007 Elsevier B.V. All rights reserved.

Functionalisation versus mineralisation of some N-heterocyclic compounds upon UV-illumination in the presence of un-doped and iron-doped TiO_2 photocatalysts

Navio, JA; Macias, M; Garcia-Gomez, M; Pradera, MA

Applied Catalysis B-Environmental, **82** *(*2008) 225-232

Heterogeneous photocatalytic oxidation of some N-heterocyclic compounds (4-picoline, and 6- and 8-methylquinoline) in oxygenated solvents (water or acetonitrile), containing dispersed photocatalyst (un-doped or iron-doped titanium dioxide), was investigated under UV-illumination in a photochemical reactor. This work aimed to correlate experimental parameters such as structural aspects of the substrates, photocatalyst chemical and surface properties. illumination times, and the nature of the solvent with the extent of mineralisation of the substrates and, also, possible selective methyl group functionalisation. Analysis of the products resulting from heterogeneous photocatalytic oxidation of 6- and 8-methylquinoline suspensions in oxygenated acetonitrile with illumination periods of <24 h detected, in both cases, the corresponding formyl derivatives quinoline-6- and -8-carbaldehyde, though at low levels. The presence of water appeared to inhibit heterogeneous photocatalytic functionalisation. However, the heterogeneous photocatalytic degradation of such compounds in water proceeds via polyhydroxylated intermediates which consequently undergo mineralisation, which, from a pollution control perspective is beneficial. The physicochemical properties of the photocatalyst were also shown to be influential. Particularly, differences in the affinity to, and mode of adsorption of the substrate compounds studied gave rise to differences in the extent of oxidation. Analysis of photogenerated oxidation products enabled some mechanistic insight into the course of the semiconductor-mediated reaction. The results obtained allow a useful comparison of the functionalisation of N-Heterocyclic compounds via heterogeneous photocatalytic processes in the absence of water, to those carried out in the presence of water, which gave complete tnineralisation. (C) 2008 Elsevier B.V. All rights reserved.

Highly photoactive ZnO by amine capping-assisted hydrothermal treatment

Colon, G; Hidalgo, MC; Navio, JA; Melian, EP; Diaz, OG; Rodriguez, JMD
Applied Catalysis B-Environmental, **83** (2008) 30-38

ZnO nanoparticles have been prepared by amine template assisted sol-gel precipitation and further hydrothermal treatment. We have investigated the effect of different pH values achieved by means of triethylamine (TEA) addition in the final surface and structural properties. Two sets of samples were obtained after thermal treatment, one with no hydrothermal pre-treatment and a second hydrothermally pre-treated. Surprisingly the precipitate obtained after the amine addition also exhibits good photocatalytic properties. It has been stated that calcination treatment leads in both sets of samples to a significant improvement in the photocatalytic properties of the studied systems. Therefore, interesting comparison has been performed between hydrothermal pre-treated and direct thermal treated samples. Surface and morphological features notably differ from ZnO prepared using different synthetic route. Wide Surface and structural characterization of the samples have been carried out, and correlations with precipitation pH are pointed out from this characterization. In all cases. the amine templated ZnO obtained exhibit high conversion values for phenol photo-oxidation reaction. Further calcination treatment in all of the studied samples clearly leads to photocatalytic conversions higher than that exhibited by TiO_2 Degussa P25. This fact is even more significant if we consider that hydrothermally and calcined ZnO exhibit almost null surface area values. leading to a startling intrinsic photoactivity. The structural excellence (crystallinity, lack of defects, crystallite size, etc.) of such systems is clearly responsible for their high photoactivity values. (C) 2008 Elsevier B.V. All rights reserved.

Role of water in the CO oxidation reaction on Au/CeO_2: Modification of the surface properties

Romero-Sarria, F; Penkova, A; Martinez, LM; Centeno, MA; Hadjiivanov, K; Odriozola, JA
Applied Catalysis B-Environmental, **84** (2008) 119-124

A metallic monolith coated with 1% Au/CeO_2 Catalyst has been calcined at 300 degrees C and tested in the CO oxidation reaction both in "dry" and "wet" conditions. The light-off curves show a positive effect of the presence of water in the reactive feed on the catalytic activity. With the aim to explain these observations, a FTIR CO adsorption study at liquid nitrogen temperature was performed over a similar powder catalyst. At this low temperature the oxygen mobility from the bulk to the surface is minimized and then surface phenomena are evidenced. Both, the effect of different pre-treatments of the catalysts and the presence of pre-adsorbed water on the surface have been examined. The studies reveal that the previous treatment of the sample deeply affects the surface species and the gold particle size. The water addition provokes oxidation of the surface and improves the CO oxidation activity. (c) 2008 Elsevier B.V. All rights reserved.

Titania-supported gold catalysts: Comparison between the photochemical phenol oxidation and gaseous CO oxidation performances

Centeno, MA; Hidalgo, MC; Dominguez, MI; Navio, JA; Odriozola, JA
Catalysis Letters, **123** (2008) 198-206

A series of Au/TiO_2 samples with gold loadings ranging from 0.11% to 1.26% have been prepared by deposition-precipitation, characterised by means of XRD, S-BET, XRF, TEM, XPS and DR UV-Vis techniques and tested in the gaseous CO oxidation and photocatalytic degradation of phenol in aqueous media. The catalytic performances of the solids on both reactions depend on the gold content. Besides this, the gold particle size plays a determinant role in the catalytic activity for the CO reaction, but apparently its influence on the photocatalytic activity appears to be negligible and only very small gold particles seem to participate on the photocatalytic process. On the other hand, the electronic properties of the solids, measured by its band gap energy, are a key factor in the photochemical activity but do not have a clear influence in the CO oxidation reaction.

CO and VOCs oxidation over Pt/SiO_2 catalysts prepared using silicas obtained from stainless steel slags

Dominguez, MI; Barrio, I; Sanchez, M; Centeno, MA; Montes, M; Odriozola, JA
Catalysis Today, **133** (2008) 467-474

Stainless steels slags are mainly composed of low specific surface area calcium silicates together with a variable amount of metallic cations dispersed in such silicate matrix. These silicates due to their heavy metals content have to be considered as hazardous wastes that cannot be reclaimed easily. An alternative to reclamation is the production of valuable materials designed to accomplish processes without economic profit as the abatement of VOCs. In this paper we describe a method for obtaining high specific surface area (up to 290 m(2) g(-1)) metal-doped SiO_2 and SiO_2/ $Al2O_3$ supports for catalytic applications using as raw materials stainless steel slags. The acid digestion of these slags followed by a hydrothermal treatment results in transition metal oxides doped silicas and silica-aluminas that are used as support for platinum catalysts. The prepared catalysts are active in the total oxidation of CO and toluene, showing comparable activities to those shown by Pt catalysts supported on commercial SiO_2.(c) 2007 Elsevier B. V. All rights reserved.

The effect of ultrasound in the synthesis of clays used as catalysts in oxidation reactions

Perez, A; Centeno, MA; Odriozola, JA; Molina, R; Moreno, S
Catalysis Today, **133** (2008) 526-529

The effect of ultrasound in the modification of a Colombian bentonite pillared with mixed solutions of Al-Ce and Al-Ce-Fe was obtained. The solids were characterized by means of X-ray diffraction (XRD) and X-ray fluorescence (XRF) techniques. The catalysts were very efficient in the phenol oxidation reaction in diluted aqueous medium under mild experimental conditions (298 K and atmospheric pressure) and in the CO oxidation reaction. The use of ultrasound showed a clear effect in the synthesis of this type of solids allowing to make their synthesis in a shorter period of time and conserving the physical-chemical characteristics as well as catalytic activity in the oxidation reactions. (C) 2007 Elsevier B.V. All rights reserved.

Preparation of Au-CeO_2 and Au-Al_2O_3/AISI 304 austenitic stainless steel monoliths and their performance in the catalytic oxidation of CO

Martinez, LM; Frias, DM; Centeno, MA; Paul, A; Montes, M; Odriozola, JA
Chemical Engineering Journal, **136** (2008) 390-397

The use of austenitic stainless steel (AISI 304) as metallic substrate for monolithic catalytic devices is explored in this work as well as an alternative procedure to the washcoating of Al_2O_3 and CeO_2 supported Au catalysts. Thermal treatment of the metallic surface ensured a good adherence of the catalysts. Some preparation parameters, like the number of dipping and drying steps, were controlled in order to obtain an homogeneous and adherent layer of catalyst. The resulting surfaces were characterized by X-ray diffraction (XRD), N-2 Sorption and scanning electron microscopy (SEM), and were tested in the CO oxidation reaction. The highest conversion to CO_2 was obtained with the monolith coated with 1% Au-CeO_2 in the presence of water. (C) 2007 Elsevier B.V. All rights reserved.

Catalytic growth of carbon nanotubes on stainless steel: Characterization and frictional properties

Abad, MD; Sánchez-López, JC; Berenguer-Murcia, A; Golovko, VB; Cantoro, M; Wheatley, AEH; Fernandez, A; Johnson, BFG; Robertson, J
Diamond and Related Materials, **17** (2008) 1853-1857

Carbon nanotubes (CNTs) have been grown both on a sample of stainless steel (317-2R) and on the same steel coated with cobalt colloid nanoparticles. Both materials are suitable supports for the growth of vertically aligned carbon nanotubes, although a more sparse growth of significantly thicker carbon nanotubes is observed in the case of the bare steel. We find that carbon nanotubes grown directly on the stainless steel support show very poor tribological behaviour whereas the support using nanoparticles for carbon nanotube growth displayed interesting tribological properties with friction coefficients of approximately 0.1-0.2. The modified CNT material (studied by Raman spectroscopy) adheres to both mating surfaces avoiding direct contact between asperities and plough so the friction and wear processes decrease greatly. (C) 2008 Elsevier B.V. All rights reserved.

Degradation of phenylmercury compounds by heterogeneous photocatalysis over alpha-Fe_2O_3

Navio, JA; Cerrillos, C; Macias, M; Pradera, MA
Journal of Advanced Oxidation Technologies, **11** (2008) 411-416

We report here on the degradation of diphenylmercury and monophenylmercury chloride in air-equilibrated aqueous solutions by heterogeneous photocatalysis over alpha-Fe_2O_3. Photocatalysis proceeded via sequential de-phenylation leaving inorganic mercury. GC-MS analysis of the products revealed that photocatalytic degradation involved hydroxylation of the phenyl rings. Mechanistic features and photocatalytic activity were also studied and are reported upon.

Nanostructured Ti-M mixed-metal oxides: Toward a visible light-driven photocatalyst

Kubacka, A; Fernandez-Garcia, M; Colon, G
Journal of Catalysis, **254** (2008) 272-284

In this report we investigate the structure-activity relationship in Ti-M (M = V, Mo, Nb, W) mixed-metal oxides with anatase structure used for the photoelimination of toluene under sunlight-type excitation. These systems were prepared by a microemulsion method, and their physicochemical properties were characterized by a multitechnique approach using X-ray diffraction-Rietveld, photoelectron spectroscopy, and Raman and UV-visible spectroscopy. The preparation method allowed the incorporation of up to around 20 at % of Mo, Nb, and W, whereas a significantly inferior solubility limit, below 5 at % was observed for V. The presence of nonpunctual defects, intimately related to the existence of MOx clustering, produced electronic mid-gap states involved in charge recombination and appeared to be the most negative factor influencing photoactivity. The maximization of photoactivity occurred for Ti-M samples with the highest doing level, together with a minimum structural disturbance of the anatase-type structure. The physicochemical bases for the photoactivity behavior of the Ti-M samples as function of the M content and, in particular, the presence of partial (for a specific Ti-M series) or global maxima are discussed. (C) 2008 Elsevier Inc. All rights reserved.

Morphology changes induced by strong metal-support interaction on a Ni-ceria catalytic system

Gonzalez-DelaCruz, VM; Holgado, JP; Pereniguez, R; Caballero, A
Journal of Catalysis, **257** (2008) 307-314

The state of the nickel in a Ni/CeO_2 catalyst during hydrogen reduction, steam and dry reforming of methane, have been studied by means of in situ XAS spectroscopy. The catalyst was prepared by a combustion method and, after calcination, very small (about 10 nm) and homogeneous cubic particles of NiO are formed. Once reduced in hydrogen at high temperature (750 degrees C), the catalyst is active in both steam and dry reforming reactions of methane, but much more stable for the dry reforming reaction. In situ XAS analysis reveals that under reaction conditions at high temperature, the nickel remains completely reduced to Ni(0). However, under strongly reducing conditions (hydrogen or dry reforming at 750 degrees C), the Ni K-edge X-ray absorption spectrum undergoes unexpected modifications that, according to the parameters obtained by fitting analysis, come from changes in the size and morphology of nickel particles, which are now flattened and strongly stabilized on the partially reduced ceria surface. These morphology changes reflect a kind of strong metal-support interaction (SMSI), and could account for the higher stability observed for the dry reforming reaction. The flattened particles are not stable after cooling down to room temperature in hydrogen, while the coke deposited during the dry reforming reaction seems to block the particles, which partially remain even after cooling down to room temperature. (C) 2008 Elsevier Inc. All rights reserved.

Reactivity of lanthanum substituted cobaltites toward carbon particles

Hueso, JL; Caballero, A; Ocaña, M; Gonzalez-Elipe, AR
Journal of Catalysis, **257** (2008) 334-344

This work reports on the reactivity toward carbon of a $La_{0.5}Sr_{0.5}CoO_3$-delta perovskite prepared by spray pyrolysis. It is shown that this perovskite presents a moderate activity for the thermal oxidation of carbon, producing a decrease in its temperature of combustion of ca. 150 degrees C and a significant increase in the selectivity toward CO_2. Different experiments were carried out with electron energy loss spectroscopy (EELS) and X-ray photoemission spectroscopy (XPS) for the perovskite and its physical mixture with a high-surface area carbon material. In the physical mixture, the cobalt at the surface was partially reduced to Co^{2+} even at room temperature. XPS demonstrated a species of oxygen with low electron density at the catalyst surface. This species seemed to play a significant role in the oxidation processes at the perovskite surface. A model is proposed to account for the changes exhibited by the catalyst during its reaction with carbon. (c) 2008 Elsevier Inc. All rights reserved.

Apatite and Portland/apatite composite cements obtained using a hydrothermal method for retaining heavy metals

Dominguez, MI; Carpena, J; Borschnek, D; Centeno, MA; Odriozola, JA; Rose, J
Journal of Hazardous Materials, **150** (2008) 99-108

Apatite and Portland/apatite composite cements containing steelwork dusts have been prepared using a low temperature hydrothermal method (200 degrees C, 48 h). The produced solids were characterized by means of XRD, IR, and SEM-EDX, and the remaining liquid was analyzed by ICP. The results clearly show the capability of these cements to inertise the heavy metals contained in steelwork dusts, that is Fe, Pb, Mo, Cr, Mn, Ni, and Zn. In the case of apatitic cements, Fe, Mg, Cr, Mn, and Pb coming from steel dust replaced Ca in the divalent cation position of the apatite structure, while Si and Mo replaced P in tetrahedral position. The average crystal size of the apatite-containing dust is smaller than in pure apatite synthesized using the same procedure, which is related to the magnesium content of the dust, since magnesium seems to inhibit the crystal growth. XRD diagrams of composite cements show only peaks corresponding to phases observed in the single cements, and in that no new phases are found. However, EDX analysis reveals the introduction of cations coming from Portland cement into the apatite structure. From the results of water analysis it could be concluded that the capability of retention is higher in composite matrices than in the pure apatite one. In conclusion, the obtained data allow stating that the proposed method, the hydrothermal synthesis of steelwork dust containing cement, is a reliable one for immobilization of toxic residues containing heavy leachable cations. (c) 2007 Elsevier B.V. All rights reserved.

Photocatalytic degradation of 2,4-dichlorophenoxyacetic acid using nanocrystalline cryptomelane composite catalysts

Lemus, MA; Lopez, T; Recillas, S; Frias, DM; Montes, M; Delgado, JJ; Centeno, MA; Odriozola, JA
Journal of Molecular Catalysis A-Chemical, **281** (2008) 107-112

2,4-Dichlorophenoxyacetic acid is a common systemic herbicide used in the control of broadleaf weeds. It is the third-most widely used herbicide in the world. 2,4-D heterogeneous photocatalysis has emerged as a useful process to aid remediation of wastewater contamination. Manganese oxide with 2 x 2 tunnel structure, cryptomelane show good results in the photodegradation of 2,4-D and excellent performance in the photodegradation of methylene blue. The later as a consequence of the S-Mn interaction that favours the adsorption step in the photodegradation process. The existence of microporous manganese oxide minerals with the OMS structure may be an acceptable environmental solution for the remediation of wastewaters. (C) 2007 Elsevier B.V. All rights reserved.

Photocatalytic Degradation of 2,4-Dichlorophenoxyacetic Acid Over ZrO_2, Cu/ZrO_2 and Fe/ZrO_2 Photocatalysts Synthesized by Sol Gel Method

Alvarez, M; Lopez, T; Odriozola, JA; Gonzalez, RD
Journal of Nanoscience and Nanotechnology, **8** (2008) 6414-6418

Photocatalytic oxidation of 2,4-dichlorophenoxyacetic acid was performed over ZrO_2, Cu/ZrO_2 and Fe/ZrO_2 catalysts prepared by the sol-gel method. The samples were annealed at 400 degrees C. Textural and electronic characterization was carried out using BET and UV-Vis in order to establish the relationship between surface, pore volume and E. with the photoactivity of the materials. The degradation of the acid was followed by UV-Vis spectroscopy. The disappearance of the herbicide in solution follows approximately pseudo-first order kinetics. The apparent rate constants were calculated for the three catalysts. The results reveal that Fe/ZrO_2 exhibits the best photoactivity for the degradation of 2,4-dichlorophenoxyacetic acid.

Visible-light driven TiO_2 photocatalysts from Ti-oxychloride precursors

Sampedro, R; Colon, G; Fernandez-Garcia, M
Journal of Photochemistry and Photobiology A-Chemistry, **199** (2008) 136-143

Series of nanosized anion-containing TiO_2-base materials with anatase-type structure were synthesized from N, Cl-containing precursors using two preparation methods, calcination and hydrotreatment. Samples were conditioned by a final calcination step in order to get free of surface anion impurities and their structural properties characterized by a combined X-ray diffraction (XRD), scanning (SEM) and transmission (TEM) microscopy, X-ray energy dispersive (XEDS), X-ray photoelectron (XPS), and diffuse reflectance infrared Fourier transform (DRIFFS) Study. The structural characterization was used to interpret the UV-vis spectra. The resulting joint information allowed the rationalization of the photocatalytic activity observed for the visible-light-assisted liquid-phase degradation of phenol. We founded that maximization of photoactivity is not related with the net absorption power of our systems in the visible range but mostly driven by a combination of two characteristics; the adequate morphological properties and the presence of negatively charged N-containing species. (C) 2008 Elsevier B.V. All rights reserved.

Fast CO_2 sequestration by aerogel composites

Santos, A; Ajbary, M; Kherbeche, A; Pinero, M; De la Rosa-Fox, N; Esquivias, L
Journal of Sol-Gel Science and Technology, **45** (2008) 291-297

The increasingly evident impact of anthropogenic CO_2 emissions on climate change and associated environmental effects is stimulating the search for viable methods to remove this gas. One of the most promising strategies is the long-term storage of CO_2 in inert, insoluble and thermodynamically-stable materials. This strategy mimics the natural reactions that transform silicates into carbonates regulating the cycle of CO_2 on the surface of the Earth, operating on a geological time-scale. Consequently, the aim is to accelerate these reactions to be applicable on the timescale of human lives. We present the various technologies developed or proposed to date, based on this particular approach. The principal limiting factor is that high pressures and temperatures are required to produce appropriate materials capable of CO_2 sequestration and storage. Nevertheless, the synthetic materials known as aerogels can be modified in shape, size and chemical functionality so as to catalyse the process of CO_2 elimination through silicates (of Ca or Mg), considerably reducing the reaction time and working at atmospheric pressure and temperature.

Synthesis, characterization, and photodegradation behavior of single-phase anatase TiO_2 materials synthesized from Ti-oxychloride precursors

Colon, G; Sampedro, P; Fernandez-Garcia, M; Chen, HY; Hanson, JC; Rodriguez, JA
Langmuir, **24** (2008) 11111-11118

Single-phase anatase-TiO_2 nanomaterials with a size of ca. 10 nm and variable quantities of anion impurities were prepared using a novel pathway based on the use of amorphous ammonium Ti-oxychloride precursors synthesized using Ti/Cl initial ratios between 1 and 6. The precursor nature and evolution under thermal treatment were studied using chemical analysis, XRD, XPS, DRIFTS, and mass spectrometry. The nature and concentration of anatase-TiO_2 materials anion impurities were analyzed by XPS and DRIFTS. It is shown that negatively charged impurities located in substitutional positions of the anatase network are maximized for a sample synthesized using a Ti/Cl 1:1 atomic ratio and are responsible for the elimination of liquid-phase (phenol) and gas-phase (isopropanol or methylcyclohexane) pollutants under sunlight excitation. A link is established among the initial chemical characterization of the precursors, the final morphological, structural, and chemical composition of the oxide materials, and their photochemical properties.

Acidity characterization of a titanium and sulfate modified vermiculite

Hernandez, WY; Centeno, MA; Odriozola, JA; Moreno, S; Molina, R

Materials Research Bulletin, **43** (2008) 1630-1640

A natural vermiculite has been modified with titanium and sulfated by the intercalation and impregnation method in order to optimize the acidity of the clay mineral, and characterization of samples were analyzed by X-ray fluorescence (XRF), X-ray diffraction (XRD), nitrogen adsorption isotherms, diffuse reflectance infrared Fourier transform spectroscopy (DRIFTS) and temperature programmed desorption with ammonia (TPD-NH3). All the modified solids have a significantly higher number of acidic sites with respect to the parent material and in all of these, Bronsted as well as Lewis acidity are identified. The presence of sulfate appears not to increase the number of acidic centers in the modified clay. For the materials sulfated with the intercalation method, it is observed that the strength of the acidic sites found in the material increases with the nominal sulfate/metal ratio. Nevertheless, when elevated quantities of sulfur are deposited, diffusion problems in the heptane reaction appear.

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

Growth and characterization of the ZnO/ZnS bilayer obtained by chemical spray pyrolysis

Lopez, MC; Espinos, JP; Leinen, D; Martin, F; Centeno, SP; Romero, R; Ramos-Barrado, JR

Applied Surface Science, **255** (2008) 2118-2124

ZnO/ZnS bilayer antireflection coatings have been prepared by spray pyrolysis using aqueous solutions of zinc acetate and thiourea or zinc chloride and thiourea. The structure, surface morphology, chemical composition and optical transmittance of the bilayer have been examined as a function of the composition of the initial solution. X-ray photoelectron spectroscopy analysis and Ar ion-beam sputter etching was carried out to obtain a depth pro. le of bilayer. Neither carbon nor other by-products, which could alter the optical transmittance of the bilayer were found in either the interface or bulk. The differences between the bilayers arise from the annealing of the ZnS underlayer, as well as the precursor used to prepare it. (C) 2008 Elsevier B. V. All rights reserved.

On the argon and oxygen incorporation into SiOx through ion implantation during reactive plasma magnetron sputter deposition

Van Hattum, ED; Boltje, DB; Palmero, A; Arnoldbik, WM; Rudolph, H; Habraken, FHPM

Applied Surface Science, **255** (2008) 3079-3084

The incorporation of argon in SiOx (0 <= x <= 2) during reactive plasma magnetron sputter deposition using a O-2/Ar plasma and a silicon sputter cathode has been investigated and related to the flux of argon ions created in the plasma afterglow region on the growth surface. The argon concentration in the grown films appears to be mainly a function of the x-value, independent of the extent of ion bombardment on the growing surface, and only slightly dependent on the substrate temperature during the growth (<400 degrees C). The argon concentration amounts to 4.0 at.% for the x = 0. film. It shows a maximum above 5 at.% for an x-value around 0.3, and decreases monotonously for increasing x-values until it is essentially 0 for x = 2.0. It is proposed that the measured concentration of argon is a result of implantation and subsequent desorption. The latter process is suggested to be dependent on the x-value. The independence of the concentration of incorporated argon on the relative ion flux is explained by a quasi-saturation state of the process. The incorporation of oxygen as a result of oxygen ion implantation, similar to the Ar incorporation, becomes apparent since values for x > 2 are reached. (C) 2008 Elsevier B.V. All rights reserved.

Synthesis of Spherical Down- and Up-Conversion $NaYF_4$-Based Nanophosphors with Tunable Size in Ethylene Glycol without Surfactants or Capping Additives

Nunez, NO; Miguez, H; Quintanilla, M; Cantelar, E; Cusso, F; Ocaña, M

European Journal of Inorganic Chemistry, **2008 -** 19 (2008) 4517-4524

A very simple route for the synthesis of spherical down-conversion (DC) and up-conversion (UC) $NaYF_4$-based nanophosphors is described which consists of a precipitation reaction at rather low temperature (max. 120 degrees C) from solutions containing sodium fluoride and appropriate Ln precursors in a common solvent (ethylene glycol/water mixtures), without the use of any other additive (complexing agent or surfactant). The role played by the nature of the yttrium precursor and the solvent on the morphological characteristics of the nanoparticles is discussed. The size of the nanospheres, which crystallized in the cubic alpha-NaYF4 phase, could be tuned within the 45-155 nm range by adjusting the reaction parameters (temperature and ethylene glycol/water ratio). The applicability of this method is illustrated for the synthesis of Eu-III-doped (DC), Tb-III-doped (DC) and Yb-III/Er-III codoped (UC) NaYF4 nanophosphors, whose luminescent properties were also analysed. (C) Wiley-VCH Verlag GmbH & Co. KGaA, 69451 Weinheim, Germany, 2008).

Microstructural and chemical characterisation techniques for nanostructured and amorphous coatings

Godinho, V; Fernandez-Ramos, C; Martinez-Martinez, D; Garcia-Lopez, J; Sanchez-Lopez, JC; Fernandez, A

European Physical Journal-Applied Physics, **43** (2008) 333-341

A full characterization of amorphous or nanostructured coatings at the microstructural level has some intrinsic difficulties associated with the lack of long range order and reference compounds, which often make difficult their study. Only by the combination of different characterization techniques is possible in many cases to achieve valuable chemical and structural information. In this paper, three different systems were used to illustrate how the combination of characterization techniques, as TEM associated to ED or EELS, EFTEM, SEM, XPS, RBS and XRD was determinant to correlate microstructure with deposition parameters and properties in such complex systems. The coatings were deposited on silicon and AISI M2 steel substrates by magnetron sputtering under different Ar/N-2 gas mixtures from Ti and C targets (system 1 and 2) or a Si target (system 3). In each case, the performed characterization allowed to get a deeper understanding of the whole system and explain their mechanical response. The studied systems are: (i) Ti-TiN-CNx multilayered coatings: the chemical and structural analysis shows that a gradual enrichment in nitrogen and nitride phases from the metallic substrate to the CNx top layer is responsible for the improvement of the adhesion properties. (ii) Ti-C-N: the existence of a nanocrystalline TiC phase embedded in an amorphous carbon matrix is demonstrated by the microstructural and chemical analysis for samples prepared under pure Ar. When N-2 is introduced in the gas phase, the nanocrystalline structure is not seen and the chemical composition is enriched in amorphous non-stoichiometric CNx. (iii) SiOxNy: although the coatings present similar composition, small differences in microstructure are observed, which can be responsible for different mechanical properties.

Influence of the chemical and electronic structure on the electrical behavior of zirconium oxynitride films

Carvalho, P; Chappe, JM; Cunha, L; Lanceros-Mendez, S; Alpuim, P; Vaz, F; Alves, E; Rousselot, C; Espinos, JP; Gonzalez-Elipe, AR

Journal of Applied Physics, **103** (2008) 104907 -104921

This work is devoted to the investigation of decorative zirconium oxynitride, ZrOxNy, films prepared by dc reactive magnetron sputtering, using a 17:3 nitrogen-to-oxygen-ratio gas mixture. The color of the films changed from metallic-like, very bright yellow pale, and golden yellow, for low gas mixture flows [from 0 to about 9 SCCM (SCCM denotes cubic centimeter per minute at STP)] to red brownish for intermediate gas flows (values up to 12 SCCM). Associated to this color change there is a significant decrease of brightness. With further increase of the reactive gas flow, the color of the samples changed from red brownish to dark blue (samples prepared with 13 and 14 SCCM). The films deposited with gas flows above 14 SCCM showed only apparent colorations due to interference effects. This change in optical behavior from opaque to transparent (characteristic of a transition from metallic to insulating-type materials), promoted by the change in gas flow values, revealed that significant changes were occurring in the film structure and electronic properties, thus opening new potential applications for the films, beyond those of purely decorative ones. Taking this into account, the electrical behavior of the films was investigated as a function of the reactive gas flow and correlated with the observed chemical, electronic, and structural features. The variations in composition disclosed the existence of four different zones, which were correlated to different crystalline structures. For the so-called zone I, x-ray diffraction revealed the development of films with a B1 NaCl face-centered cubic zirconium nitride-type phase, with some texture changes. Increasing the reactive gas flow, the structure of the films is that of a poorly crystallized overstoichiometric nitride phase, which may be similar to that of Zr_3N_4, but with some probable oxygen inclusions within nitrogen positions. This region was characterized as zone II. Zone III was indexed as an oxynitride-type phase, similar to that of gamma-Zr_2ON_2 with some oxygen atoms occupying some of the nitrogen positions. Finally, occurring at the highest flow rates, zone IV was assigned to a ZrO_2 monoclinic-type structure. The composition/structure variations were consistent with the chemical bonding analysis carried out by x-ray photoelectron spectroscopy, which showed oxygen doping in both Zr_3N_4- and ZrNtype grown films. The electronic properties of the films exhibited significant changes from zone to zone. Resistivity measurements revealed a very wide range of values, varying from relatively highly conductive materials (for zone I) with resistivity values around few hundreds of mu Omega cm to highly insulating films within zones III and IV, which presented resistivity values in the order of 10(15) mu Omega cm. Regarding zone II, corresponding to oxygen doped Zr_3N_4-type compounds, the observed behavior revealed resistivity values increasing steeply from about 10(3) up to 10(15) mu Omega cm, indicating a systematic transition from metallic to insulating regimes. (C) 2008 American Institute of Physics.

Sorption properties of mesoporous multilayer thin films

Fuertes, MC; Colodrero, S; Lozano, G; Gonzalez-Elipe, AR; Grosso, D; Boissiere, C; Sanchez, C; Soler-Illia, GJDAA; Miguez, H
Journal of Physical Chemistry C, **112** (2008) 3157 -3163

The vapor sorption properties of multilayers made of ordered mesoporous thin films with tailored composition and mesostructure are herein investigated. Optical reflectance measurements versus partial pressure of several vapors are performed to analyze the interplay between the affinity to and the accessibility of the different types of layers in the structure. We find that the behavior of a mesoporous oxide layer within the multilayer largely differs from that of the isolated thin film, its sorption properties being determined by the interaction with neighboring films. An explanation of the phenomena observed in these complex systems is provided in terms of the pore size, the affinity of each type of layer to specific compounds, and the effect of neighboring layers in the sorption properties of bilayers by an independent environmental ellipsometric study.

Plasmas and atom beam activation of the surface of polymers

Lopez-Santos, C; Yubero, F; Cotrino, J; Barranco, A; Gonzalez-Elipe, AR
Journal of Physics D-Applied Physics C, **41** (2008) 225209 -225220

Wetting properties of polyethylene terephthalate (PET) and low-density polyethylene polymers have been investigated after treatment with a microwave (MW) plasma discharge at low pressure and a dielectric barrier discharge at atmospheric pressure. Experiments have also been carried out in situ with an atom source installed in an x- ray photoemission spectrometer (XPS). The water contact angle measured on both polymers experienced a significant decrease after activation, but a progressive recovery up to different values after ageing. Standard chemical analysis by XPS showed that the plasma and oxygen beam treatments produced an increase in the concentration of -C(O) x functional groups at the outermost surface layers of the treated polymers. Besides, the oxygen distribution between the topmost surface layer and the bulk has been obtained by non- destructive XPS peak shape analysis. Atomic force microscopy analysis of the surface topography showed that, except for PET treated with the MW plasma and the atom beam, the surface roughness increased after the plasma treatments. Wetting angle variations, oxygen content and distribution, surface roughness and evolution of these properties with time are comparatively discussed by taking into account the basic processes that each type of activation procedure induces in the outmost surface layers of the treated polymers.

Reversible superhydrophobic to superhydrophilic conversion of Ag@TiO_2 composite nanofiber surfaces

Borras, A; Barranco, A; Gonzalez-Elipe, AR
Langmuir, **24** (2008) 8021-8026

A new type of superhydrophobic material consisting of a surface with supported Ag@TiO_2 core-shell nanofibers has been prepared at low temperature by plasma-enhanced chemical vapor deposition (PECVD). The fibers are formed by an inner nanocrystalline silver thread which is covered by a TiO_2 overlayer. Water contact angles depend on the width of the fibers and on their surface concentration, reaching a maximum wetting angle close to 180 degrees for a surface concentration of similar to 15 fibers mu m(-2) and a thickness of 200 nm. When irradiated with UV light, these surfaces become superhydrophilic (i.e., 0 degrees contact angle). The decrease rate of the contact angle depends on both the crystalline state of the titania and on the size of the individual TiO_2 domains covering the fibers. To the best of our knowledge, this is one of the few examples existing in the literature where a superhydrophobic surface transforms reversibly into a superhydrophilic one as an effect of light irradiation.

Preillumination of TiO_2 and Ta_2O_5 photoactive thin films as a tool to tailor the synthesis of composite materials

Sanchez-Valencia, JR; Borras, A; Barranco, A; Rico, VJ; Espinos, JP; Gonzalez-Elipe, AR
Langmuir, **24** (2008) 9460-9469

Illumination of TiO_2 thin films with UV light is known to induce the transformation of the surface of this material from partially hydrophobic into fully hydrophilic. The present work shows that this transformation is accompanied by other effects that may be used to control the synthesis of composite materials. For this purpose, TiO_2 and Ta_2O_5 transparent thin films with a columnar structure and open pores were prepared by electron evaporation at glancing angles. Transparent TiO_2 thin films with micropores (i.e., pores smaller than 2 nm) prepared by plasma enhanced chemical vapor deposition (PECVD) were also used. All these films became hydrophilic upon UV illumination. Rhodamine 6G and Rhodamine 800 dyes were irreversibly adsorbed within the columns of the TiO_2 and Ta_2O_5 thin films by immersion into a water solution of these molecules. Isolated and aggregated molecules of these two dyes were detected by visible absorption spectroscopy. The infiltration adsorption efficiency was directly correlated with the acidity of the medium, increasing at basic pHs as expected from simple considerations based on the concepts of the point of zero charge (PZC) in colloidal oxides. The infiltration experiments were repeated with columnar TiO_2 and Ta_2O_5 thin films that were subjected to preillumination with UV light. It was found that this treatment produced a modification in the type (isolated or aggregated) and amount of dye molecules incorporated into the pores. Moreover, the selective adsorption of a given dye in preilluminated areas of the films permitted the lithographic coloring of the films. Preillumination also controls the UV induced deposition of silver on the Surface of the microporous TiO_2 thin films. It was found that the size distribution of the formed silver nanoparticles was dependent on the preillumination treatment and that a well-resolved surface plasmon resonance at around 500 nm was only monitored in the preilluminated films. A model is proposed to account for the effects induced by UV preillumination on the TiO_2 and Ta_2O_5 oxide surfaces. The possibilities of this type of light treatment for the tailored synthesis of nanocomposite thin films (i.e., dye-oxide, metal nanoparticles-oxide) are highlighted.

Optical properties of Zr and ZrO_2 films deposited by laser ablation

Prieto-Lopez, LO; Yubero, F; Machorro, R; De La Cruz, W
Microelectronics Journal, **24** (2008) 1371-1373

Optical properties of Zr and ZrO_2 films in the energy range from 1.5 to 100eV were obtained by quantitative analysis of reflection electron energy loss spectroscopy (REELS) and ellipsometry. The films were prepared oil (I 1 1) silicon substrates by reactive laser ablation using a zirconium target. For the growth of ZrO_2 films a pressure of 5 m Torr of oxygen in the growth chamber was used. The substrate temperature during deposition was 400 degrees C. The deposits were Studied ex situ by X-ray diffraction (XRD) and in situ by X-ray photoelectron spectroscopy (XPS) and REELS. The ZrO_2 films were found to be polycrystalline With monoclinic structure. The XPS results showed that the oxygen pressure used is the optimal control to produce ZrO_2 films by laser ablation. A gap of 5eV for the ZrO_2 film W IS measured by REELS. (C) 2008 Elsevier Lid. All rights reserved.

Nanostructural control in solution-derived epitaxial $Ce_{1-x}Gd_xO_2$-y films

Coll, M; Gazquez, J; Sandiumenge, F; Puig, T; Obradors, X; Espinos, JP; Huhne, R
Nanotechnology, **19** (2008) 395601-395607

A novel mechanism based on aliovalent doping, allowing fine tuning of the nanostructure and surface topography of solution-derived ceria films, is reported. While under reducing atmospheric conditions, non-doped ceria films are inherently polycrystalline due to an interstitial amorphous Ce_2C_3 phase that inhibits grain growth, a high quality epitaxial film can be achieved simply by doping with Gd^{3+} cations. Gd^{3+} <-> Ce^{4+} substitutions within the lattice are accompanied by charge-compensating oxygen vacancies throughout the volume of the crystallites acting as an efficient vehicle to reduce the barrier for grain boundary motion caused by interstitial Ce_2C_3. In this way, the original nanostructure is self-purified by pushing the amorphous Ce_2C_3 phase towards the free surface of the film. Once a full epitaxial cube-on-cube oriented ceria film is obtained, its surface morphology is dictated by the interplay between faceting on low energy {110} and/or {111} pyramidal planes and truncation of those pyramids by (001) ones. The development of the latter requires the suppression of their polar character which is thought to be achieved by charge compensation between the dopand and oxygen along < 100 > directions.

UV irradiation effects on TiO_2 thin films

Fernandez-Rodriguez, M; Rico, VJ; Gonzalez-Elipe, AR; Alvarez-Herrero, A
Physica Status Solidi C-Current Topics in Solid State Physics, **5** (2008) 1164-1167

This paper presents the behaviour of a standard optical coating to be used in aerospace applications when exposed to ultraviolet (UV) irradiation. Ellipsometric measurements are carried out in order to monitor the effects produced on the optical properties of the TiO_2 film when it is exposed to a 500 W Xenon lamp during the time intervals of 1 hour, 22 hours and 42 hours. The ellipsometric measurements show that main changes occur in the real part of the refractive index after the first hour of exposure to UV irradiation. To assess a possible relation between the hydrophilicity that the UV irradiation typically induces on the TiO_2 film, and the variation of the optical properties of the film, the water contact angle on the TiO_2 optical coating was also measured after irradiation under similar conditions.

Interface effects in the Ni 2p x-ray photoelectron spectra of NiO thin films grown on oxide substrates

Preda, I; Gutierrez, A; Abbate, M; Yubero, F; Mendez, J; Alvarez, L; Soriano, L
Physical Review B, **77** (2008) 075411

We report the Ni 2p x-ray photoelectron spectra of NiO thin films grown on different oxide substrates, namely, SiO_2, Al_2O_3, and MgO. The main line of the Ni 2p spectra is attributed to the bulk component, and the shoulder at 1.5 eV higher binding energies to the surface component. The spectra of the NiO thin films show strong differences with respect to that of bulk NiO. The energy separation between the main peak and the shoulder increases with the substrate covalence. This indicates the strong covalent interactions between the NiO thin films and the oxide substrates, and reflects changes in the bonding at the interface from a more ionic to a more covalent interaction. These conclusions are supported by cluster model calculations with a reduced O 2p-Ni 3d hybridization.

In situ XPS studies of laser induced surface cleaning and nitridation of Ti

Lahoz, R; Espinos, JP; de la Fuente, GF; Gonzalez-Elipe, AR
Surface & Coatings Technology, **202** (2008) 1486-1492

A titanium foil has been subjected to laser irradiation "in situ" in a pre-chamber of an X-ray photoemission spectrometer under different atmospheres (vacuum, Ar, 02, air, N-2 and H-2). As a result of these treatments, a high amount of the carbon contamination layer was removed and other changes in composition were induced. Nitridation was achieved by laser irradiation under nitrogen. The most effective treatment protocol included an initial cleaning procedure induced by irradiation in vacuum, followed by a second irradiation process performed under nitrogen. Partial nitridation is also observed when irradiating under synthetic air. Lateral and depth analysis of the nitrogen concentration around the laser spot has been also carried out. It is found that the outermost layers present a similar concentration of nitrogen. In addition, the measured nitrogen profile indicates that the amount of nitrogen within the laser spot region is relatively lower than within the immediately surrounding area. Almost no nitrogen remains in the spot area after sputtering for 30 min. A model is proposed to account for the observed titanium surface nitridation processes. (c) 2007 Elsevier B.V. All rights reserved.

Tribological behaviour of titanium carbide/amorphous carbon nanocomposite coatings: From macro to the micro-scale

Sanchez-Lopez, JC; Martinez-Martinez, D; Lopez-Cartes, C; Fernandez, A
Surface & Coatings Technology, **202** (2008) 4011-4018

The tribological behaviour of nanocomposite coatings made of nanocrystalline metal carbides and amorphous carbon (a-C) prepared by PVD/CVD techniques is found to be very dependant on the film deposition technique, synthesis conditions and testing parameters. Focusing in the TiC/amorphous carbon-based nanostructured system, this paper is devoted to an assessment of the factors governing the tribological performance of this family of nanocomposites using a series of TiC/a-C films prepared by magnetron sputtering technique varying the power applied to each target (titanium or graphite) as model system to establish correlations between film microstructure and chemical compositions and tribological properties measured by a pin-on-disk tribometer. The film microstructure goes from a quasi - polycrystalline TiC to a nanocomposite formed by nanocrystals of TiC embedded in an amorphous carbon matrix as observed by transmission electron microscopy (TEM). The nanocrystalline/amorphous ratio appears to be the key-parameter to control the tribological properties and its quantification has been done by electron energy-loss spectroscopy (EELS). A significant change in the tribological performance is observed for nanocomposites with amorphous carbon phase contents above 60-65%. The friction coefficient decreases from 0.3 to 0.1 and the film wear rates by a factor of 10. Examination of the wear scars on ball and film surfaces by laser micro-Raman spectroscopy has allowed to determine the presence of metallic oxides and carbonaceous compounds responsible of the observed friction behaviour. The revision of the literature results in view of the conclusions obtained enabled to explain their apparent dispersion in the tribological performance. (c) 2008 Elsevier B.V. All rights reserved.

Comparative performance of nanocomposite coatings of TiC or TiN dispersed in a-C matrixes

Martinez-Martinez, D; Lopez-Cartes, C; Fernandez, A; Sanchez-Lopez, JC
Surface & Coatings Technology, **203** (2008) 756-760

Titanium carbide (TiC) and nitride (TiN) are two of the most used materials in the field of protective coatings, due to their optimal mechanical and tribological properties. The addition of the second phase can provide extra benefits to the coating, like improved hardness, reduced friction and/or oxidation resistance. In this work, we present two series of coatings in which hard crystalline TiC and TiN phases are mixed at the nanometric level with a soft lubricant phase like amorphous carbon (a-C). Both series of TiC/a-C and TiN/a-C nanocomposite coatings were prepared by double magnetron sputtering of C and Ti(N) targets in a Ar atmosphere (P = 5 x 10(-3) Torr) by changing the power ratio applied to each magnetron. The chemical composition has been measured by electron energy loss spectroscopy, and the phase composition changes gradually from pure C to pure TiC or TiN through nanocomposite structures with variable phase contents. These structures are confirmed by transmission electron microscopy and diffraction techniques. like X-ray diffraction and electron diffraction. The mechanical and tribological properties are found to be mainly controlled by the hard/soft phase ratio present in the coating. The changes in hardness values follow similar trends in both types of nanocomposite samples. Introducing a small amount of TiN or TiC into a-C matrix causes a hardness reduction, but further addition of crystalline phase makes increase the hardness. The best tribological properties are found for nanocomposite coatings (both TiN/a-C and TiC/a-C) with high amount of a-C (> 65%), showing low friction values (f similar to 0.1) and high wear resistance (k about 10(-7) mm(3) N-1 m(-1)).

However, coatings with 50-60% a-C show a good compromise between tribological and mechanical properties. (C) 2008 Elsevier B.V. All rights

Preparation and properties of $La_{1-x}Ag_yMnO_3$+delta thin epitaxial films

Gorbenko, OY; Melnikov, OV; Kaul, AR; Koroleva, LI; Babushkina, NA; Taldenkov, AN; Inyushkin, AV; Barranco, A; Szymczak, R

Thin Solid Films, **516** (2008) 3783-3790

We report here the preparation and properties of $La_{1-x}Ag_yMnO_3$+delta thin epitaxial films. The original two-step preparation procedure was developed. At first, $La_{1-x}MnO_3$+delta were grown epitaxially by metal-organic chemical vapor deposition on the single-crystal substrates (001) and (110) $SrTiO_3$, (001) $LaAlO_3$, (111) and (001) $ZrO_2(Y_2O_3)$. Treatment by the vapor of the metallic silver in the oxygen atmosphere (at 1 bar and 20 bar) was the second step resulting in the selective absorption of silver by $La_{1-x}MnO_3$+delta phase. The value of y depended on the process conditions and revealed different kinetics of the silver absorption for (001) and (110) orientation of $La_{1-x}MnO_3$+delta films. The films prepared were characterized by X-ray diffraction, scanning electron microscopy with energy-dispersion X-ray analysis, high resolution transmission electron microscopy, X-ray photoelectron spectroscopy, electrical resistivity and magnetoresistance measurements in a four-probe configuration. We have found that metal-insulator transition temperature (T-p) in the series $La_{1-x}Ag_xMnO_3$+delta possessed a maximum of 380 K at x=0.15. Thus, T-p of $La_{1-x}AgMnO_3$+delta films was significantly higher than ever reported in the literature for the $La_{1-x}Ag_xMnO_3$+delta ceramics. $La_{1-x}Ag_xMnO_3$+delta films demonstrated the important role of the ferromagnetic fluctuations above Curie temperature T, resulting in the sign change of the resistivity curve temperature slope dR/dT and a significant shift of T-p well above T-c. The maximum of the magnetoresistance on the temperature scale was close to dR/dT maximum. The intrinsic magnetoresistance values as high as 22% at 310 K and 50% at 280 K were measured in the magnetic field of 1 T in the series of $La_{1-x}AgyMnO_3$+delta epitaxial films. (c) 2007 Elsevier B.V. All rights reserved.

NANOPARTÍCULAS Y NANOCOMPOSITES PARA APLICACIONES TECNOLÓGICAS / NANOPARTICLES AND NANOCOMPOSITES FOR TECHNOLOGICAL APPLICATIONS

Pt/TiO2 brain biocompatible nanoparticles: GBM treatment using the C6 model in Wistar rats

Lopez, T; Recillas, S; Guevara, P; Sotelo, J; Alvarez, M; Odriozola, JA

Acta Biomaterialia, **4** (2008) 2037-2044

In the present work we synthesized inorganic oxide nanoparticle carriers of platinum compounds and tested their therapeutic effect on animal models in which C6 glioma cells have been inoculated. TiO_2-containing Pt(NH3)(4)Cl-2 complexes were synthesized using sol-gel methods. The platinum species are chemically bonded to the TiO_2 carrier, as shown by Fourier transform infrared spectroscopy of probe molecules. Treatment with TiO2-Pt nanoparticles reduces tumour growth rate by up to 56%, showing that a synergistic effect exists between the TiO_2 carrier and the platinum drug. (C) 2008 Acta Materialia Inc. Published by Elsevier Ltd. All rights reserved.

Permanent magnetism in thiol capped nanoparticles, gold and ZnO

Crespo, P; Garcia, MA; Fernandez-Pinel, E; De la Venta, J; Merino, JM; Quesada, A; Hernando, A; Fernandez, A; Penades, S
Acta Physica Polonica A, **113** (2008) 515-520

In spite of the diamagnetic behavior exhibited by bulk ZnO and Au, a ferromagnetic-like behavior is induced in nanoparticles of both systems by appropriate surface functionalization. By capping with thiol derivatized molecules, magnetic hysteresis is observed even at room temperature, whereas the magnetization has a very little temperature dependence. Capping induces an alteration of their electronic configuration that depends on the capping molecule, as evidenced by X-ray absorption spectroscopy, that strongly affects their magnetic properties.

Photoconducting Bragg Mirrors based on TiO_2 Nanoparticle Multilayers

Calvo, ME; Colodrero, S; Rojas, TC; Anta, JA; OcaÑa, M; Miguez, H
Advanced Functional Materials, **18** (2008) 2708-2715

A synthetic route to building photoconducting films of TiO_2 nanoparticles that display bright structural color is presented. The color arises as a result of the periodic modulation of the refractive index, which is achieved by controlling the degree of porosity of each alternate layer through the particle size distribution of the precursor suspensions. The suspensions are cast in the shape of a film by spin-coating, which allows tailoring of the lattice parameter of the periodic multilayer, thus tuning the Bragg peak spectral position (i.e., its color) over the entire visible region. Photoelectrochemical measurements show that the Bragg mirrors are conductive and distort the photocurrent response as a result of the interplay between photon and electron transport.

Synthesis of Supported Single-Crystalline Organic Nanowires by Physical Vapor Deposition

Borras, A; Aguirre, M; Groening, O; Lopez-Cartes, C; Groening, P
Chemistry of Materials, **20** (2008) 7371-7373

Fe^{3+} intercalation/deposition on vermiculites and interaction with pyrrole: a Mossbauer spectroscopic investigation

Ramirez-Valle, V; Lerf, A; Wagner, FE; Poyato, J; Perez-Rodriguez, JL
Clay Minerals, **43** (2008) 487-499

The Fe^{3+} uptake from aqueous and methanol solutions of FeCl(3)6H(2)O in two vermiculites from Santa Olalla and Ojen (Spain) and in a montmorillonite from Wyoming has been investigated by Mossbauer spectroscopy at room temperature and 4.2 K. The samples were further characterized by X-ray diffraction. The low temperature Mossbauer spectra reveal the deposition of akaganeite and perhaps some ferrihydrite on the external surface of the clay minerals. The room temperature spectra exhibit two Fe^{3+} quadrupole doublets in addition to the Fe^{2+} components of the structural iron in the sheet silicates. On treatment in >= 0.04 M Fe^{3+} solutions the Fe3+ quadrupole splittings of 0.90 mm/s and 0.55 mm/s can be assigned to the mineral akaganeite; at smaller Fe^{3+} concentrations one of these doublets has a quadrupole splitting similar to that of the Fe^{3+} in the original vermiculites, the other one a quadrupole splitting of 0.6-0.7 mm/s. which can be considered as a hint for an uptake of Fe dimers in the interlayer space irrespective of the solvent used for iron deposition. Preliminary results show that the adsorption of pyrrole in all of our Fe^{3+}-containing samples, regardless of the preparation in aqueous or methanol solution, results in the formation of polypyrrole and a concomitant reduction of some of the Fe^{3+}. An uptake of pyrrole into the interlayer space has been observed only in the Fe^{3+}-containing Wyoming montmorillonite and in the Ojen vermiculite treated with the methanol solution of iron chloride.

The behavior of Fe in ground and acid-treated vermiculite from Santa Olalla, Spain

Maqueda, C; Romero, AS; Morillo, E; Perez-Rodriguez, JL; Lerf, A; Wagner, FE
Clays and Clay Minerals, **56** (2008) 380-388

The preparation of porous materials from clay minerals by selective leaching is of interest because it yields residues with large specific surface areas that can be used as adsorbents of contaminants or as catalysts. Grinding produces surface modifications and therefore may significantly influence the leaching behavior. The aim of this paper is to study the effect of grinding and leaching on the structure of the vermiculite from Santa Olalla, Spain, using Fe-57 Mossbauer spectroscopy, X-ray diffraction, infrared spectroscopy, and specific surface area (S-BET) measurements. The study shows that grinding destroys the long range order of the vermiculite, but leaves the local structure in the environment of the Fe atoms intact, at least up to a grinding time of 10 min. The Mossbauer study shows that there is no Fe 3 in the tetrahedral sheets and that grinding does not lead to a significant oxidation of the structural Fe. Vermiculite ground for 4 min and leached with 1 M HCl solution at 80 degrees C over a 24 h period was decomposed to X-ray amorphous silica with a very large specific surface area (S-BET = 720 m(2)g(-1)) and with total pore volume of 0.586 cm(3) g(-1), whereas an unground sample leached with the same acid concentration yielded a specific surface area of only 504 m(2) g(-1). Most of the Mg^{2+} and Al^{3+} are removed from the ground sample after leaching with 1 M HCl, while large percentages of Fe_2O_3 remain with the X-ray amorphous silica. In unground vermiculite leached with 1 M HCl, a considerable amount of vermiculite remains in the residue. A sample ground for 4 min and treated with 0.25 M HCl also shows the typical vermiculite Mossbauer spectrum with an Fe^{2+}/Fe^{3+} ratio similar to that of the unground vermiculite. The samples ground for 2 or 4 min and treated with 1 M HCl solution have an orange color and, according to the Mossbauer spectra, only Fe3+ remains. Mossbauer spectra of these samples taken at 4.2 K reveal the presence of akaganetite.

Brown ceramic pigments based on chromium(III)-doped titanite obtained by spray pyrolysis

Lyubenova, TS; Ocaña, M; Carda, J
Dyes and Pigments, **79** (2008) 265-269

Cr-doped titanite ($CaTiSiO_5$) pigments were synthesized through spray pyrolysis of aerosols generated from aqueous solutions containing colloidal silica, calcium chloride, titanium(IV) oxychloride and chromium(III) nitrate. This process yielded amorphous powders with spherical morphology and broad size distribution (<10 mu m) after thermal decomposition at 600 degrees C. The titanite phase was obtained by further calcination at 800 degrees C without any addition of flux agents. The brown color of the pigments can be attributed mainly to the existence of Cr(IV) ions occupying both, octahedral positions of Ti(IV) and tetrahedral position of Si(IV), together with a small amount of Cr(III) present as Cr_2O_3. The optimum pigment obtained by this method corresponded to a Cr/titanite mole ratio of 0.04. (C) 2008 Elsevier Ltd. All rights reserved.

Influence of the Capping Molecule on the Magnetic Behavior of Thiol-Capped Gold Nanoparticles

Crespo, P; Guerrero, E; Muñoz-Marquez, MA; Hernando, A; Fernandez, A
IEEE Transactions on Magnetics, **44** (2008) 2768-2771

Gold nanoparticles with an average particle size below 3 nm have been synthesized and stabilized with different thiol-derivatized molecules for studying the influence of the capping molecule on the magnetic behavior. Thiolated-alkane chains with different lengths as well as a thiol-containing biomolecule (tiopronin) have been selected as protecting shells for the synthesized NPs. Magnetic characterization indicates that the appearance of a ferromagnetic-like behavior is related not only with the formation of Au-S bonds linking the protective molecules to the nanoparticle surface but also with the formation of the nanoparticle itself as well as with the geometry of the capping molecule. The later seems to determine whether the protective monolayer shell is ordered or not. The simultaneous presence of Au-Au and Au-S bonds together with a reduced particle diameter, and the formation of an ordered monolayer protective shell, have been proved to be key parameters for the ferromagnetic-like behavior exhibited by thiol-functionalized gold NPs.

Nitriding study of titanium silicide intermetallics obtained by mechanical alloying

Cordoba, JM; Alcala, MD; Sayagues, MJ; Aviles, MA; Real, C; Gotor, FJ
Intermetallics, **16** (2008) 948-954

Titanium and silicon powder blends were ball-milled under an inert atmosphere and subsequently annealed in a nitrogen atmosphere. $Ti_{62.5}Si_{37.5}$, $Ti_{55.6}Si_{44.4}$, and $Ti_{50}Si_{50}$ mixtures suffered a mechanically induced self-propagating reaction during milling. The products of the combustion were Ti_5Si_3 for the 5 mixture and a combination of intermetallic phases for the $Ti_{55.6}S_{44.4}$ and $Ti_{50}Si_{50}$ mixtures. The $Ti_{33.3}Si_{66.7}$ blend did not show an MSR process, but prolonged milling allowed the formation of a mixture of stable C_{54}-$TiSi_2$ and metastable C_{49}-$TiSi_2$ by a diffusion reaction. The nitriding study showed a different behaviour for C_{54}-$TiSi_2$ and

Ti_5Si_3. C_{54}-$TiSi_2$ nitriding took place in a two-step process: the first corresponded to the formation of TiN and Si and the second to the silicon nitriding leading to the formation of alpha- and beta-Si_3N_4. However, silicon and titanium nitriding primarily occurred simultaneously during the annealing of Ti_5Si_3, and the final product was a mixture of TiN and alpha-Si_3N_4 (C) 2008 Elsevier Ltd. All rights reserved.

Influence of particle size on electrochemical and gas-phase hydrogen storage in nanocrystalline Mg

Friedrichs, O; Kolodziejczyk, L; Sanchez-Lopez, JC; Fernandez, A; Lyubenova, L; Zander, D; Koster, U; Aguey-Zinsou, KF; Klassen, T; Bormann, R

Journal of Alloys and Compounds, **463** (2008) 5394-545

Nanocrystalline Mg powders of different particle size were obtained by inert gas evaporation and studied during electrochemical and gas-phase hydrogen cycling processes. The samples were compared to dehydrided samples obtained by mechanical milling of MgH_2 with and without 2 mol% Nb_2O_5 as catalyst. The hydrogen overpotential of the pure Mg, which is a measure of the hydrogen evolution at the electrode surface, was observed to be reduced with smaller particle sizes reaching values comparable to samples with Nb_2O_5 additive. On the other hand gas-phase charging experiments showed the capacity loss with smaller particle sizes due to oxidation effects. These oxidation effects are different depending on the synthesis method used and showed a major influence on the hydrogen sorption kinetics. (C) 2007 Elsevier B.V. All rights reserved.

Polymorphic transformation from body-centered to face-centered cubic vanadium metal during mechanosynthesis of nanostructured vanadium nitride determined by extended x-ray absorption fine structure spectroscopy

Lopez-Flores, V; Roldan, MA; Real, C; Paez, AM; Castro, GR

Journal of Applied Physics, **104** (2008) 023519

The pathway for vanadium nitride (VN) formation obtained by milling treatment has been traced out. At the initial stages of the process, the reactant, vanadium metal, showing body-centered cubic (bcc) structure, becomes highly distorted. Simultaneously, the formation of a small nucleus of the product, VN, takes place. X-ray absorption spectroscopy (XAS) has allowed the quantification of the distortion degree as well as the detection of the VN nucleus in the early stages of their formation, while other standard structural characterization techniques are unable to detect such phenomena. For increasing milling times, apart from the expected increase in the size of the VN nucleus, a polymorphic transformation from bcc to fcc vanadium metal has been recorded. This phase might play a key role in the overall synthesis process and could be a reaction intermediate in other solid state processes involving V metal. The sensitivity of XAS to noncrystalline domains and to highly distorted environments, as well as the use of high resolution x-ray diffraction, has provided the relevant information to understand the whole reaction process. (C) 2008 American Institute of Physics.

Bioactivity of wollastonite/aerogels composites obtained from a TEOS-MTES matrix

Toledo-Fernandez, JA; Mendoza-Serna, R; Morales, V; de la Rosa-Fox, N; Pinero, M; Santos, A; Esquivias, L
Journal of Materials Science-Materials in Medicine, **19** (2008) 2207-2213

Organic-inorganic hybrid materials were synthesized by controlled hydrolysis of tetraethoxysilane (TEOS), methyltrimethoxysilane (MTES), synthetic wollastonite powders and polydimethylsiloxane (PDMS) in an ethanol solution. Aerogels were prepared from acid hydrolysis of TEOS and MTES with different volume ratio in ethanol, followed by addition of wollastonite powder and PDMS in order to obtain aerogels with 20 wt% of PDMS and 5 wt% of CaO of the total silica. Finally, when the wet gels were obtained, they were supercritically dried at 260 C and 90 bar, in ethanol. In order to obtain its bioactivity, one method for surface activation is based on a wet chemical alkaline treatment. The particular interest of this study is that we introduce hybrid aerogels, in a 1 M solution of NaOH, for 30 s at room temperature. We evaluate the bioactivity of TEOS-MTES aerogel when immersed in a static volume of simulated body fluid (SBF). An apatite layer of spherical-shaped particles of uniform size smaller than 5 microns is observed to form on the surface of the aerogels after 25 days soaking in SBF.

Surface and interlayer structure of vermiculite intercalated with methyl viologen

Kulhankova, L; Capkova, P; De Valle, VR; Poyato, J; Perez-Rodriguez, JL; Lerf, A
Journal of Molecular Modelling, **14** (2008) 1183-1189

Molecular modeling using empirical force field revealed the differences between the surface and interlayer arrangement of the dye guest molecules in vermiculite intercalated with the divalent methyl viologen cation (MV2+). Conformation and anchoring of MV2+ cations on the silicate layer in the interlayer space of vermiculite host structure is different from that on the crystal surface. A preferential position has been found for the anchoring of guests on the silicate layer. Anyway the arrangement of guests in the interlayer space as well as on the crystal surface exhibits a high degree of disorder due to a certain flexibility in guest molecules arrangement and first of all due to the presence of water molecules in the interlayer space. The presence of water disturbs not only the regularity in guest positions and orientations but also in conformation of guest molecules in the interlayer space of the host structure.

Electronic structure, magnetic properties, and microstructural analysis of thiol-functionalized Au nanoparticles: role of chemical and structural parameters in the ferromagnetic behaviour

Guerrero, E; Munoz-Marquez, MA; Fernandez-Pinel, E; Crespo, P; Hernando, A; Fernandez, A
Journal of Nanoparticle Research, **10** (2008) 179-192

Gold nanoparticles (NPs) have been stabilized with a variety of thiol-containing molecules in order to change their chemical and physical properties; among the possible capping systems, alkane chains with different lengths, a carboxylic acid and a thiol-containing biomolecule (tiopronin) have been selected as protecting shells for the synthesized NPs; the NPs solubility in water or organic solvents is determined by the protecting molecule. A full microstructural characterization of these NPs is presented in the current research work. It has been shown that NPs capped with alkanethiol chains have a marked ferromagnetic behaviour which might also be dependent on the chain length. The simultaneous presence of Au-Au and Au-S bonds together with a reduced particle diameter, and the formation of an ordered monolayer protective shell, have proved to be key parameters for the ferromagnetic-like behaviour exhibited by thiol-functionalized gold NPs

Spectral response of opal-based dye-sensitized solar cells

Mihi, A; Calvo, ME; Anta, JA; Miguez, H
Journal of Physical Chemistry C, **112** (2008) 13-17

Herein we present an experimental study of the spectral dependence of the photogenerated current of opal-based solar cells. We analyze the incident photon-to-current conversion efficiency (IPCE) for dye-sensitized solar cells in which colloidal crystals are introduced in different configurations. We prove that a dye-sensitized nanocrystalline titanium oxide electrode moulded in the shape of an inverse opal shows a decrease of efficiency for the spectral region in which a photonic stop band opens up. Contrarily, when a standard thin film of disordered titania nanocrystallites is coupled to an inverse opal, the mirror effect of the photonic crystal at band gap frequencies increases the light harvesting efficiency of the cell and thus the IPCE. This effect is further demonstrated by coupling an inverse opal multilayer to a homogeneous electrode, with two well-defined spectral ranges of increased photogenerated current being detected.

Thiol-immobilized silver nanoparticle aggregate films for surface enhanced Raman scattering

Caro, C; Lopez-Cartes, C; Zaderenko, P; Mejias, JA
Journal of Raman Spectroscopy, **39** (2008) 1162-1169

We report a novel method for the fabrication of films of silver nanoparticle aggregates that are strongly attached to Si substrates (Thiol-immobilized silver nanoparticle aggregates or TISNA). The attachment is achieved by chemically modifying the surface of a Si(100) surface in order to provide SH groups covalently linked to the substrate and then aggregating silver nanoparticles on these thiol covered surfaces. The transmission electron microscopy (TEM), scanning electron microscopy (SEM) and atomic force microscopy (AFM) characterization show a high coverage with single nanoparticles or small clusters and a partial coverage with fractal aggregates that provide potential hot spots for surface enhanced Raman scattering (SERS). We have confirmed the SERS activity of these films by adsorbing rhodamine 6G and recording the Raman spectra at several concentrations. By using the silver-chloride stretching band as an internal standard, the adsorbate bands can be normalized in order to correct for the effects of focusing and aggregate size, which determine the number of SERS active sites in the focal area. This allows a quantitative use of SERS to be done. The adsorption-desorption of rhodamine 6G on TISNA films is reversible. These features make our TISNA films potential candidates for their use in chemical sensors based on the SERS effect. Copyright (c) 2008 John Wiley & Sons, Ltd.

Changes in the structure of composite colloid-polymer xerogels after cold isostatic pressing

Esquivias, L; Morales-Florez, V; Mosquera, MJ; de la Rosa-Fox, N
Journal of Sol-Gel Science and Technology, **47** (2008) 194-202

Monolithic gels, prepared from different mixtures of colloidal silica in a sol solution containing tetraethoxysilane under powerful ultrasonic agitation (sonosols), were compacted at an isostatic pressure of 390 MPa. Then N-2 adsorption-desorption data were used to construct structural models of the gels using Monte-Carlo calculations on the basis of random close-packing (RCP) premises. Structural information on these composites obtained before compaction indicates that the characteristic uniform structure of silica colloid gel undergoes profound modification when it is mixed with silica sonogel. From a structural point of view, the behaviour under compaction of the sonogel phase, which exhibits a significant degree of microporosity, depends on the relative concentration of the colloidal phase. Two hierarchic levels of micropores were discerned. After compression, the size of the elementary particles-and their aggregates-of the sonogel phase increases from 1.6 to 2.1 nm radius when the colloidal phase content is increased from 30 to 82% by weight. For an intermediate content, 50% of the volume reduction is caused by compression of the sonogel phase at the micropore level.

Improvement of the bioactivity of organic-inorganic hybrid aerogels/wollastonite composites with TiO_2

Fernandez, JAT; Mendoza-Serna, R; Santos, A; Pinero, M; de la Rosa-Fox, N; Esquivias, L
Journal of Sol-Gel Science and Technology, **45** (2008) 261-267

Organic-inorganic hybrid aerogels containing P and Ti have been synthesized by supercritical drying of alkogels prepared by hydrolysis and poly-condensation of metalo-organic precursors under high-power ultrasound. These materials become bioactive when doped with Ca. Wollastonite particles ($CaSiO_3$) were added as an active phase, instead of incorporating Ca into the aerogel atomic network. These particles had previously been precipitated and were then added to the sol. The aerogels were studied by Fourier transform infrared analysis, scanning electron microscopy coupled with energy dispersive spectroscopy and X-ray diffraction and N-2 adsorption. The stress-strain behaviours were evaluated under compression to obtain the Young's modulus. It was found that the incorporation of TiO2 into wollastonite-P_2O_5 hybrid aerogels increased their capacity to form apatite and, consequently, improving their bioactive response.

Reactivity of CO_2 traps in aerogel-wollastonite composites

Santos, A; Ajbary, M; Toledo-Fernandez, JA; Morales-Florez, V; Kherbeche, A; Esquivias, L
Journal of Sol-Gel Science and Technology, **48** (2008) 224-230

Synthetic wollastonite has been used as the active phase embedded into two different silica aerogel composites. These composites are different in respect of the route used for the synthesis of the wollastonite powder. Texture and composition of both types of composite have been characterized. In addition, several factors (pH, reaction time, CO_2 saturation, etc.)

that could help to optimize the carbonation process at room temperature and pressure have been studied. Under the same conditions, both composites confirm previous results showing efficiencies as CO2 sequesters between 80% and 100% in only 15 min of gas flow. The textural characteristics of the aerogel, together with the grain size of the synthetic wollastonite powder, not only increase the speed of the reaction, but also inhibit the appearance of a passivating layer on the surface of the wollastonite grains attacked by the CO2. This is an outstanding feature as it insists on a cutting-edge challenge of the CO2 research: its economical availability.

New production of TiCxN1-x-based cermets by one step mechanically induced self-sustaining reaction: Powder synthesis and pressureless sintering

Cordoba, JM; Alcala, MD; Aviles, MA; Sayagues, MJ; Gotor, FJ
Journal of the European Ceramic Society, **28** (2008) 2085-2098

TiCxN1-x-based powdered cermets were synthesized by a one step mechanically induced self-sustaining reaction (MSR) process from mixtures of elemental powders, and subsequently sintered by a pressureless method. The composition and microstructure of the ceramic and binder phases before and after the sintering process were studied by X-ray diffraction, scanning and transmission electron microscopy, and electron diffraction. The powdered cermets showed excellent binder dispersion and a nanometer character for the ceramic and binder particles. The TiCxN1-x stoichiometry was consistently richer in carbon than expected from the raw powder composition. An important amount of titanium was present in the binder after MSR synthesis, and intermetallic Ti-Ni or Ti-Co phases were obtained in some cases. After sintering, the binder phase was always constituted by intermetallic compounds. The morphology of the ceramic phase in the final bodies was dependent on the C/N ratio of TiCxN1-x and its growth primarily occurred through a coalescence process. The presence of titanium in the binder reduced hard particle solubility in the melted binder and its grain growth. (c) 2008 Elsevier Ltd. All rights reserved.

Thermal study of polypyrrole complexes with vermiculites of different layer charge

Ramirez-Valle, V; Lerf, A; Wagner, FE; Poyato, J; Perez-Rodriguez, JL
Journal of Thermal Analysisand Calorimetry, **92** (2008) 43-51

We have studied the synthesis of polypyrrole-clay nanocornposites by the in situ oxidative polymerization of pyrrole in the interlayer space of vermiculites with different layer charges from Santa Olalla and Ojen, Spain. Moreover, the influence of different interlayer cations (Na^+, Mg^{2+}, Fe^{3+}) on the interaction between pyrrole and the vermiculites was studied. The resulting materials were characterized by means of DTA-TG, XRD, FTIR and Mossbauer spectroscopy. In all samples polymerization of pyrrole was observed, presumably triggered by the structural iron. In most cases it was found to be externally deposited. An uptake of pyrrole in the interlayer space and PPy formation is observed in the case of the Fe3+-intercalated Ojen vermiculite, which has a lower layer charge than the Santa Olalla vermiculite.

Thermal characterization of montmorillonite clays saturated with various cations

Balek, V; Benes, M; Subrt, J; Perez-Rodriguez, JL; Sanchez-Jimenez, PE; Perez-Maqueda, LA; Pascual-Cosp, J

Journal of Thermal Analysis and Calorimetry, **92** (2008) 191-197

Emanation thermal analysis (ETA), thermogravimetry and high temperature XRD were used to characterize the thermal behavior during dehydration of natural Na montmorillonite (Upton Wyoming, USA) and homoionic montmorillonite (MMT) samples saturated with different cations, i.e. Li^+, Cs^+, NH^{4+}, Mg^{2+} and Al^{3+}. ETA results characterized radon mobility and microstructure changes that accompanied the mass loss of the samples due to dehydration on heating in air. A collapse of interlayer space between the silicate sheets after water release from the MMT samples was characterized by a decrease of the radon release rate, Delta E. Decreases in c-axis basal spacing (d(001)) values determined from XRD patterns for the different montmorillonite samples follow the sequence: Mg-MMT>AI-MMT>Li-MMT>Na-MMT>NH4-MMT>Cs-MMT The decrease of the radon release rate (Delta E) determined by ETA that characterized microstructure changes due to collapse of interlayer space corresponded well to differences in the c-axis basal spacing (Delta d(001)) values determined from the XRD patterns before and after samples dehydration.

Nanoparticle-based one-dimensional photonic crystals

Colodrero, S; Ocaña, M; Miguez, H

Langmuir, **24** (2008) 191-197

Herein we present a fast, reliable method for building nanoparticle-based ID photonic crystals in which a periodic modulation of the refractive index is built by alternating different types of nanoparticles and by controlling the level of porosity of each layer. The versatility of the method is further confirmed by building up optically doped photonic crystals in which the opening of transmission windows due to the creation of defect states in the gap is demonstrated. The potential of this new type of structure as a sensing material is illustrated by analyzing the specific color changes induced by the infiltration of solvents of different refractive indexes.

Response of nanoparticle-based one-dimensional photonic crystals to ambient vapor pressure

Colodrero, S; Ocaña, M; Gonzalez-Elipe, AR; Miguez, H

Langmuir, **24** (2008) 9135-9139

Herein we report an analysis of the variation of the optical properties of different nanoparticle-based one-dimensional photonic crystal architectures versus changes in the ambient vapor pressure. Gradual shift of the optical response provides us with information on the sorption properties of these structures and allow us to measure precise adsorption isotherms of these porous multilayers. The potential of nanoparticle-based one-dimensional photonic crystals as base materials for optical sensing devices is demonstrated in this way.

Surface plasmon resonance and magnetism of thiol-capped gold nanoparticles

Guerrero, E; Munoz-Marquez, MA; Garcia, MA; Crespo, P; Fernandez-Pinel, E; Hernando, A; Fernandez, A

Nanotechnology, **19** (2008) 175701-175706

Surface plasmon resonance measurements and magnetic characterization studies have been carried out for two types of thiol-capped gold nanoparticles (NPs) with similar diameters between 2.0 and 2.5 nm and different organic molecules linked to the sulfur atom: dodecanethiol and tiopronin. In addition, Au NPs capped with tetraoctyl ammonium bromide have also been included in the investigation since such capping molecules weakly interact with the gold surface atoms and, therefore, this system can be used as a model for naked gold NPs; such particles presented a bimodal size distribution with diameters around 1.5 and 5 nm. The plasmon resonance is non-existent for tiopronin-capped NPs, whereas a trace of such a feature is observed for NPs covered with dodecanethiol molecules and a bulk-like feature is measured for NPs capped with tetralkyl ammonium salts. These differences would indicate that the modification of the surface electronic structure of the Au NPs depends on the geometry and self-assembling capabilities of the capping molecules and on the electric charge transferred between Au and S atoms. Regarding the magnetization, dodecanethiol-capped NPs have a ferromagnetic-like behaviour, while the NPs capped with tiopronin exhibit a paramagnetic behaviour and tetralkyl ammonium-protected NPs are diamagnetic across the studied temperature range; straight chains with a well-defined symmetry axis can induce orbital momentum on surface electrons close to the binding atoms. The orbital momentum not only contributes to the magnetization but also to the local anisotropy, giving rise to permanent magnetism. Due to the domain structure of the adsorbed molecules, orbital momentum is not induced for tiopronin-capped NPs and the charge transfer only induces a paramagnetic spin component.

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

Characterization of iron oxide-based pigments by synchrotron-based micro X-ray diffraction

Herrera, LK; Cotte, M; de Haro, MCJ; Duran, A; Justo, A; Perez-Rodriguez, JL

Applied Clay Science, **42** (2008) 57-62

The characterization of iron in microsamples by conventional X-ray diffraction is difficult due to its low concentration in thin layers and its low reflecting power relative to other phases. Synchrotron radiation can provide unique information because of high intensity, sample penetration, small beam diameter and fast data collection. In this study, micro X-ray diffraction (mu-XRD) data were obtained of two samples taken from wall paintings at San

Agustin's Church in Cordoba. Crystalline iron phases such as goethite, lepidocrocite and hematite in the cross-section of the painting thin layers were identified. with a good spatial resolution. Conventional XRD only detected hydrocerussite and cerussite rather than the full range of iron phases found in the mu-XRD experiments. (c) 2008 Elsevier B.V. All rights reserved.

Studies of deterioration of the tin–mercury alloy within ancient Spanish mirrors

Herrera, LK, Duran, A., Franquelo, M.L., Jiménez de Haro, Justo, A., Pérez Rodríguez, J.L.
Journal of Cultural Heritage, **9** (2008) 41-46

Glass backed with a tin–mercury alloy, commonly called the amalgam mirror, was the dominant mirror used from the 15th century until the beginning of the 20th century. In this work, a qualitative analysis of the crystalline phases of the alloy surface of ancient mirrors was done using the grazing incidence X-ray diffraction technique (GID). Their morphologies were studied by scanning electron microscopy (SEM), and the elemental analyses were done by energy dispersive X-ray spectrometry (EDX). X-ray photoelectron spectroscopy (XPS) was used to characterize the atomic composition of the surfaces. Our results indicate that the amalgam is composed of a binary alloy of tin and mercury ($Hg_{0.1}Sn_{0.9}$). Mercury is volatile and slowly evaporates, leaving finely divided particles of tin that are easily oxidized, forming romarchite (SnO) and cassiterite (SnO_2). (C) 2008 Elsevier Masson SAS. All rights reserved.

Degradation of gold and false golds used as gildings in the cultural heritage of Andalusia, Spain

Duran, A; Perez-Rodriguez, JL; de Haro, MCJ; Herrera, LK
Journal of Cultural Heritage, **9** (2008) 184-188

The causes and degree of alteration of metals such as gold, tin, silver and bronze powders from ornamental implements of Andalusia Cultural Heritage have been studied. The unaltered gold is lost due to the alteration of the material used to adhere the leaf gold on the ceramic. Tin is transformed to romarchite and is lost due to a similar alteration as with the gold leaf adhesive. Silver is altered to Ag2S due to environmental contamination. Part of the bronze powders and silver used in Huercal-Overa altarpiece are altered to atacamite and AgCl, respectively, due to an unsuitable cleaning process. (C) 2008 Elsevier Masson SAS. All rights reserved.

Roman ceramics of hydraulic mortars used to build the Mithraeum house of Merida (Spain)

Franquelo, ML; Robador, MD; Ramirez-Valle, V; Duran, A; de Haro, MCJ; Perez-Rodriguez, JL
Journal of Thermal Analysis and Calorimetry, **92** (2008) 331-335

Roman ceramics of two hydraulic mortars used to build the pond and water channel of Mithraeum house from Merida (Spain) have been studied. The sizes of the ceramic fragments found were different in both of the samples studied, showing different behaviour in the reactions with the lime. The X-ray diffraction of the ceramic shows the presence of quartz, mica (biotite), anorthite and hematite accompanied by amorphous phase, being observed scarce vitrification. The presence of mica confirms a firing temperature for manufacturing the ceramic below 900 degrees C. In one of the ceramics studied, X-ray diffraction did not show calcite. However, in the FTIR appear bands that could be assigned to carbonates absorptions and likewise, carbonates were identified in the DTA-TG curves. Ca and small quantities of Si and Al were also identified by SEM-EDX on the surface of the pores that could be due to an amorphous phase formed in the reaction of lime with the Si and Al of the ceramic. On the other hand, in other ceramic samples carbonates (about 10%) were detected. The carbonates have been found filling the pores, sometimes accompanied by a new calcium-aluminium-silicate phase produced by the reaction between the lime and the amorphous phase of the ceramic. The carbonates and the new phases formed inside the pores are responsible for the decrease of the porosity and for the formation of new phases during the heating of the ceramics.

Study by thermal analysis of mortars belonging to wall paintings corresponding to some historical buildings of Sevillian art

Duran, A; Robador, MD; de Haro, MCJ; Ramirez-Valle, V
Journal of Thermal Analysis and Calorimetry, **92** (2008) 353-359

Mortars taken from the walls of three historical buildings in Seville: Pond of Patio de las Doncellas in Real Alcazar of Seville, the Monastery of Santa Maria de las Cuevas and the Church of El Salvador were investigated. The techniques employed were thermogravimetry (TG), differential thermal analysis (DTA), XRD, FTIR, SEM with EDAX, Bernard calcimeter, granulometry, mercury intrusion porosimetry and mechanical strength tests. The majority of the studied mortars consist of calcite and silica. Gypsum was detected in samples of four mortars from the Santa Maria de las Cuevas Monastery and two from the El Salvador Church, whose samples were taken from the upper layers of the walls, but gypsum was not detected in the internal mortars layers. Only in two of the samples of the Monastery, the presence of cellulosic material as an organic additive was detected. All the studied mortars could be regarded hydraulic, so much by results from ratios between mass loss due to CO_2 and H_2O, hydraulic module and assays of compressive strength. The values obtained by these three techniques are related, providing good agreements between them. These results give useful information that aids in understanding the technology of historic mortars, and how to plan the restoration of these wall paintings.

Copper alloys deterioration due to anthropogenic action

Duran, A; Perez-Rodriguez, JL; Herrera, LK; Jimenez-de-Haro, MC; Robador, MD; Justo, A; Blanes, JM; Perez-Ferrer, JC
Revista de Metalurgia, **44** (2008) 85-91

Results are presented from several samples taken from leaves of the Pardon Portico of Mosque-Cathedral of Cordoba, where an alteration on their surface was detected. Metal samples analyzed using X-ray microanalysis and powder x-ray diffraction were predominantly constituted by copper with some amounts of zinc attributed to brass, whereas other samples were also constituted by copper, tin and lead attributed to bronze. Surface samples were analyzed using the same techniques. In addition Fourier transform infrared spectroscopy was also used. The main compound identified in all the surface of the leaves is copper chloride hydroxide (atacamite). Lead chlorides have also been found. These data show that the sudden alteration that appears may be attributed to the use of some cleaning product containing chloride. Other compounds detected in the surface were gypsum, quartz and oxalates coming from environmental contamination.

Non-destructive analysis of cultural heritage artefacts from Andalusia, Spain, by X-ray diffraction with Gobel mirrors

Duran, A; Herrera, LK; de Haro, MCJ; Justo, A; Perez-Rodriguez, JL
Talanta, **76** (2008) 183-188

The characterization of the phases present in artefacts has been normally carried out using XRD (Bragg-Brentano geometry) that requires sampling from artworks, being a destructive technique. However, X-ray diffraction with Gobel mirrors permits directly to study rough artefacts without sampling. Grazing incidence attachments can be used to characterize as much the superficial layer as the underlying ones in flat samples to obtain information about the depth profile of some samples. The combination of Gobel mirrors and measure at low fixed incidence angles allow to obtain information about the depth profile of bent samples. This work reports the alteration processes on the surface of the following cultural heritage artefacts: a rivet and a nail extracted from Pardon Gateway, located in the North facade of Mosque-Cathedral of Cordoba; a Roman arrow and a button from a Roman jacket obtained from an excavation in Baena (Cordoba); organ pipe from Cathedral of Zaragoza; lead seals from Seville City Hall collection. The main objective of this paper is the study through a totally non-destructive analytical method, Xray diffraction with Gobel mirrors, of the superficial alteration of some metallic artefacts from cultural heritage. This knowledge allows us the election of appropriate methods to carry out the restoration of these artefacts. (C) 2008 Elsevier B.V. All rights reserved.

Microanalysis of Gothic mural paintings (15th century) in Slovenia: Investigation of the technique used by the Masters

Kriznar, A; Ruiz-Conde, A; Sanchez-Soto, PJ
X-Ray Spectrometry, **37** (2008) 360-369

The present article focuses on an interdisciplinary research on cultural heritage concerning the microanalysis of Gothic mural paintings made during the 15th century in Slovenia. The samples were chosen from the churches of Crngrob (1453), Mirna (1463-1465), Mevkuz (1465) and Mate (1467), attributed to two of the most important Gothic painters of that period of time: Master Bolfgang and Master of Mate. The chemical and phase composition of all the mortars, number of their layers and selection of the pigments were of interest. For this purpose, fragments of mural paintings were studied with several instrumental techniques: optical microscopy (OM), SEM-EDX, x-ray powder diffraction (XRD) and Fourier transform infrared spectroscopy (FTIR). In early artworks, the mortar was made using a mixture of lime and more or less clean sand. Later, crushed lime-rock or marble instead of sand was added to lime. The pigments identified by EDX microanalysis of cross sections previously studied by OM, are of earth or mineral origin. Therefore, they are durable in fresco and lime techniques: lime white, yellow and red natural or burned ochres, green earth and azurite. The results confirmed the high technical quality of both painters and the relationships between the teacher and the disciple. Master Bolfgang and Master of Mate combine three basic techniques of mural painting: fresco, secco and lime techniques. This kind of investigation and methodology allow us to know better the Central European Art and the Slovenian Art in the Adriatic zone, as well as the general map of European Art in the 14-15th centuries. Copyright (C) 2008 John Wiley & Sons, Ltd.

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

Pyroelectric potassium hydrogen malate with polarized hydrogen bond chains and aligned dipole moments

Gomes, ED; Belsley, MS; Criado, A; Rodrigues, VH; Costa, MMR
Applied Physics Letters, **93** (2008) 222903-222903

A spontaneous polarization of 16 mu C/cm(2) at room temperature has been found in the semiorganic crystal potassium hydrogen malate ($KHC_4H_4O_5$ center dot H_2O). This high polarization results from a structural arrangement of oriented dipoles formed by the potassium cations and the COO- group from the malate anion, and long hydrogen bonded polarized chains created by the hydrogen >L-malate anion via O-H center dot O interactions, directed along the polar sixfold axis. The material shows a second harmonic generation with a rotationally averaged effective second order susceptibility equal to 0.70 of potassium dihydrogen phosphate at an incident wavelength of 1064 nm.

Relation between growth dynamics and the spatial distribution of intrinsic defects in self-assembled colloidal crystal films

Lozano, G; Miguez, H
Applied Physics Letters, **92** (2008) 091904-091907

Herein we establish a clear relation between the parameters that govern the growth dynamics and the structural quality of colloidal crystal films. We report an optical analysis of the spatial distribution of intrinsic defects in colloidal crystal films and correlate our results with a theoretical model describing the growth dynamics of such lattices. We find that the amount of defects fluctuates periodically and decreases along the growth direction of the lattice. We demonstrate that these spatial variations are a direct consequence of the temporal oscillations of the crystal film formation velocity, which are inherent to the colloidal particle deposition process.

Influence of deuteration, electric field and uniaxial stress on tricritical phase transition of TGSe: Calorimetric study

Romero, FJ; Gallardo, MC; Manchado, J; Koralewski, M; Del Cerro, J
Ferroelectrics, **363** (2008) 100-109

The tricritical phase transition of ferroelectric triglycine selenate (TGSe) has been investigated under the influence of weak uniaxial stress and electric fields by means of a high sensitive calorimetric technique. The effect of deuteration on the latent heat has been also analysed.

Mechanical alloying of Fe100-x-yNbxBy (x=5, 10; y=10, 15): From pure powder mixture to amorphous phase

Ipus, JJ; Blazquez, JS; Franco, V; Conde, A
Intermetallics, **16** (2008) 1073-1082

The mechanical alloying process of $Fe_{75}Nb_{10}B_{15}$ and $Fe_{85}Nb_5B_{10}$ systems has been studied from an initial mixture of elemental powders. The amorphization process is monitored by X-ray diffraction and Mossbauer spectrometry. An amorphous phase is formed after 400 h milling only for $Fe_{75}Nb_{10}B_{15}$ alloy, whereas a bcc supersatured solid solution is the final product after milling $Fe_{85}Nb_5B_{10}$ alloy. For both cases, a dispersion of similar to 10% in the Fe content of the powder particles persists after 400 h milling. Powder particle size, Cr content and lattice parameter of bcc phase are larger for the alloy with the highest Nb content. (C) 2008 Elsevier Ltd. All rights reserved.

An equivalent time approach for scaling the mechanical alloying processes

Ipus, JJ; Blazquez, JS; Franco, V; Millan, M; Conde, A; Oleszak, D; Kulik, T
Intermetallics, **16** (2008) 470-478

Dynamics of a single ball into a planetary ball mill is analyzed leading to a cubic dependence of the power transferred during milling with the rotational speed, Omega. This leads to the definition of an equivalent time to describe the state of ball milled powders independently of Omega. Mechanical alloying of $Fe_{75}Ge_{20}Nb_5$ composition is studied by a combination of experimental techniques (differential scanning calorimetry, scanning electron microscopy, energy dispersive X-ray spectrometry, X-ray diffraction, Mossbauer spectrometry and vibrating sample magnetometry) and results evidence a good agreement with the predictions of the equivalent time approach. (C) 2007 Elsevier Ltd. All rights reserved.

A phenomenological fitting curve for the magnetocaloric effect of materials with a second-order phase transition

Dong, QY; Zhang, HW; Sun, JR; Shen, BG; Franco, V
Journal of Applied Physics, **16** (2008) 116101-116104

The magnetic entropy change of polycrystalline samples Gd, La(Fe0.92Co0.08)(11.83)Al-1.17, LaFe10.8Si2.2, Mn5Ge2.7Ga0.3, Nd2AlFe13Mn3, and TbCo2 with a second-order phase transition has been investigated. A uniform phenomenological function that describes the magnetic entropy change is found for these materials. This could be of great benefit for the design of magnetic refrigerators. The field dependence of the critical exponent for the variation in the maximum entropy change with field is studied. The critical exponent value of 2/3, which is predicted by the mean field theory, is only satisfied for moderate field values. The refrigerant capacity is analyzed and compared to the predictions of the fitting function. (C) 2008 American Institute of Physics.

Influence of Ge addition on the magnetocaloric effect of a Co-containing Nanoperm-type alloy

Franco, V; Blazquez, JS; Conde, A
Journal of Applied Physics, **103** (2008) 07B316

The influence of the partial substitution of B by Ge on the magnetocaloric response of $Fe_{78}Co_5Zr_6B_1$0Cu_1 is studied. Ge addition produces a reduction in the temperature at which the peak entropy change takes place, as well as a slight decrease in the magnitude of the peak, $|\Delta S_M^{pk}|$. The refrigerant capacity, RC, and its field dependence is also analyzed: although Ge addition increases RC of the Co-containing alloy, the largest RC value corresponds to the Co- and Ge-free alloy. This will be discussed on the basis of the recently proposed universal curve for the magnetic entropy change, which is also followed by the FeZrBCu(Co,Ge) alloy series. ©2008 American Institute of Physics

Magnetic permeability of (FeCoGe)(88)Zr6B5Cu1 alloys: Thermal stability in a wide temperature range

Blazquez, JS; Conde, CF; Franco, V; Conde, A; Kiss, LF
Journal of Applied Physics, **103** (2008) 07E721

Temperature dependence, from room temperature up to 1000 K, of the initial permeability (μ) of $Fe_{83-x}Co_xGe_5Zr_6B_5Cu_1$ (x=5 and 20) alloys at different stages of devitrification is reported. As nanocrystallization progresses, room temperature μ decreases but high temperature one increases, leading to an improvement of its thermal stability extended from room temperature up to 915 K, characterized by a temperature coefficient of permeability ~0.1%/K (μ~4000) and 0.04%/K (μ~800) for 5 and 20 at. % Co containing alloys, respectively.

Magnetocaloric response of FeCrB amorphous alloys: Predicting the magnetic entropy change from the Arrott-Noakes equation of state

Franco, V; Conde, A; Kiss, LF
Journal of Applied Physics, **104** (2008) 033903-033905

The magnetic entropy change in $Fe_{92-x}Cr_8B_x$ (x=12,15) amorphous alloys has been studied. Increasing the B content, both the peak entropy change and the Curie temperature of the alloy increase. This is in agreement with an increase in the average magnetic moment per iron atom. The thermal and field dependences of the magnetic entropy change curves have been analyzed with the use of the Arrott-Noakes equation of state. It is shown that determining the parameters in this equation of state (through fitting the magnetization data) allows prediction of the field and temperature dependences of the magnetic entropy change curves in a broad temperature range around the Curie temperature. (c) 2008 American Institute of Physics.

Instantaneous growth approximation describing the nanocrystallization process of amorphous alloys: A cellular automata model

Blazquez, JS; Franco, V; Conde, CF; Millan, M; Conde, A
Journal of Non-Crystalline Solids, **354** (2008) 3597-3605

A cellular automata simulation based on an instantaneous growth approximation is developed to model the nanocrystallization kinetics. In this frame, the time required for a nucleus to grow up to its maximum size is neglected in comparison with the time required for the crystallization process. This approach allows a simple interpretation of the very low values of Avrami exponent found for nanocrystallization processes, <= 1, in the theoretical frame of Johnson-Mehl-Avrami-Kolmogorov theory. Kinetics and microstructure predictions from the simulations are compared with experimental data for FeCoNbB alloys and a good qualitative agreement is found. (C) 2008 Elsevier B.V. All rights reserved.

Analysis of the mechanically alloyed Fe-85-Nb-5-B-10 powder using a non-unique lattice parameter

Ipus, JJ; Blazquez, JS; Conde, A; Krasnowski, M; Kulik, T
Journal of Non-Crystalline Solids, **354** (2008) 5132-5134

X-ray diffraction patterns of mechanically alloyed $Fe_{85}Nb_5B_{10}$ powder were fitted using whole powder pattern decomposition procedure to resemble the presence of alpha-Fe type crystals with different Nb content. To do so, a distribution of lattice parameters was proposed based on the asymmetry of the diffraction maxima and the broadening of the distribution of the powder particles composition. Analogously, a set of discrete sextets was used to represent the different local Fe environments. (C) 2008 Elsevier B.V. All rights reserved.

Nanocrystallization effects on the specific heat of Fe-Co-Nb-B amorphous alloy

Blazquez, JS; Millan, M; Conde, CF; Franco, V; Conde, A; Lozano-Perez, S
Journal of Non-Crystalline Solids, **354** (2008) 5135-5137

Specific heat at constant pressure, C-p, was measured on amorphous, nanocrystalline and fully crystalline samples of $Fe_{60}Co_{18}Nb_6B_{16}$ alloy. Magnetic and calorimetric measurements agree, describing a continuously decreasing Curie temperature of the amorphous phase. A clear enhancement of Cp over the Dulong-Pettit limit has been observed (from 14% to 25 %). Part of the enhancement is due to magnetic (mainly amorphous phase) and electronic contributions, although an excess volume can be inferred from the high value of the slope of Cp versus temperature. (C) 2008 Elsevier B.V. All rights reserved.

Phase composition-dependent physical and mechanical properties of $Yb_xZr_{1-x}O_{2-x}/2$ solid solutions

Hartmanova, M; Kubel, F; Bursikova, V; Lomonova, EE; Holgado, JP; Navratil, V; Navratil, K; Kundracik, F

Journal of Physics and Chemistry of Solids, **69** (2008) 805-814

The paper represents a detailed insight into the correlation between changes of the phase composition of crystalline $Yb_xZr_{1-x}O_{2-x}/2$ solid solutions and their structural, electrical, mechanical and optical properties. Particularly, the effect of the crystal growth conditions and stabilizer amount in the range of 1.5-13.8 mol% of Yb_2O_3 are studied in terms of Rietveld analysis of powder X-ray diffraction data, electrical conductivity measured by impedance spectroscopy, absorption coefficient and refractive index measurements, Vickers microhardness (classical technique) as well as the plastic microhardness and effective elastic modulus (DSI-depth-sensing indentation technique). Potential applications of the investigated systems Lire discussed in view of the results obtained. (C) 2007 Elsevier Ltd. All rights reserved.

A universal curve for the magnetocaloric effect: an analysis based on scaling relations

Franco, V; Conde, A; Romero-Enrique, JM; Blazquez, JS

Journal of Physics-Condensed Matter, **20** (2008) 285207-285211

The universal character of the recent experimentally found master curve for the magnetic entropy change, Delta S-M, in studies of the magnetocaloric response of materials is analytically justified by using scaling arguments. The validity of the obtained scaling relations is checked against experimental data as well as the mean field and Heisenberg models. The curves are unique for each universality class. It is shown that the universal curve can be practically constructed in two different ways, reducing the number of required parameters with respect to the previous phenomenological derivation. This opens the possibility of an inexpensive screening of the performance of magnetocaloric materials, as it allows extrapolations to magnetic fields or temperatures not available in some laboratories.

High-temperature mechanical properties of porous $NaMgF_3$ derived from directionally solidified $NaMgF_3$-NaF eutectics

Ramirez-Rico, J; de Arellano-Lopez, AR; Martinez-Fernandez, J; Larrea, A; Orera, VM

Journal of the European Ceramic Society, **28** (2008) 2451-2457

Porous $NaMgF_3$ ceramics have been fabricated by leaching a NaF-$NaMgF_3$ eutectic in distilled water, producing $NaMgF_3$ with 53% of connected porosity. The eutectic was fabricated using the Bridgman technique at growth rates of 8, 10 and 15 mm/h. The microstructure and composition of the resulting material has been studied by means of X-ray diffraction and SEM. Compression mechanical tests have been performed at different temperatures up to 750 degrees C, both in constant strain rate and constant stress loading. The microstructure consists of plate-like grains with cylindrical pores in approximately hexagonal packing. Pores are perpendicular in adjacent grains. The compressive strength is found to be rather independent of growth rate, in the range studied. Small differences can be explained using a minimum solid area (MSA) model and differences in the microstructure. In creep experiments, no steady-state regime was observed. Instead, the strain exhibited a series of accelerations that could be associated with damage propagation. (c) 2008 Elsevier Ltd. All rights reserved.

Transport properties and microstructure changes of talc characterized by emanation thermal analysis

Perez-Maqueda, LA; Balek, V; Poyato, J; Subrt, J; Benes, M; Ramirez-Valle, V; Buntseva, IM; Beckman, IN; Perez-Rodriguez, JL

Journal of Thermal Analysis and Calorimetry, **92** (2008) 253-258

Thermal behavior of talc samples (from locality Puebla de Lillo, Spain) were characterized by emanation thermal analysis (ETA), DTA and TG. The ETA, based on the measurement of radon release rate from samples, revealed a closing up of surface micro-cracks and annealing of microstructure irregularities of the talc samples on heating in the range 200-500 degrees C. For ground talc sample a crystallization of non-crystalline phase formed by grinding, into orthorhombic enstatite was characterized as a decrease of radon mobility in the range 785-825 degrees C and by a DTA exothermal effect with the maximum at 830 degrees C. ETA results characterized the microstructure development of the talc samples on heating and served to evaluate their radon mobility and transport properties on heating and cooling. Transport properties of the talc samples were evaluated by using ETA experimental data measured during heating to 600 and 1300 degrees C, respectively, and subsequent cooling to room temperature.

High temperature coercivity of Nb-containing HITPERM alloys: Effect of Cu addition

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

Materials Letters, **62** (2008) 780-783

Hysteresis loops of nanocrystalline samples of Fe39Co39Nb6B16-yCuy (y=0, 1) HITPERM-type alloys were measured from room temperature up to 773K. The alloy with Cu shows a nearly constant value of coercivity (similar to 135A/m) in all the studied temperature range, whereas for the Cu-free alloy, the coercivity increases from 125A/m at 300K up to 190A/m at 773K. Room temperature Mossbauer spectra can be interpreted on the basis of the presence of three different regions: amorphous, crystalline and interface. The observed narrocrystalline microstructure is similar for the two alloys, although bigger crystallites are found in the alloy without Cu. The very small grain size ensures the averaging out of the magnetocrystalline anisotropy but, as the expected value of magnetostriction constant for the crystalline phase is similar to 60ppm, the magnetoelastic anisotropy cannot be neglected. (c) 2007 Elsevier B.V. All rights reserved.

Comment on "Observation of higher-order diffraction features in self-assembled photonic crystals"

Dorado, LA; Depine, RA; Miguez, H

Physical Review A, **78** (2008) 037801-037803

The purpose of this Comment is to show that we find that the conclusions presented in a paper by Nair and Vijaya [Phys. Rev. A 76, 053805 (2007)], concerning the perfect periodic ordering of self-assembled photonic crystals, are not supported and contradict previous studies of this matter.

Tailoring of magnetocaloric response in nanostructured materials: Role of anisotropy

Franco, V; Pirota, KR; Prida, VM; Neto, AMJC; Conde, A; Knobel, M; Hernando, B; Vazquez, M
Physical Review B, **77** (2008) 104434-104440

The magnetocaloric response of an ensemble of oriented uniaxial magnetic objects, perpendicularly magnetized to their easy axes, for temperatures close to the blocking temperature is calculated with the aim of demonstrating that the control of the sample's microstructure makes up an effective way to tailor its magnetocaloric response. Coexisting positive and negative magnetocaloric effect (MCE) is found for a model material with a single magnetic phase transition. Both MCE regimes are controlled by the magnitude of the applied magnetic field. As a proof of concept, experimental results for arrays of self-assembled ferromagnetic nanowires embedded into highly ordered nanoporous anodic alumina templates are shown, suggesting the validity of the numerical calculations.

Test of validity of the V-type approach for electron trajectories in reflection electron energy loss spectroscopy

Yubero, F; Pauly, N; Dubus, A; Tougaard, S
Physical Review B, **77** (2008) 245405

An electron reaching the detector after being backscattered from a solid surface in a reflection electron energy loss spectroscopy (REELS) experiment follows a so-called V-type trajectory if it is reasonable to consider that it has only one large elastic scattering event along its total path length traveled inside the solid. V-type trajectories are explicitly assumed in the dielectric model developed by Yubero [Phys. Rev. B 53, 9728 (1996)] for quantification of electron energy losses in REELS experiments. However, the condition under which this approximation is valid has not previously been investigated explicitly quantitatively. Here, we have studied to what extent these REELS electrons can be considered to follow near V-type trajectories. To this end, we have made Monte Carlo simulations of trajectories for electrons traveling at different energies in different experimental geometries in solids with different elastic scattering properties. Path lengths up to three to four times the corresponding inelastic mean free paths have been considered to account for 80-90% of the total electrons having one single inelastic scattering event. On this basis, we have made detailed and systematic studies of the correlation between the distribution of path lengths, the maximum depth reached, and the fraction of all electrons that have experienced near V-type trajectories. These investigations show that the assumption of V-type trajectories for the relevant path lengths is, in general, a good approximation. In the rare cases, when the detection angle corresponds to a scattering angle with a deep minimum in the cross section, very few electrons have experienced true V-type trajectories. However, even in these extreme cases, a large fraction of the relevant electrons have near V-type trajectories.

Experimental and theoretical analysis of the intensity of beams diffracted by three-dimensional photonic crystals

Dorado, LA; Depine, RA; Schinca, D; Lozano, G; Miguez, H
Physical Review B, **78** (2008) 075102

An analysis of the diffracted beams emerging from three-dimensional photonic crystals is herein presented. The wave vectors of nonspecular beams are calculated for a triangular two-dimensional lattice and the change in their directions as a function of the wavelength is confirmed experimentally for the case of face-centered-cubic colloidal crystals illuminated under normal incidence. A fluctuating behavior of beam intensity as a function of the wavelength of the incident light is predicted for perfectly ordered lattices. As it is the case for specularly reflected and ballistically transmitted beams, this modulation arises from multipole resonances of the sphere ensemble that are smoothed out via the diffuse light scattering produced by imperfections in the crystalline structure. When optical extinction is introduced in order to model the effect of imperfections, it is possible to accurately reproduce experimental observations.

Synthesis, characterization and ionic conductivity of Sr1.5Sb0.5O3-y (y similar to 0.25)

Chinarro, E; Mather, GC; Caballero, A; Saidi, M; Moran, E
Solid State Sciences, **10** (2008) 645-650

We describe the synthesis, structural and microstructural characterization of a strontium antimonate, Sr1.5Sb0.5O3-y (y similar to 0.25), with a cubic, double-perovskite structure and a large concentration of oxygen vacancies with no apparent long-range order. High resolution electron microscopy indicates, however, that short-range ordering phenomena may occur. Electrical conductivity is independent of oxygen partial pressure (pO(2)) for pO(2) < 10(-1.25) atm, typical of ionic transport (sigma similar to 10(-4) S cm(-1) at 600 degrees C), whereas the conductivity is dominated by p-type charge carriers at higher pO(2). (C) 2007 Elsevier Masson SAS. All rights reserved.

Influence of Mn content on the microstructure and hyperfine interaction parameters of amorphous and nanocrystalline hitperm-TYPE FeCoMnNbB alloys

Benaini, H; Blazquez, JS; Conde, CF; Conde, A; Ochin, P
Reviews on Advanced Materials Science, **18** (2008) 549-552

Effects of Mn addition on the devitrification kinetics, microstructure and hyperfine interaction parameters of FeCoMnNbB alloys were investigated. As-cast and nanocrystalline samples were studied by different experimental techniques and results were correlated. Mn alloying provoked a significant lowering of the Curie temperature of the amorphous phase. No big changes were observed in the microstructure of the nanocrystalline alloys with the Mn addition.

Microstructure and magnetic properties of mo containing nanoperm-type alloys

Conde, CF; Conde, A

Reviews on Advanced Materials Science, **18** (2008) 565-571

The influence of composition changes on the devitrification process, microstructure and magnetic properties of (Fe,Co)MoB(Cu) alloys was investigated. Amorphous and nanocrystalline samples were studied by differential scanning calorimetry, thermomagnetic gravimetry, X-ray diffraction, transmission electron microscopy and vibrating sample magnetometry and obtained results are correlated. Cu addition increases the thermal stability and the crystalline fraction of the nanocrystalline microstructure and improves the soft magnetic properties of the alloy. As B content increases the thermal stability of the nanocrystalline microstructure decreases and for the 20 at.% B alloy boride crystals are formed during the first crystallization stage. Saturation magnetization decreases and Curie temperature of the amorphous phase increases with B content. Co addition lowers the volume fraction of nanocrystals and as Co content increases in the alloy nanocrystals are enriched by Co, Curie temperature of the amorphous phase increases, linearly with Co content, and saturation magnetization and coercive field of nanocrystalline alloys increase as well.

Cis-Fused bicyclic sugar thiocarbamates. Reactivity towards amines

Lopez, O.; Zafra, E.; Maya, I.; Fuentes, J.; Dianez, M.J.; Estrada, M.D.; Perez-Garrido, S.; Fernández-Bolanos, J.G.

Tetrahedron, **51** (2008) 11789-11796

1,2-cis-Fused bicyclic sugar thiocarbamates of gluco and manno configurations have been prepared by treatment of the corresponding O-unprotected amino sugars and glycopyranosyl amines with thiophosgene. The reactivity of these compounds towards amines has been studied in order to determine whether these compounds could act as latent isothiocyanates; it is shown that 1,2-cis-fused bicyclic sugar thiocarbamates are more stable than their trans analogues, and are not transformed into thioureas upon treatment with amines. An unprecedented isomerization of a peracetylated glucopyranoso[2,1-d]oxazolidine-2-thione into a glucopyranoso[2,1-d]thiazolidin-2-one in DMF is also reported. The structure of this thiazolidin-2-one was confirmed by X-ray crystallography.

OTROS / OTHERS

Self-assembled polyhydroxy fatty acids vesicles: a mechanism for plant cutin synthesis
Heredia-Guerrero, JA; Benitez, JJ; Heredia, A
Bioessays, **30** (2008) 273-277

A simulation of the mass-transfer effects on the kinetics of solid-gas reactions
Ortega, A
International Journal of Chemical Kinetics, **40** (2008) 217-222

Carbothermal synthesis of silicon nitride(Si_3N_4): Kinetics and diffusion mechanism
Ortega, A; Alcala, MD; Real, C
Journal of Materials Processing Technology, **195** (2008) 224-231

Fabrication, chemical etching, and compressive strength of porous biomimetic SiC for medical implants
Torres-Raya, C; Hernandez-Maldonado, D; Ramirez-Rico, J; Garcia-Ganan, C; de Arellano-Lopez, AR; Martinez-Fernandez, J
Journal of Materials Research, **23** (2008) 3247-3254

Reaction-formation mechanisms and microstructure evolution of biomorphic SiC
Varela-Feria, FM; Ramirez-Rico, J; de Arellano-Lopez, AR; Martinez-Fernandez, J; Singh, M
Journal of Materials Science, **43** (2008) 933-941

Crystallization behaviour of (GeS2)(0.1)(Sb2S3)(0.9) glass
Svadlak, D; Zmrhalova, Z; Pustkova, P; Malek, J; Perez-Maqueda, LA; Criado, JM
Journal of Non-Crystalline Solids, **354** (2008) 3354-3361

Po(IV) Hydration: A quantum chemical study
Ayala, R.; Martínez, J.M.; Pappalardo, R.R.; Muñoz-Páez, A. and Sánchez-Marcos, E.
Journal of Physical Chemistry B, **112** (2008) 5416-5422

The Role of Hydroxyl Groups in the Self-Assembly of Long Chain Alkylhydroxyl Carboxylic Acids on Mica
Benitez, JJ; Heredia-Guerrero, JA; Serrano, FM; Heredia, A
Journal of Physical Chemistry C, **112** (2008) 16968-16972

Ar+NO microwave plasmas for Escherichia coli sterilization
Hueso, JL; Rico, VJ; Frias, JE; Cotrino, J; Gonzalez-Elipe, AR
Journal of Physical D-Applied Physics, **41** (2008) 0920021 -0920024

Getting more out of $X_2T_2O_7$ compounds with thortveltite structure: The bond-valence model
Alba, MD; Becerro, AI; Chain, P; Escudero, A; Gonzalez-Carrascosa, T
Journal of Solid State Chemistry, **181** (2008) 340-344

Kinetic analysis of precipitation in a quasi-binary Cu-1% at CoTi Alloy
Donoso, E.; Diaz, G.; Criado, J.M.
Journal of Thermal Analysis and Calorimetry, **91** (2008) 491-495

Critical study of the isoconversional methods of kinetic analysis
Criado, JM; Sanchez-Jimenez, PE; Perez-Maqueda, LA
Journal of Thermal Analysis and Calorimetry, **92** (2008) 199-203

Kissinger kinetic analysis of data obtained under different heating schedules
Sanchez-Jimenez, PE; Criado, JM; Perez-Maqueda, LA
Journal of Thermal Analysis and Calorimetry, **92** (2008) 427-432
Syntesis by reactive grinding of molibdenum iron bimetallic nitride
Roldan, MA; Ortega, A; Palencia, I; Real, C
Revista de Metalurgia, **44** (2008) 13-18

A simple and precise linear integral method for isoconversional data
Ortega, A
Thermochimica Acta, **474** (2008) 81-86

Influence of mass-transfer effect on isoconversional calculations
Ortega, A
Thermochimica Acta, **475** (2008) 65-71

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

Comportamiento plástico en compresión uniaxial de cermets Ti(C,N)-CO
Gallardo López, A.; Morales Rodríguez, A.; Domínguez Rodríguez, A.; Córdoba, J.M.; Gotor, F.J.
Actas del XI Congreso Nacional de Propiedades Mecánicas de Sólidos, **103** (2008) (pages 2)

Permanent in thiol capped nanoparticles, gold and ZnO
Crespo, P., García, M.A., Fernández-Pinel, E., De la Venta, J., Merino, J.M., Quesada, A., Hernando, A., Fernández, A., Penades, S.
Acta Physica Polonica A, **113** (2008) 515-520

Integration of photonic crystals in dye sensitized solar cells
Colodrero, S; Mihi, A; Calvo, ME; Ocana, M; Miguez, H
Active Photonic Crystals II, **7031** (2008) 3107-3107

La calcarenita de Carmona, Cueva de la Batida: Estratigrafía, mineralogía y sistema poral
Herrero Fernández, H., García Talegón, J., Justo, A., Pérez Rodríguez, J.L., Iñigo, A.C.
Carel, **6** (2008) 2355-2367

Effect of the layer charge on the thermal behaviour of NH_4^+-vermiculites
Jiménez de Haro, M.C., Justo Erbez, A., Pérez Maqueda, L.A., Lerf, A., Wagner, F.E., Pérez Rodríguez, J.L.
Mineralogia Polonica, (2008) 74

Thermal behaviour of lead-containing bentonite from Gador
Benitez Guerrero, M., Pascual Cosp, J., Balek, V., Benes, M., Subrt, J., Pérez Rodríguez, J.L., Pérez Maqueda, L.A.
Mineralogia Polonica, (2008) 46

Mesoporous hybrid thin films: Building blocks for complex materials with spatial organization
Soler-Illia, G.J., Angelomé, P.C, Fuertes, C. Wolosiuk, A., Bilmes, S.A., López-Alcaraz, F.J., Míguez, H.
Organic-Inorganic Hibrid Materials, (2008) 75-84

Elasticity and inelasticity of biomorphic composite SiC/Si fabricated from Sapele Wood
K. Kardashev, T.S. Orlova, B.I. Smirnov, A.R. de Arellano-López, J. Martínez-Fernández
XLVII International Conference Actual Problems of Strength, (2008) 89-91

3.3. LIBROS Y OTRAS PUBLICACIONES / BOOKS AND OTHER PUBLICATIONS

Comportamiento plástico en compresión uniaxial de cermets Ti(C,N)-CO
Gallardo López, A.; Morales Rodríguez, A.; Domínguez Rodríguez, A.; Córdoba, J.M.; Gotor, F.J.
En: *Pms 2008. Actas del XI Congreso Nacional de Propiedades Mecánicas de Sólidos*. Cádiz, España. Servicio de Publicaciones de la Universidad de Cadiz. 2008. Pag. 67-68
ISBN: 978-84-9828-2

Doping and Alloying Effects on DLC Coatings
Sánchez López, J.C.; Fernández Camacho, A.
En: *Tribology of Diamond-like carbon films. Fundamentals and Applications.* Donnet, Christophe; Erdemir, Ali (Eds.) 2008. Springer Science+business Media, LCC. Nueva York, EE.UU. pp. 311-338
ISBN: 978-0-387-30264-5

Characterization of mortars in medieval mural paintings in Slovenia
Kriznar, A., Ruiz Conde, A., Sánchez Soto, P.J.
En: *Rehabilitación del Patrimonio Arquitectónico y Edificación. Centro Internacional de* Conservación del Patrimonio (CICOP). Sevilla, España. pp. 69-74
ISBN: 978-0-612-3459-Z

Materiales cerámicos y vítreos
Sánchez Soto, P.J.
En: *Innovaciones en las tecnologías de la información aplicadas a la conservación de Patrimonio.* Asociación de Gestores Culturales de Extremadura. G. Durán y José J. de Sanjosé (Eds.). Mérida, España. pp. 65-78
ISBN: 978-84-612-7554-0

Técnicas Instrumentales Aplicadas a la Caracterización y Análisis de Materiales del Patrimonio Histórico y Cultural
Ruiz Conde, A.
En: *Innovaciones en las tecnologías de la información aplicadas a la conservación de Patrimonio.* Asociación de Gestores Culturales de Extremadura. G. Durán y José J. de Sanjosé (Eds.). Mérida, España. pp. 79-86
ISBN: 978-84-612-7554-0

Estudio de materiales y técnicas de realización utilizadas en obras de arte y sus procesos de alteración
Pérez Rodríguez, J.L., Justo, A., Poyato, J., Durán, A., Jiménez de Haro, M.C., Sigüenza, B., Herrera, L.K., Odriozola, C., Herrero Fernández, H., Franquelo, M.L.
En: *La investigación sobre Patrimonio Cultural.* Red Temática del CSIC del Patrimonio Histórico y Cultural, Saiz Jiménez, C. y Rogelio Candelero, M.A. (Eds.) Sevilla.

3.4. PATENTES / PATENTS

Solar to electric energy conversion device base don a light absorbing electrode coupled to a one-dimensional photonic crystal

Inventores: H. Míguez, S. Colodrero
N. de solicitud: US61046212
País de prioridad: España
Fecha de prioridad: 5/Mayo/2008
Entidad titular: Nanologica y CSIC

Dispositivo y su uso para la medidad de porosidades en láminas delgadas, materiales nanoestruturados

Inventores: A. Barranco, A. Borrás, J.R. Sánchez-Valencia, A.R. González-Elipe, J.P. Espinós, F. Yubero, J. Cotrino
N. de solicitud: P300001178
País de prioridad: España
Fecha de prioridad: 26/Mayo/2008
Entidad titular: CSIC

Método de prospección y caracterización de materias primas

Inventores: P.J. Sánchez Soto, A. Ruiz Conde y E. Garzón Garzón
N. de solicitud: P200803674
País de prioridad: España
Fecha de prioridad: 23/Diciembre/2008
Entidad titular: CSIC y Universidad de Almería

Dispositivo de hipertermia y su utilización con nanopartículas
Inventores: M.A. Muñoz Márquez, E. Guerrero, A. Fernández Camacho
N. de solicitud: P200702084. Extensión PCT: PCT/IB2008/002780
País de prioridad: España
Fecha de prioridad: 25/7/2008
Entidad titular: CSIC y Midatech Andalucia, S.L.

Fabricación de cerámicas porosas y materiales multifásicos a partir de precursores celulósicos
Inventores: J. Martínez Fernández, A.R. de Arellano-López, F.M. Valera Feria
N. de solicitud: P20080743
País de prioridad: España
Fecha de prioridad: 14/3/2008
Entidad titular: Universidad de Sevilla

3.5. CONGRESOS Y REUNIONES INTERNACIONALES
INTERNATIONAL CONGRESS AND MEETINGS

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

First International Conference on Functional Nanocoatings
30 Marzo-2 Abril [Budapest, Hungria]
Asunción Fernández Camacho [Miembro del Comité Científico]

35th International Conference on Metallurgical coatings and Thin Films | ICMTF2008
28 Abril-2 Mayo [San Diego, EUA]
Asunción Fernández Camacho [Miembro del Comité Científico]

5th European Topical Conference in Hard Coatings
22-25 Junio [Lisboa, Portugal]
Juan Carlos Sánchez López [Miembro del Comité Científico]
Asunción Fernández Camacho [Miembro del Comité Científico]

Workshop on Recent Development in the Processing and Applications of Structural Metals and Alloys
23-27 Junio [Como, Italia]
Asunción Fernández Camacho [Miembro del Comité Científico]

Nanomaterials and Nanotechnology Meeting | NANOSTRAVA 2008
2-5 Septiembre [Ostrava, Repúplica Checa]
Pedro José Sánchez Soto [Miembro del Comité Científico]

Workshop on Complex Solid State Reactions for Energy Efficient Hydrogen Storage
18-19 Septiembre [Sevilla, España]
Emilie Deprez [Miembro del Comité Organizador Local]
Inmaculada Rosa Cejudo [Miembro del Comité Organizador Local]
Asunción Fernández Camacho [Miembro del Comité Científico]
Carlos López Cartes [Miembro del Comité Científico]

IV Bienal del GERMN – I Reunión Ibérica de RMN
21-23 Septiembre [Sevilla, España]
Mª Dolores Alba Carranza [Miembro del Comité Organizador Local]

4th European Meeting on Solar Chemistry and Photocatalysis: Environmental Applications | SPEA-5
4-8 Octubre [Sicilia, Italia]
José Antonio Navío Santos [Miembro del Comité Científico]

International Workshop on Advanced Nanostructured Materials and Thin Films for Industrial Applications
21-24 Octubre [Nottingham, Reino Unido]
Asunción Fernández Camacho [Miembro del Comité Científico]

7th International Conference on Diffusion in Materials | DIMAT
28-30 Octubre [Lanzarote, España]
Juan Carlos Sánchez López [Miembro del Comité Científico]
Asunción Fernández Camacho [Miembro del Comité Científico]

Nanobusiness'08
18 Noviembre [Sevilla, España]
Instituto de Ciencia de Materiales de Sevilla

COMUNICACIONES EN CONGRESOS Y REUNIONES / COMMUNICATIONS IN CONGRESS AND MEETINGS

2nd Symposium Hydrogen & Energy
21-25 Enero [Braunwald, Suiza]

"Microstructural and Chemical Study of $2LiBH_4$+MgH_2 Reactive Hydride Composite for H_2 Storage", E. Deprez, A. Justo, D. Martínez-Martínez, T.C. Rojas, A. Fernández, U. Bösenberg, M. Dornhein, R. Bormann. Poster

International Congress of Glass Science in Art and Conservation

5-7 Marzo [Valencia, España]

"Studies of Tin-Mercury Alloy and Corrosion Compounds of Ancient Spanish Mirrors", L.K. Herrera, A. Durán, M.C. Jiménez de Haro, M.L. Franquelo, A. Justo. Comunicación Oral

International Congress of Glass Science in Art and Conservation

10-14 Marzo [Montego Bay, Jamaica]

"Multidisciplinary Evaluation of Fracture Surfaces: A Case Study in Sapphire", J.M. Cepero, A.R. de Arellano-López, J. Martínez-Fernández, S.M. Wiederhorn, D. Black, J.P. Guin. Comunicación Oral

"Study of the Mechanical Properties of BioSiC made with Artificial Precursors", M.A. Bautista, A.R. de Arellano López, J. Martínez-Fernández, J.M. López Cepero. Póster

Marie Curie Training

Marzo [Sevilla, España]

"Caracterización de Materiales del Patrimonio Andaluz", L.K. Herrera. Comunicación Oral

First International Conference on Functional Nanocoatings

30 Marzo-2 Abril [Budapest, Hungria]

"Tailored Synthesis of Nanocomposites based on the Ti-C-N system with controlled Mechanical and Tribological properties", D. Martínez Martínez, J.C. Sánchez López, A. Fernández. Conferencia Invitada

"Mechanical and Tribological properties of nc-TiAlN/a-Si_3N_4 Thin Films: From Macro to the Nanoscale", V.C. Fortio, D. Philippon, D. Aranyi, P. Nagy, J.C. Sánchez López, M.P. Delplancke-Ogletree, A. Fernández Camacho. Poster

"Microstructural and Chemical Characterization of Nanostructured and Amorphous Nitride Coatings", A. Fernández, C. Fernández, V.C. Fortio. Comunicación Oral

AICHE 2008 Spring National Meeting

6-10 Abril [New Orleans, EUA]

"Supported Gold Catalysts for CO Oxidation in Microchannel Reactors", L.M. Martínez T., F. Romero-Sarria, M.I. Domínguez, M.A. Centeno, J.A. Odriozola, M. Montes. Comunicación Oral

"Computational Fluid Dynamics Study of Heat Transfer in a Microchannel Reactor for Fischer-Tropsch Synthesis", G. Arzamendi, P.M. Dieguez, M. Montes, J.A. Odriozola, E. Falabella, L. Gandia. Póster

"Zeolitic Coatings onto Fecralloy Microchannels: Washcoating Vs. In Situ Growing", A. Eleta, L. Costa, M. Montes, J.A. Odriozola. Póster

Nanospain 2008. NanoIberian Conference

14-18 Abril [Braga, Portugal]

"Nanoparticle based One-Dimensional Photonic Crystals", M. Calvo Roggiani, S. Colodrero, M. Ocaña, H. Míguez. Comunicación Oral

XVITH International Symposium on Non-Oxide and New Optical Glasses

21-25 Abril [Montpellier, Francia]

"Studies of Tin-Mercury Alloy and Corrosion Compounds of Ancient Spanish Mirrors", L.K. Herrera, A. Durán, M.L. Franquelo, M.C. Jiménez de Haro, A. Justo, J.L. Pérez Rodríguez. Comunicación Oral

35th International Conference on Metallurgical coatings and Thin Films | ICMTF2008

28 Abril-2 Mayo [San Diego, EUA]

"Comparative performace of nanocomposite coatings of TiC or TiN dispersed in a-C matrixes", D. Martínez, C. López Cartes, A. Fernández, J.C. Sánchez López. Comunicación Oral

"Microstructural and Compositional Studies of TiAlSiN Nanostructured Coatings", V.C. Fortio, T.C. Rojas, F.J. Ferrer, J. García, A. Justo, M.P. DelPlancke-Ogletree, C. López Cartes, A. Fernández. Comunicación Oral

IEEE International Magnetic Conference |INTERMAG2008

4-8 Mayo [Madrid, España]

"Influence of the Capping Molecule on the Magnetic behavior of Thiol Capped Gold Nanoparticle", P. Crespo, E. Guerrero, M.A. Muñoz, A. Hernando, A. Fernández. Poster

2nd International Corrosion Meeting | INTERCORR 2008

12-16 Mayo [Madrid, España]

"Coating Systems for Carbon Steel Protection Against Biocorrosion and Biofouling in Seawater. A Laboratory and Field Study", H.A. Videla, L.K Herrera, M. Pereyra, C.A. Giudice. Comunicación Oral

37th Symposium on Archaeometry

24-27 Mayo [Siena, Italia]

“Study of Face Front of Altar Made of Ceramic Tile Panels (16-17th Centuries) in some Monuments of the Cultural Heritage in Spain: the Italian Influence”, A. Ruiz-Conde, J.J. Lupión, M.Arjonilla, G. Durán, P.J. Sánchez Soto. Póster

E-MRS 2008 Spring Meeting

26-30 Mayo [Estrasburgo, Francia]

“Optically Active Polymers and Nanocomposits for the Fabrication of Photonic Devices”, F.J. Aparicio, A. Barranco, I.K. Blaszczyk Lezak, A.I. Borrás, J. Cotrino, A.R. González-Elipe. Comunicación Oral

“Optical and Electrical Properties of WC-C and TiBC-C Nanocomposite Thin Films Deposited by Magnetron Sputtering”, M.D. Abad, J.C. Sánchez-López, N. Cusnir, R. Sanjinés. Comunicación Oral

6th European Stainless Steel Science and Market Congress

10-13 Junio [Helsinki, Finlandia]

“Behaviour of Ferritic Stainless Steel at High Temperature”, M.A. Heredia, C. Luna, J.F. Almagro, O. Sanz, A. Paúl, J.A.Odriozola. Comunicación Oral

“High Temperature Behaviour of 22Cr-5Al Stainless Steel in Wet Air and CO_2 Atmospheres”, A. Paúl, M. Montes, J.A. Odriozola. Comunicación Oral

“Mechanical Properties and Corrosion Resistence of W Bearing Superduplex Stainless Steels”, C. Muñoz, A. Paúl, A. Gallardo, J.A. Odriozola. Comunicación Oral

“Corrosion Resistence of Powder Sintered Ferritic Stainless Steel”, S.A. Cruz, R. Poyato, A. Paúl, J.A. Odriozola. Comunicación Oral

XVII International Synchrotron Radiation Conference | SR2008

15-20 Junio [Novosibirsk, Rusia]

“Structural study of Pd-Me/TiO_2 (Me=Co, Mn) nanosystem by XAFS”, V.V. Kriventsov, D.I. Kochubey, B.N. Novgorodov, D.P. Ivanov, E.P. Yakimchuk, O.V. Bukhtenko, M.V. Tsodikov, N. Yu. Kozitsyna, M.N. Vargaftik, I.I. Moiseev, G. Colón, M.C. Hidalgo, J.A. Navío, S.G. Nikitenko. Poster

International Symposium on "Catalysis for Clean Energy and Sustainable Chemistry | CCESC

17-20 Junio [Madrid, España]

"Integration of Methanol Steam Reforming and Combustion in a Microchannel Reactor for H_2 Production: a CFD Simulation Study", G. Arzamendi, P.M. Dieguez, M. Montes, M.A. Centeno, J.A. Odriozola, L.M. Gandía. Comunicación Oral

2nd International Conference on Advanced Nanomaterials | ANM 2008

22-25 Junio [Aveiro, Portugal]

"Microstructural characterization and magnetic behavior of thiol-and phosphine-functionalized gold cluster and nanoparticles", E. Guerrero, M.A. Muñoz-Márquez, P. Crespo, A. Hernando, J.C. Conesa, A. Fernández. Póster

XXI Simposio Iberoamericano de Catálisis

22-27 Junio [Málaga, España]

"Catalizadores Monolíticos de Acero Austenítico Tipo AISI 304 con Oro-Criptomelano para la Oxidación de CO", L.M. Martínez T., F. Romero-Sarria, M. Montes, M.A. Centeno, J.A. Odriozola. Póster

"Catalizadores Oro/Hidroxiapatito. Síntesis y Caracterización", M.I. Domínguez, F. Romero-Sarria, M.A. Centeno, J.A. Odriozola. Comunicación Oral

"Catalizadores de Níquel Soportado con Arquitectura Molecular Controlada para Reformado de Metano", D. Hufschmidt, L.F. Bobadilla, F. Romero-Sarria, M.A. Centeno, J.A. Odriozola, M. Montes, E. Falabella. Comunicación Oral

"Nanopartículas de Oro en Titania Modificada: Propiedades del Soporte y Actividad Catalítica", F. Romero-Sarria, R.S. Avellaneda, M.I. Domínguez, M.A. Centeno, J.A. Odriozola. Póster

"Características Estructurales y Superficiales de Catalizadores NiSn/ γ-Al_2O_3 para la reacción de Reformado de Metanol", F. Romero-Sarria, R.S. Avellaneda, M.I. Domínguez, M.A. Centeno, J.A. Odriozola. Póster

"Síntesis y Caracterización de Sistemas Mixtos Tipo $Ce_{1-x}Eu_xO_{2-x/2}$, para ser Empleados como Soportes Activos en la Reacción de Oxidación Catalítica de CO", W.Y. Hernández, M.A. Ceneno, F. Romero Sarria, J.A. Odriozola. Póster

"Influencia de la Atmósfera de Calcinación en la Actividad Catalítica de Catalizadores 1% Au/CeO_2", S.A. Cruz, L.M. Martínez T., F. Romero Sarria, M.A. Centeno, J.A. Odriozola. Póster

"Preparación y Caracterización de Nanopartículas de Oro Soportadas sobre Esferas Monodispersas de Sílica Funcionalizadas con Grupos Amino", A. Penkova, J.M. Martínez-Blanes, M.A. Centeno, K. Hadjiivanov, J.A. Odriozola. Póster

"Hidrotalcitas Comerciales Mg-Al como Precursores de Catalizadores para la Transesterificación con Metanol de Aceite de Girasol", I. Campo, A. Navajas, L.F. Bobadilla, M.A. Centeno, J.A. Odriozola, G. Arzamendi, L.M. Gandia. Póster

"Efecto del Tamaño de Agregado sobre Algunas Propiedades de Montmorillonitas Pilarizadas con Al", O.H. Laguna, M.A. Centeno, J.A. Odriozola, S. Moreno, R. Molina. Póster

"Nanomedicina Catalítica: Funcionalización de Criptomelano Biocompatible y Nanoestructurado para Tratamiento de Cáncer", T. López, E. Ortiz-Islas, J. Manjarrez, P. Arteafa-López,l P. Quintana, M. Montes, P. Navarro, J.A. Odriozola. Comunicación Oral

"Nanomedicina catalítica: Catalizadores Nanoestructurados Pt/SiO_2 para Alquilación Catalítica de ADN de Células Cancerígenas", T. López, E. Ortíz-Islas, M. Alvarez, J.A. Odriozola, S. Recillas. Comunicación Oral

"IR Study of CO adsorption for the Characterization of Fe2+ Cations in Ferrierite as Catalysts for NO_x SCR with NH_3", I. Malpartida, E. Ivanova, M. Mihaylov, K. Hadjiivanov, F. Romero-Sarria, O. Marie, M. Daturi. Comunicación Oral

"Síntesis y Caracterización del Polímero Mixto Fe+Al_{13}-NO_3 y su Inserción en un Mineral Arcilloso", I. Malpartida, E. Ivanova, M. Mihaylov, K. Hadjiivanov, F. Romero-Sarria, O. Marie, M. Daturi. Comunicación Oral

Conference on Recent Development in the Processing and Applications of Structural Metals and Alloys

23-27 Junio [Como, Italia]

"Infrared, Raman and SEM Characterization on Magnetron Puttered Silicon Oxyde and Silicon Oxynitride Films", V.C. Fortio, C. Fernández Ramos, V.N. Denisov, E.A. Vinogradov, A. Fernández. Póster

International Conference on Surface X-ray and Neutron Scattering | SXNS10

2-5 Julio [Paris, Francia]

"Preferential Adsorption from Binary Mixtures of Alkanes and Alcohols: The Decane-Heptanol System", M.D. Alba, M.A. Castro, S.M. Clarke, C. Millán, S. Medina, M.M. Orta, E. Pavón, A.C. Perdigón. Póster

8th Conference on Solid State Chemistry

6-11 Julio [Bratislava, República Eslovaca]

"Nitrogen doping of anatase by room temperature ball milling of titania", M.J. Diánez, L.A. Pérez Maqueda, J.M. Criado, J. Subrt. Póster

3rd International School of Advanced Plasma Technology

28-31 Julio [Varena, Italia]

"Preparation of N-TiO_2 Thin Films by Plasma Enhanced Chemical Vapour Deposition (PECVD)", P. Romero, A. Barranco, J. Cotrino, J.P. Espinós, A.R. González-Elipe. Comunicación Oral

Gordon Research Conference on Biomineralization 2008

10-15 Agosto [New London, EUA]

"Processing, microstructure and mechanical properties of biomimetic silicon carbide developed for medical applications", J. Martínez. Póster

Congress of the International Union of Crystallography

23-31 Agosto [Osaka, Japón]

"Soft Synthesis and Crystallographic Characterization of Calcium Magnesium mixed Carbonates", J.M. Criado, L.A. Pérez Maqueda, M.J. Diánez Millán. Comunicación Oral

"Structure of sodium L-malate monohydrate", M.D. Estrada, A. Criado, S. Pérez-Garrido, M.J. Diánez, E. de Matos Gomes, M. Belsley. Póster

"X-ray structure and hydrogen bonding study of taurine and N-(glucitol-1-yl)taurine", M.J. Diánez, M.D. Estrada, S. Pérez Garrido. Póster

European Congress on Molecular Spectroscopy

31 Agosto-5 Septiembre [Opatija, Croacia]

"Study of the Dehydroxylation-Rehydroxylation of Pyrophyllite by Spectrometric and Thermal Analysis Methods", L.A. Pérez-Maqueda, A. Durán, P.E. Sánchez Jiménez, M.L. Franquelo, J.L. Pérez Rodríguez. Comunicación Oral

14th European Microscopy Congress |EMC2008

1-5 Septiembre [Aache, Alemania]

"Contribution of Electron Microscopy Techinques to the Chemical and Structural Characterization of TiC/a-C Nanocomposites Coatings", C. López Cartes, D. Martínez, J.C. Sánchez López, A. Fernández Camacho. Comunicación Oral

"Influence of Si on the structure and properties of multifunctional bioactive nanostructured films", I.A. Bashukova, A.N. Sheveiko, N.A. Gloushankova, B.N. Marvrin, T.C. Rojas, D.V. Shtansky. Comunicación Oral

Nanomaterials and Nanotechnology Meeting | NANOSTRAVA 2008

2-5 Septiembre [Ostrava, República Checa]

"Characterization of nanoparticles at the environment: a case study at the Canary Islands (Spain) by airbone dust accumulation contribution", I. Menéndez, J.L. Díaz-Hernández, A. Ruiz-Conde, P.J. Sánchez Soto. Comunicación Oral

"Formation of nanostructured powders by dry grinding: a particle size model", P.J. Sánchez Soto, E. Garzón, A. Ruiz-Conde. Poster

11th International Symposium "Order, Disorder and Oxide Properties" | ODPO2008

5-9 Septiembre [Rostov na Donu, Rusia]

"Study of local structure of Pd-Me(3d)/TiO2 nanocatalytic system prepared from bimetallic complexes", V.V. Kriventsov, D.A. Ziuzin, D.P. Ivanov, I.E. Beck, B.N. Novgorodov, D.I. Kochubey, O.V. Bukhtenko, M.V. Tsodikov, N. Yu. Kozitsyna, M.N. Vargaftik, I.I. Moiseev, J.A. Navío, S.G. Nikitenko. Póster

Fractography of Advanced Ceramics 2008

7-10 Septiembre [Donu Stara Lesna, Eslovaquia]

"AFM study of typical surface features in room-temperature fracture of sapphire", J.M. López-Cepero Borrego, A.R. de Arellano-López, J. Martínez-Fernández, J.P. Guin, S.M. Wiederhorn. Comunicación Oral

59Th Meeting of ISE. Electrochemistry Down to the Molecular Level: Interface Science for Life and Technology

7-12 Septiembre [Sevilla, España]

"Electrochemical Properties of a Porphyrin Infiltrated into a Columnar TiO2 Thin Film Modified ITO Electrode", M. Cano, P. Castillero, J.M. Pedrosa, L. Camacho, A.R. González-Elipe, A. Barranco, J.R. Sánchez Valencia. Comunicación Oral

Society of Photo-Optical Instrumentation Engineers: Optics + Photonics | SPIE

7-12 Septiembre [San Diego, EAU]

"Integration of Photonic Crystals in Dye Sensitized Solar Cells", S. Colodrero, A. Mihi, M. Calvo, M. Ocaña, H. Míguez. Comunicación Oral

The 59th Annual Meeting of the International Society of Electrochemistry

7-12 Septiembre [Sevilla, España]

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

11th International Conference on Plasma Surface Engineering

15-19 Septiembre [Garmisch-Partenkirchen, Alemania]

“Bonding structure and mechanical properties of Ti-B-C coatings”, M.D. Abad, D. Cáceres, Y.S. Pogozhev, D.V. Shtansky, J.C. Sánchez-López. Comunicación oral

“N-doping of TiO2 thin films prepared by plasma enhanced chemical vapour deposition”, A. R. González-Elipe, P. Romero Gómez, A. Barranco, J. Cotrino, J.P. Espinós. Comunicación oral

“Thermal Stability and Oxidation Resistance of Nanocomposite TiC/a-C Protective Coatings”, D. Martínez, C. López Cartes, R. Gago, A. Fernández, J.C. Sánchez López. Póster

“Microstructural and Chemical Characterization of Nanostructured and Amorphous Nitride Coatings”, A. Fernández, C. Fernández, V.C. Fortio. Póster

“Tribological behavior of Titanium Carbide/Amorphous Carbon Nanocomposite Coatings”, J.C Sánchez López, D. Martínez, C. López Cartes, A. Fernández. Conferencia Invitada

“In-Situ XPS Study of the Plasma Activation of PET and LDPE Polymers”, M.C. López Santos, A. Barranco, F. Yubero, J. Cotrino, A.R. González-Elipe. Comunicación Oral

“Modelling of Capacitively Coupled Radio-Frequency Discharges in Nitrogen”, L. Marques, C. Pintassilgo, M.C. López Santos, J. Cotrino, L.L. Alves. Póster

“Sterilization of Escherichia Coli Colonies by Means of Ar+NO Microwave Plasmas”, J.L. Hueso, V. Rico, J. Frías E., J. Cotrino, A.R. González-Elipe. Póster

“Water Plasma Effect on the Surface Modification of Carbon Residues from Petrochemical Refinery Processes”, J.L. Hueso, V. Rico Gavira, J. Cotrino, J.P. Espinós, A.R. González-Elipe. Póster

“Influence of the nanocrystalline/amorphous carbon ratio in the tribo-mechanical properties of nanostructured WC/a-C coatings”, J.C. Sánchez-López, M.D. Abad, M.A. Muñoz-Márquez, S. ElMrabet, A. Justo. Póster

“Thermal evolution of WC/C nanostructured coatings by Raman and in situ XRD analysis”, S. ElMrabet, M.D. Abad, C. López-Cartes, D. Martínez Martínez, J.C. Sánchez-López. Póster

XXVII Congreso Argentino de Química “Dr. Pedro José Aymonino”

17-19 Septiembre [Tucumán, Argentina]

“Oxidación de CO sobre Catalizadores de MnO_x-CeO_2 y Au/MnO_x-CeO_2”, O.D. Alessandro, W.Y. Hernández, M.A. Centeno, R.M. Torres, J.E. Sambeth, H. Thomas. Póster

IV Bienal del GERMN-I Reunión Ibérica de RMN

21-23 Septiembre [Sevilla, España]

“Study of the Transformation Mechanism of Kaolinite to Illite at High Pressure by ^{29}Si and ^{27}Al MAS NMR”, M. Mantovani, A. Escudero, A.I. Becerro. Póster

4th Mid-European Clay Conference | MECC 2008

22-27 Septiembre [Zalopane, Polonia]

“Effect of the Layer Charge on the Thermal Behaviour of NH4+-vermiculites”, M.C. Jiménez de Haro, A. Justo, J. Poyato, L.A. Pérez-Maqueda, A. Lerf, F.E. Wagner, J.L. Pérez Rodríguez. Comunicación Oral

“Effect of sonication on the redox state of vermiculites”, J.L. Pérez-Rodríguez, V. Ramírez del Valle, J. Poyato, A. Lerf, E. Wagner. Póster

“Thermal behavior of lead-containing Bentonita from Dador”, M. Benitez-Guerrero, J. Pascual Cosp, V. Balek, M. Benes, J. Subrt, J.L. Pérez-Rodríguez, L.A. Pérez Maqueda. Póster

Sixth International Conference on Inorganic Materials

28-30 Septiembre [Dresden, Alemania]

“Microcharacterization of Cermets (TiCxN1-x-M, M=Ni, Co) using HRSEM, ED/HRTEM, EELS and EFTEM Tecniques”, M.J. Sayagués, J.M. Córdoba, M.D. Alcalá. Póster

“Synthesis of Bimetallic Diborides of Transition Metals by Mechanically Induced Self-Sustaining Reactions”, M.A. Avilés, J.M. Córdoba, M.J. Sayagués, M.D. Alcalá, F.J. Gotor. Póster

XVIII International Conference on Chemical Reactors | CHEMREACTOR 18

29 Septiembre-3 Octubre [Malta]

“Methane Steam Reforming in a Micrhochannel Reactor for GTL Intensification: A Computational Fluid Dynamics Simulation Study”, G. Arzamendi, P.M. Dieguez, M. Montes, J.A. Odriozola, E.F. Sousa-Aguilar, L.M. Gandía. Comunicación Oral

5th European Meeting on Solar Chemistry and Photocatalysis: Environmental Applications | SPEA-5

4-8 octubre [Palermo, Italia]

“ZnO Activation by Using Activated Carbon as a Support: Characterization and Photoreactivity”, E. Pulido Melián, O. González Díaz, J.M. Doña, G. Colón, J. Arana, J.A. Herrera Melián, J.A. Navío, J. Pérez Peña. Poster
“Effect of Sulphate Pre-treatment on the Photocatalytic Activity of Different Gold-modified TiO_2”, M. Maicu, M.C. Hidalgo, G. Colón, J.A. Navío. Poster

“N-Containing TiO_2 Nanocatalysts: Structural and Electronic Parameters Influencing Photoactivity”, P. Sampedro-Tejedor, A. Kubacka, G. Colón, M. Fernández-García. Poster

“Mechanochemical Synthesis of Visible Light Sensitive N-Doped Titanium Dioxide”, J. Subrt, L. Szatmary, M.J. Diánez, J.M. Criado. Comunicación Oral

14th International Symposium on Biodeterioration and Biodegradation | IBBS14

6-11 Octubre [Alessio Siculo, ME, Italia]

“Understanding Microbial Inhibition of Corrosion”, H.A. Videla, L.K. Herrera. Póster

“Surface Analysis and Materials Characterization for the Study of Biodeterioration and Weathering Effects of Cultural Property”, L.K. Herrera, H.A. Videla. Comunicación Oral

“Role of iron Reducing Bacteria in Corrosion and Protection of Carbon Steel”, L.K. Herrera, H.A. Videla. Póster

International Workshop on Advanced Nanostructured Materials and Thin Films for Industrial Applications

21-24 Octubre [Nottingham, Reino Unido]

“Tribological and Mechanical Characterization of TiAlSiN Nanocomposite Thin Films”, D. Philippon, V.C. Fortio, J.C. Sánchez López, D.V. Shtansky, M.P. DelPlancke-Ogletree, A. Fernández. Comunicación Oral

Synchrotron Radiation in Art and Archeology

22-24 Octubre [Barcelona, España]

“Characterization of Azurite and Malachite Pigments by Combined Application of XRD and XRF in the Cross Sections from Spanish Baroque Paintings”, L.K. Herrera, S. Montalbani, G. Chiavari, M. Cotte, A. Duran, A. Justo, J.L. Pérez- Rodríguez. Comunicación Oral

“Identification of Cellulose Fibres Belonging to Spanish Cultural Heritage Using Synchrotron Radiation High Resolution X-Ray Diffraction”, L.K. Herrera, A. Duran, M.C. Jiménez de Haro, M.L. Franquelo, A. Justo, J.L. Pérez-Rodríguez. Comunicación Oral

Hysitron European Workshop & User Meeting 2008
19-20 Octubre [Ismaning, Alemania]

"Mechanical characterization of Ti-Al-Si-N thin films through nanoindentation", C. Paternoster, V. Godinho, M. Haidopoulo, A. Fernández. Póster

Congreso International de Metalurgia y Materiales
28-31 Octubre [Santiago, Chile]

"Evaluaciones Microcalorimétricas en Aleaciones de Cu-4Ti Templadas y Deformadas en Frío", E. Donoso, J.M. Criado. Comunicación Oral

"Modificación de un horno doméstico de microondas para el tratamiento de materiales de alta temperatura bajo atmósfera controlada", J.M. Criado, M.J. Diánez, L.A. Pérez-Maqueda. Comunicación Oral

International Workshop on Advanced Nanostructured Materials and Thin Films for Industrial Applications
10-13 Noviembre [Nothingham, Reino Unido]

"Tribological and mechanical characterization of TiAlSiN nanocomposite thin films", D. Philippon, V. Godinho, J.C. Sánchez-López, D. Shtansky, M.P. Delplancke-Ogletree, A. Fernández. Comunicación Oral

"Nanostructured Materials and Microstructure Group", A Fernández, J.C. Sánchez-López, C. López-Cartes, T.C. Rojas, D. Philippon, S. ElMrabet, M.A. Muñoz Márquez, V. Godinho, M.D. Abad, E. Deprez, G. Arzac, I. Rosa. Póster

"Mechanical Properties of Ti-Al-Si-N thin films at scale", V. Godinho, D. Aranny, P.M. Nagy, D. Philippon, E. Kalman, A. Fernández, M.P. Ogletree. Póster

CHRESP I
27-30 Noviembre [Ljubljana, República de Eslovenia]

"Differences and similarities in the materials and techniques of medieval mural paintings in the coastal región of Slovenia", A. Kriznar, A. Ruiz-Conde, P.J. Sánchez Soto. Póster

II Simposio Latinoamericano Procesos Avanzados de Oxidación | SILAPAO 2008
27-28 Noviembre [Medellin, Colombia]

"Efecto de pre-tratamientos de sulfatación en la actividad catalítica de Au", M. Maicu, M.C. Hidalgo, G. Colón, J.A. Navío. Comunicación Oral

3.6. CONGRESOS Y REUNIONES NACIONALES
NATIONAL CONGRESSES AND MEETINGS

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

XI Congreso Nacional de Tratamientos Térmicos y de Superficies
12-13 Marzo [Valencia, España]
José Antonio Odriozola Gordón [Miembro del Comité Técnico y Científico]

COMUNICACIONES EN CONGRESOS Y REUNIONES
COMMUNICATIONS IN CONGRESS AND MEETINGS

V Reunión del Grupo Especializado de Física del Estado Sólido (GEFES)
6-8 febrero [Santiago de Compostela, España]

“Aplicaciones de las técnicas espectroscópicas al estudio tribológico de sistemas nanoestructurados de Carbono”, J.C. Sánchez López, D. Martínez Martínez, M.D. Abad Roldán, C. Fernández Ramos, Asunción Fernández Camacho. Conferencia Invitada.

9 Reunión Nacional de la Red Temática de Patrimonio Histórico y Cultural del CSIC
2-3 Marzo [Sevilla, España]

“Investigación Interdisciplinar sobre el Estado de Conservación de Negativos Fotográficos”, G. Durán, M. Arjonilla, A. Ruiz-Conde, P.J. Sánchez Soto. Póster

“Las Pinturas Murales Medievales en la Zona Litoral de Eslovenia: Materiales y Técnicas”, Kriznar, A., Ruiz-Conde, A, Sánchez Soto, P.J. Póster

“Estudio de Materiales y Técnicas de Realización Utilizadas en Obras de Arte y sus Procesos de Alteración”, Pérez Rodríguez, J.L., Justo, A., Poyato, J., Durán, A., Jiménez de Haro, M.C., Sigüenza, B., Herrera Quintero, L.K., Odriozola, C., Herrero Fernández, H., Franquelo, M.L. Póster

XI Congreso Nacional de Tratamientos Térmicos y de Superficie | TRATERMAT 2008
12-13 Marzo [Valencia, España]

“Estudio del Efecto de la Modificación Superficial de Monolitos Metálicos en el Anclaje de Catalizadores”, L.M. Martínez T., O. Sanz, A. Paúl, M.A. Centeno, J.A. Odriozola. Póster

“Propiedades Mecánicas y Resistencia a la Corrosión en Aceros Inoxidables Superdúplex con Contenidos Elevados de W”, C. Muñoz, A. Paúl, R. Poyato, J.A. Odriozola. Póster

X Reunión del Grupo Especializado de Polímeros
15-19 Junio [Sevilla, España]

“Ventajas de los Métodos de Control Inteligente de la Temperatura para el Estudio de la Descomposición Térmica de Polímeros”, P.E. Sánchez-Jiménez, L.A. Pérez-Maqueda, J.M. Criado. Póster

X Congreso Nacional de Materiales
18-20 Junio [San Sebastián, España]

“Comportamiento de los aceros inoxidables ferríticos a altas temperaturas”, M.A Heredia, C. Luna, J.F. Almagro, O. Sanz, A. Paúl, J.A. Odriozola. Comunicación Oral

“Activación Superficial mediante Plasmas de LDPE y PET”, M.C. López Santos, J. Cotrino, F. Yubero, A. Barranco, A.R. González-Elipe. Comunicación Oral

“Capas Coloreadas y Fluorescentes preparadas mediante Polimerización mediante Plasmas de Moléculas de Colorantes”, F.J. Aparicio, A. Barranco, I.K. Blaszczyk Lezak, A.R. González-Elipe. Comunicación Oral

“Sensibilización en el Visible de Capas de TiO2 preparadas mediante PVD y PECVD”, P. Romero, J.P. Espinós, J. Cotrino, A. Barranco, A.R. González-Elipe. Comunicación Oral

II Congreso Nacional de Pulvimetalurgia 2008
13-15 Julio [San Sebastián, España]

“Sinterización mediante Spark Plasma de aceros inoxidables ferríticos con dispersión de óxidos”, S.A Cruz, R. Poyato, A. Paúl, J.A. Odriozola. Comunicación Oral

XI Congreso Nacional de Propiedades Mecánicas de los Sólidos
9-12 Septiembre [El Bosque, Cádiz, España]

“Comportamiento Plástico en Compresión Uniaxial de Cermets Ti(C,N)-CO”, A. Gallardo, A. Morales, A. Domínguez Rodríguez, J.M. Córdoba Gallego, M.A. Avilés, F.J. Gotor Martínez. Comunicación Oral

XLVIII Congreso Anual de la Sociedad Española de Cerámica y Vidrio
29-31 Octubre [Oviedo, España]
“Caracterización de pigmentos y soportes empleados en pinturas murales medievales en la iglesia parroquial de San Nicolás en Pangr Grm (Eslovenia)”, A. Kriznar, A. Ruiz-Conde, P.J. Sánchez Soto. Poster

“Caracterización mineralógica y química de filitas de distintos yacimientos del sureste de la Península Ibérica (Almería y Granada)”, E. Garzón, I.G. García, A. Ruiz Conde, P.J. Sánchez Soto. Poster

“Degradación de materiales cerámicos aplicados en Arquitectura: factores de influencia, mecanismos e indicadores de alteración”, J.J. Lupión, M. Arjonilla, J.J. Alarcón, A. Ruiz-Conde, P.J. Sánchez Soto. Poster

“Evolución térmica de vermiculitas con distinta composición y procedencia”, C. Marcos, Y.C. Arango, A. Ruiz-Conde, P.J. Sánchez Soto. Poster

“Investigación interdisciplinar del estado de conservación de placas fotográficas (Siglo XX) de la Facultad de Bellas Artes de la Universidad de Sevilla”, G. Durán, M. Arjonilla, A. Ruiz-Conde, P.J. Sánchez Soto. Poster

3.7. CURSOS / COURSES

MÁSTER / MASTER

MÁSTER EN ESTUDIOS AVANZADOS EN QUÍMICA

Organizado por la Universidad de Sevilla
Coordinadora: Dra. Mª Angeles Alvarez Rodríguez
Fecha de Celebración: Curso Académico 2008-09
Créditos necesarios: 60
Dirigido a: Licenciados en Química, Física, asío como, los Titulados en Ingeniería afines (Ingenieros Químicos, de Materiales, etc.)
Especialidades: Materiales para la Energía y el Medio Ambiente. Ingeniería de Superficies, Materiales Estructurales y Funcionales.
Mención de Calidad

Seminario-Laboratorio de espectroscopia Avanzada (Créditos Europeos: 8) |Dr. Ernesto Carmona (IIQ) | Dra. María Dolores Alba | Dr. Antonio M. Gil (USE) | Dra. Maria Angeles Pradera (USE) | Dr. José M. Fernández-Bolaños (USE)
Química de Polímeros. Biomateriales (Créditos Europeos: 4) | Dr. Manuel Bueno Martínez (USE) | Dr. Juan A. Galbis Pérez | Dr. Manuel Mancera Clavería (USE)
Catálisis Homogénea y Heterogénea (Créditos Europeos: 4) | Dr. Guillermo Munuera | Dr. Juan Cámpora (IIQ) | Dr. Antonio Pizzano (IIQ)
Química de Polímeros. Biomateriales (Créditos Europeos: 4) | Dr. Manuel Bueno Martínez (USE) | Dr. Juan A. Galbis Pérez | Dr. Manuel Mancera Clavería (USE)
Catálisis Homogénea y Heterogénea (Créditos Europeos: 4) | Dr. Guillermo Munuera | Dr. Juan Cámpora (IIQ) | Dr. Antonio Pizzano (IIQ)

MÁSTER EN CIENCIA Y TECNOLOGÍA DE NUEVOS MATERIALES

Máster en Ciencia y Tecnología de Nuevos Materiales

Organizado por la Universidad de Sevilla
Coordinador: Dr. Antonio Córdoba Zurita
Fecha de Celebración: Curso Académico 2008-09
Créditos necesarios: 60
Dirigido a: Licenciados en Química, Física, asío como, los Titulados en Ingeniería afines (Ingenieros Químicos, de Materiales, etc.)
Especialidades: Materiales para la Energía y el Medio Ambiente. Ingeniería de Superficies, Materiales Estructurales y Funcionales.
Mención de Calidad

Química del Estado Sólido (Créditos Europeos: 5) | Dr. Guillermo Munuera | Dr. Miguel Angel Castro | Dra. Pilar Malet
Fisica del Estado Sólido (Créditos Europeos: 5) | Dr. Alfonso Bravo | Dra. Josefa Borrego | Dr. Manuel Jiménez Melendo
Técnicas de Caracterización de Materiales (Créditos Europeos: 8) | Dra. Adela Muñoz Páez | Dr. Antonio Ramírez de Arellano | Dr. Julián Martínez Fernández | Dr. Juan M. Montes (USE) | Dr. Juan Pedro Holgado
Síntesis de Materiales y Nanoestructuras (Créditos Europeos: 7) | Dra. Asunción Fernández Camacho | Dr. Francisco J. Gotor | Dr. Juan Pedro Espinós | Dr. Manuel Ocaña
Catalizadores para la Energía y el Medio Ambiente (Créditos Europeos: 5) | Dr. Alfonso Caballero | Dr. José Antonio Navío | Dr. Miguel Angel Centeno
Materiales con Funcionalidad Superficial (Créditos Europeos: 5) | Dr. Angel Barranco | Dr. Agustín R. González-Elipe | Dr. Francisco Yubero
Corrosión y Recubrimientos Protectores (Créditos Europeos: 5) | Dr. Antonio Paúl Escolano | Dr. Juan Carlos Sánchez López | Dr. José M. Gallardo (USE) | Dr. Enrique Herrera (USE)
Recuperación y Transformación de Materiales (Créditos Europeos: 5) | Dr. Gerardo Colón | Dr. José Antonio Odriozola | Dr. Luis Pérez Maqueda
Procesado de Materiales Estructurales (Créditos Europeos: 5) | Dr. Alfonso Bravo León | Dr. Julián Martínez Fernández | Dr. José A. Rodríguez Ortiz (USE)
Comportamiento Mecánico (Créditos Europeos: 5) | Dr. Arturo Domínguez Rodríguez | Dra. Angela Gallardo López | Dr. Diego Gómez
Comportamiento Magnético (Créditos Europeos: 5) | Dr. Alejandro Conde Amiano | Dra. Clara F. Conde Amiano | Dr. Victorino Franco
Comportamiento Térmico, Dieléctrico y Óptico (Créditos Europeos: 5) | Dra. M. Carmen Gallardo Cruz | Dr. Hernán Míguez García | Dr. Jaime del Cerro
Computación en Ciencia de Materiales (Créditos Europeos: 5) | Dr. Antonio Córdoba (USE) | Dr. Agustín Galindo del Pozo (USE) | Dr. Felipe Gutiérrez Mora

CURSOS DE POSTGRADO / POSTGRADUATE COURSES

MÉTODOS FÍSICOS DE ANÁLISIS DE CAPAS FINAS Y SUPERFICIES DE SÓLIDOS


Curso de Postgrado del CSIC
Programa 2005-06

Métodos Físicos de Análisis de Capas Finas y Superficies de Sólidos

Sevilla, del 26 al 30 de junio de 2006

Este curso de postgrado pretende familiarizar a los asistentes con algunos de los métodos físicos de análisis más utilizados en la actualidad para la caracterización de capas finas y superficies. El curso, de una semana de duración, constará de clases teóricas y sesiones prácticas. Será impartido por profesores de la Universidad de Sevilla e Investigadores del CSIC, en las instalaciones y con el equipamiento científico disponible en el Instituto de Ciencia de Materiales de Sevilla y el Centro Nacional de Aceleradores.

Está dirigido a científicos e ingenieros especializados en temas de análisis, diagnóstico e investigación en materiales y superficies. También se considera especialmente adecuado para alumnos de tercer ciclo de ingenierías de materiales.

Temáticas

Aplicaciones Tecnológicas de las Películas Delgadas
Técnicas de Preparación de Películas y Recubrimientos (CVD, PVD)
Espectroscopías de Fotoemisión (XPS, UPS)
Microscopías Electrónicas de Transmisión y Barrido (TEM y SEM)
Espectroscopías Electrónicas (Auger, REELS, EDX, PEELS)
Difracción y Fluorescencia de Rayos X
Absorción de Rayos X (EXAFS, XANES)
Dispersión de Iones (ISS, RBS)
Microscopías de Aproximación de puntas (AFM, STM)

Directores:

Dr. Juan Pedro Espinós Manzorro
Instituto de Ciencia de Materiales de Sevilla
jpespinos@icmse.csic.es

Dr. Guillermo Munuera Contreras
Instituto de Ciencia de Materiales de Sevilla
Dpto. Química Inorgánica
munuera@us.es

Instituto de Ciencia de Materiales de Sevilla
c/ Américo Vespucio, 49. 41092 (Sevilla)
Telf: 954 48 95 27 • Fax: 954 46 06 65
http://www.icmse.csic.es/Cursos.htm
CUOTA DE INSCRIPCIÓN: 260 €

core level

Hay disponible un número limitado de becas para alumnos de tercer ciclo que lo soliciten (Deben adjuntar curriculum vitae y una carta de presentación de un investigador cualificado)

Organizado por el Instituto de Ciencia de Materiales de Sevilla
Directores: Dr. Guillermo Munuera y Dr. Juan Pedro Espinós
Fecha de Celebración: 23 al 27 de junio de 2008
Horas lectivas: 25 de teoría + 15 de prácticas
Dirigido a: Grado de Doctor, Estudiante de Doctorado o Especialista de Empresa

Este curso de postgrado pretende familiarizar a los asistentes con algunos de los métodos físicos de análisis más utilizados en la actualidad para la caracterización, de materiales en general, y de capas finas y superficies en particular. El curso, de carácter intensivo y una semana de duración, consta de clases teóricas y sesiones prácticas. Estas últimas, desarrolladas con grupos de reducidos de alumnos, se realizarán con el equipamiento científico disponible en el Instituto de Ciencia de Materiales de Sevilla, el Centro Nacional de Aceleradores y el Servicio de Espectroscopía de Fotoelectrones de la Universidad de Sevilla. El contenido y enfoque de los temas y otras actividades del curso son eminentemente prácticos, estando dirigido a científicos e ingenieros especializados en temas de análisis, diagnóstico, investigación en superficies, etc. También se considera especialmente adecuado para alumnos de tercer ciclo relacionados con la temática tratada.

Teoría**:**
Interacción de Fotones, Electrones e Iones con la Materia. Métodos Experimentales de Análisis de Sólidos | Dr. Guillermo Munuera
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
Los electrones como sonda en el Análisis de Superficies: Espectroscopías Auger y Reels | Dr. Francisco Yubero Valencia
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
Microscopía Electrónica de Transmisión y Barrido: Fundamentos y Aplicaciones Generales | Dra. Asunción Fernández Camacho
Microscopía Electrónica de Alta Resolución: Simulación | Dra. María Jesús Sayagués
Microscopías Efecto Túnel y Fuerzas Atómicas | Dr. José Jesús Benítez
Métodos de Determinación de Espesores de Capas Finas| Dr. Juan Pedro Espinós

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
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. Victor López Flores
Retrodispersión Rutherford | Dr. Javier García
Microscopía de Fuerzas Atómicas | Dr. Carmen López Santos

APLICACIÓN DE LA RADIACIÓN SINCROTRÓN A LA CARACTERIZACIÓN DE MATERIALES


Curso de Postgrado del CSIC
Programa 2006-07
Aplicación de la Radiación Sincrotrón a la Caracterización de Materiales
Sevilla, del 9 al 11 de Abril de 2007

Organizado por el Instituto de Ciencia de Materiales de Sevilla
Directores: Dra. Adela Muñoz Páez
Fecha de Celebración: 6 al 8 de octubre de 2008
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

Determinación Estructural bajo altas presiones con Radiación Sincrotrón | Dr. Julio Pellicer Porres, Universidad de Valencia

Aplicaciones en Química de la Radiación Sincrotrón | Dra. Sofía Díaz Moreno, Diamond, Oxford, GB

Espectroscopía de Fotoelectrones: Fotoemisión| Dr. Juan Pedro Espinós

Introducción a la Dispersión de Rayos X a bajo ángulo de Luz de Sincrotrón | Dr. Tiberio Ezquerra, IEM Madrid

Espectroscopía de Absorción de Rayos X | Dr. Jesús Chaboy Nalda, ICMA Zaragoza

Espectroscopía de Absorción de Rayos X de baja energía | Dr. Agustín R. González-Elipe

Demostración práctica de los métodos de análisis de espectroscopía EXAFS | Dr. Victor López Flores

Microscopía de Rayos X: Principios y Aplicaciones | Dra. Germa Martínez Criado, ESRF, Francia

La fuente de luz sincrotrón "ALBA" y la línea "CIRCE" de espectroscopía y de microscopía de fotoemisión | Dra. Lucía Aballe, ALBA Barcelona

Técnicas de caracterización de materiales mediante haces de iones | Dr. Francisco Yubero Valencia

DETERMINACIÓN DE ESTRUCTURAS EN SÓLIDOS REALES: TÉCNICA DE RESONANCIA MAGNÉTICA NUCLEAR

Curso de Postgrado del CSIC
Programa 2007-08

Determinación de Estructuras en Sólidos Reales: Técnica de Resonancia Magnética Nuclear

Sevilla, del 8 al 12 de septiembre de 2008

PROFESORES

Dra. Mª Dolores Alba
Dr. Miguel Angel Avilés
Dra. Ana Isabel Becerro
Dra. Teresa Blasco
Dr. Miguel Angel Castro
Dr. Pablo Chain
D. Juan I. Corredor
Dr. Laurence Delevoye
Dr. Alberto Escudero
Dr. Pedro Nieto
Dr. Jesús Sanz
Dª Esperanza Pavón

Este curso pretende suministrar los conocimientos básicos para el estudio de los sólidos reales a través de una técnica que informa acerca del orden local de los átomos de la red. Para ello, se hará una breve introducción teórica de los sólidos reales, haciendo hincapié en aquellos aspectos estructurales que demandan el empleo de técnicas instrumentales que aporten información a corto alcance. Además, se darán los principios básicos en los que se basa la resonancia magnética nuclear que irán acompañados de una colección de problemas.

HORARIO

Lunes-Jueves: 9:00-13:00 y 15:30-19:00
Viernes: 9:00-13:00

DIRIGIDO A

Alumnos de tercer ciclo e investigadores interesados en el área de RMN y Química del Estado Sólido

DIRECTORA

Dra. María Dolores Alba Carranza
alba@icmse.csic.es

SECRETARIA

Dª Margarita Adorna
Dª Ana García Martín
D. José Carlos Rivero

Instituto de Ciencia de Materiales de Sevilla
c/ Américo Vespucio, 49. 41092 (Sevilla)
Telf: 954 48 95 46 • Fax: 954 46 06 65
http://www.icmse.csic.es/cursormn.htm
CUOTA DE INSCRIPCIÓN: 150 €

Organizado por el Instituto de Ciencia de Materiales de Sevilla
Directores: Dra. María Dolores Alba Carranza
Fecha de Celebración: 8 al 12 de septiembre de 2008
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 | Dr. Miguel Angel Castro Arroyo

Conceptos Básicos | Dra. María Dolores Alba Carranza

Secuencia de Pulso Básica en RMN | Dr. Laurent Delevoye

Herramientas Matemáticas Básicas para RMN | Dr. Laurent Delevoye

Estado Sólido: Componentes Anisotrópicas| Dr. Jesús Sanz
RMN de No-Sólido No-Líquido | Dr. Pedro Nieto
RMN de Sólido de Núcleos con Espín ½ Abundantes | Dr. Miguel Angel Castro Arroyo
RMN de Sólido de Núcleos con Espín ½ y bajo gamma | Dra. Ana Isabel Becerro Nieto
RMN de Sólido de Núcleos con Espín mayor de ½ | Dra. Teresa Blasco
Profesores de Seminarios: Dra. María Dolores Alba, Dra. Ana Isabel Becero Nieto, Ldo. Pablo Chain, Ldo. Juan Isidro Corredor, Dr. Alberto Escudero, Lda. Esperanza Pavón
Profesor de Prácticas: Dr. Miguel Angel Avilés Escaño

OTROS / OTHER

Curso de Extensión Universitaria: "La Difracción de Rayos X. Introducción al Análisis de Difractogramas"

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: 2 al 27 de junio de 2008
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

14 de enero	**Aplicaciones ambientales de la fotocatálisis heterogénea. Estrategias para aumentar la actividad fotocatalítica del óxido de titanio** M. Carmen Hidalgo López Lugar: Real Academia de Ciencias, Sevilla
25 de enero	**Aceros Inoxidables: Futuros Desarollos y Usos** José Antonio Odrizola Gordón Lugar: Ciclo de Conferencias sobre Ciencia y Tecnología de Materiales. Inasmet-Tecnalia, San Sebastián
11 de febrero	**Estudio de clusters y nanopartículas de oro funcionarizadas con trifenilfosfina y tiol** Asunción Fernández Camacho Lugar: Instituto de Magnetismo Aplicado. Universidad Computense-Renfe. Madrid
30 de marzo	**Tailored synthesis of Nanocomposites base on the Ti-C-N system with controlled mechanical and tribological properties** Diego Martínez, Juan Carlos Sánchez López, Asunción Fernández Lugar: First International Conference on Functional Nanocoatings, Budapest, Hungria
27 de mayo	**Arqueometría. Técnicas Instrumentales de Caracterización de Materiales Cerámicos de Interés Arqueológico** Antonio Ruiz Conde Lugar: Sevilla
17 de septiembre	**Nanostructured oxide thin films prepared by the plasma and related methods** Agustín R. González-Elipe Lugar: EMRS Varsovia, Polonia
19 de septiembre	**N-Doping of TiO_2 Thin Films Prepared by Plasma Enhanced Chemical Vapour Deposition** A.R. González-Elipe, P. Romero, A. Barranco, J. Cotrino, J.P. Espinós Lugar: 11th International Conference on Plasma Surface Engineering. Garmisch-Partenkirchen, Alemania

11 de noviembre	**Resonancia Magnética Nuclear de Sólidos: Estudios de Interfases Sólido-Líquido** Mª Dolores Alba Carranza Lugar: Bilbao, España
16 de noviembre	**Actividades del Grupo de Investigación “Materiales Cerámicos y Vítreos” dentro de la Red Temática PHYC del CSIC** Pedro José Sánchez Soto Lugar: Universidad de Extremadura, Cáceres
16 de noviembre	**Aplicación de Técnicas Instrumentales a la Caracterizacion y Análisis de Materiales del Patrimonio Histórico y Cultural** Antonio Ruiz Conde Lugar: Universidad de Extremadura, Cáceres
18 de noviembre	**Materiales Nanoestructurados y Microestructura** Asunción Fernández Camacho Lugar: Nanobusiness2008, Sevilla
18 de noviembre	**Reactividad de Solidos** José Manuel Criado Luque Lugar: Nanobusiness2008, Sevilla

3.9. Conferencias Impartidas en el ICMS / Conferences in the ICMS

Ciclo de Conferencias / Conferences

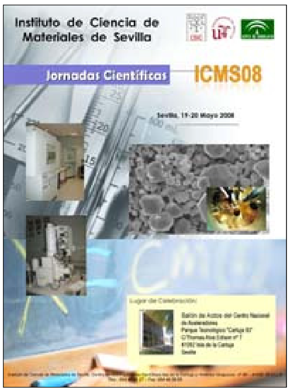
3 de julio	**Generación de nanopartículas core@shell. Estructura y propiedades** Enric Bertrán Serra Lugar: Grupo FEMAN, Departamento de Física Aplicada y Óptica. Instituto de Nanociencia y Nanotecnología, IN2UB. Universidad de Barcelona
5 de septiembre	**Utilización de la técnica RMN en el estudio de electrolitos sólidos** Jesús Sanz Lázaro Lugar: Departamento de Sólidos Iónicos. Instituto de Ciencia de Materiales de Madrid

22 de septiembre	**Espectroscopía Raman operando, determinación simultánea de estructura y actividad catalítica** Miguel Ángel Bañares González Lugar: Laboratorio de Espectroscopía Catalítica. Instituto de Catálisis y Petroleoquímica. Madrid
9 de octubre	**Control de la morfología y la respuesta óptica de oro coloidal** Luis M. Liz Marzán Lugar: Grupo de Química Coloidal. Departamento de Química Física. Universidad de Vigo
11 de noviembre	**Cristales y vidrios fotónicos por autoensamblado** Ceferino López Fernández Lugar: Grupo de Cristales Fotónicos. Instituto de Ciencia de Materiales de Madrid

Seminarios Internos / Internal Seminars

13 de marzo	**Microscopía Electrónica de Transmisión: Aportación al Estudio de Sistemas Nanoestructurados. “Últimas Tendencias”** Cristina Rojas Ruiz Lugar: Instituto de Ciencia de Materiales de Sevilla
25 de marzo	**Friction and Wear of Modern Carbon-Based Films (Environmental Effects)** Feodor M. Borodich Lugar: Cardiff University, Cardiff CF24 3AA, UK
17 de Junio	**How to design nanostructured PVD nitrides based coatings for increasing the durability of steel?** P. Steyer Lugar: INSA de Lyon, Laboratoire MATEIS, bât. L. de Vinci, 69621 Villeurbanne cedex, France
10 de Julio	**Biological Applications of Colloidal Nanoparticles** Wolfgang Parak Lugar: Philipps-Universität Marburg Fachbereich Physik, AG Biophotonik. Renthof 7, D-35032 Marburg
23 de septiembre	**Novel Nanostructured Mg-based Reactive Hydride Composites for Mobile Hydrogen Storage** Rüdiger Bormann Lugar: Institute of Materials Research, GKSS Research Centre, 21502 Geestracht, Germany

Jornadas Científicas. ICMSE 08



Sevilla, 19 y 20 de Mayo

Desarrollo de Fibras Nanoestructuras mediante Plasmas| Dr. Agustín R. González-Elipe

Nanopartículas de Oro con Funcionalización y Microestructura Controladas | Dra. Asunción Fernández Camacho

Efecto de las vacantes de oxígeno en las propiedades electrónicas, estructurales y catalíticas de sistemas de Au soportado| Ldo. Willinton Yesid Hernández Enciso

Efecto sinérgico entre sulfatación y deposición de metales nobles en la mejora de la actividad fotocatalítica de nanopartículas de oxido de titanio | Dr. Gerardo Colón Ibáñez

Efecto de los cristales fotónicos coloidales sobre la eficiencia de células solares| Ldo. Agustín Mihi Cervelló

Composites de matriz aerogel para captar y fijar CO2 | Dr. Luis Esquivias Fedriani

Síntesis por combustión: un nuevo método para la preparación de materiales nanoestructurados | Ing. Victor Manuel González de la Cruz

Microestructura, cristalografía y modelado del comportamiento mecánico en cerámicos eutécticos de Al2O3 | Ldo. Joaquin Ramírez Rico

Desarrollo de nuevos materiales refractarios por métodos mecanoquímicos | Dr. Francisco José Gotor Martínez

Algunas cuestiones pendientes acerca de la plasticidad de sólidos nanoestructurados | Dr. Diego Gómez García

Desarrollo experimental de medidas de difracción de rayos X en sólidos de baja dimensionalidad | Ldo. Santiago Medina Carrasco

Adsorción y autoensamblado de aminas y ácidos carboxílicos alifáticos en soportes modelo como surfactantes en los procesos de flotación y recuperación de minerales | Dr. José Jesús Benítez Jiménez

Estudio de muestras de Patrimonio (estratigrafías y amalgamas) por técnicas de Rayos X | Lda. Liz Karen Herrera Quintero

3.10. Tesis Doctorales/ Doctor Degree Thesis

Título: **Deposición de catalizadores sobre superficies metálicas para aplicaciones catalíticas**
Autor: Leidy Marcela Martínez Tejada
Directores: José Antonio Odriozola Gordón y Miguel Angel Centeno Gallego
Calificación: Sobresaliente “Cum Laude”
Centro: Universidad de Sevilla

Título: **Estabilidad térmica de polímeros y nanocompuestos poliméricos. Propuesta de una metodología de análisis cinético**
Autor: Pedro E. Sánchez Jiménez
Directores: Luis Allan Pérez Maqueda
Calificación: Sobresaliente “cum laude”
Centro: Universidad de Sevilla

Título: **Preparación, caracterización y modelización de cristales fotónicos coloidales para aplicaciones en células solares**
Autor: Agustín Mihi Cervelló
Directores: Hernán Míguez García
Calificación: Sobresaliente “cum laude”
Centro: Universidad de Sevilla

Título: **Development of ReflEXAFS technique: atomic structure from deep surface regions**
Autor: Victor López Flores
Directores: Adela Muñoz Páez
Calificación: Sobresaliente “cum laude”
Centro: Universidad de Sevilla

Título: **Caracterización Microestructural de Compuestos Cerámicos y Laminados para Aplicaciones Estructurales**
Autor: Joaquón Ramírez Rico
Directores: Julián Martínez Fernández, Antonio Ramírez de Arellano-López
Calificación: Sobresaliente “cum laude”
Centro: Universidad de Sevilla

COOPERACIÓN CIENTÍFICA
SCIENTIFIC COOPERATION

4

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

Chile

Síntesis de aleaciones y cermets de cobre de alta conductividad eléctrica y elevada Resistencia mecánica | J.M. Criado, L.A. Pérez-Maqueda, M.J. Diánez, P.E. Sánchez Jiménez, E. Donoso Catalán, R. Palma Hillem

Código:	2006CL0033
Organismo Financiador:	CSIC – Universidad de Chile
Periodo:	2007-2008

Colombia

Síntesis y caracterización de sistemas fotocatalíticos basados en óxidos de titanio con respuesta en el visible para su uso en fotocatálisis solar | M.C. Hidalgo, G. Colón, J.A. Navío, G.M. Restrepo, J.M. Marín, L.A. Ríos, M.I. Mejía, C.F. Granda

Código:	2006CO0001
Organismo Financiador:	CSIC – Colciencias
Periodo:	2007-2008

Elaboración de monolitos basados en arcillas pilarizadas y su potencial catalítico en la reacción de oxidación de fenol en base acuosa diluida | M.A. Centeno, J.A. Odriozola, L.M. Martínez Tejada

Código:	2006CO0014
Organismo Financiador:	CSIC – Colciencias
Periodo:	2007-2008

Hungría / Hungary

Efecto magnetocalórico en materiales amorfos y nanoestructurados | A. Conde, C.F. Conde, V. Franco, J.S. Blázquez

Código: Comisión Mixta CSIC-AHS 2006HU0015
Organismo Financiador: CSIC
Periodo: 2007-2008

Mexico

Estudio de la interacción de sistemas oxídicos nanoestructurados con moléculas orgánicas con potencial farmacológico. Hacia el diseño de dispositivos de liberación controlada "in situ" | J.A. Odriozola, M.A. Centeno

Código: 2005MX0029
Organismo Financiador: CSIC – CONACYT
Periodo: 2007-2008

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

República Checa / The Czech Republic

Nanocristalización de calcogenuros y óxidos amorfos | L.A. Pérez-Maqueda, J.M. Criado, M.J. Diánez, J. Subrt, J. Malek, V. Balek

Código: 2006CZ0023
Organismo Financiador: CSIC – Academia de Ciencias Checa
Periodo: 2007-2008

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. José Luis Pérez Rodríguez, Profesor de Investigación del CSIC.

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 Seville.

The person in charge of this Associated Unit is Dr. José Pascual Cosp from the University of Malaga and Dr. José Luis Pérez Rodríguez 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 MEDIOAMBIENTE

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, Profesor Titular 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 fotocatálisis 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

University of Cambridge		
Londres, Reino Unido	Ldo. **M. David Abad**	[1 semana]
	Dr. **Juan Carlos Sánchez López**	[1 semana]
Università degli Studi di Cagliari		
Cagliari, Italia	Dr. **José Antonio Navío Santos**	[1 semana]
Universidad Nacional		
Bogotá, Colombia	Dr. **Miguel Angel Centeno Gallego**	[1 semana]
CIDIA. Universidad de Las Palmas de Gran Canaria		
Las Palmas de Gran Canarias	Dr. **José Antonio Navío Santos**	[2 semanas]
Instituto Politecnico de Milan		
Milán, Italia	Dra. **Francisca Romero Sarria**	[1 mes]
Institute of General and Inorganic Chemistry. Bulgarian Academy of Sciences		
Sofia, Bulgaria	Dra. **Anna Dimitrova Penkova**	[1 mes]
Walter-Meissner Institut. Academia de Ciencias de Baviera		
Garching, Alemania	Dr. **Juan Poyato Ferrera**	[1 mes]
LACCO. Universidad de Poitiers		
Poitiers, Francia	Dra. **María Isabel Domínguez Leal**	[7 semanas]
Forschungszentrum Karlsruhe. Institute for Materials Research I (IMFI)		
Karlsruhe, Alemania	Lda. **Sylvia Andrea Cruz Torres**	[10 semanas]
University College of London		
Londres, Reino Unido	Lda. **Esperanza Pavón González**	[3 meses]
Institute de Physique de la Matière Complexe		
Laussane, Suiza	Ldo. **M. David Abad**	[3 meses]
GKSS (Forschungszentrum)		
Geesthacht, Alemania	Lda. **Emilie Deprez**	[3 meses]
Universitat Hannover		
Hannover, Alemania	Lda. **Marina Maicu**	[3 meses]
Faculty of Applied Sciences, Chemicals & Materials Department		
Bruselas, Bélgica	Ing. **Vanda Godinho**	[6 meses]

4.4. ESTANCIAS DE INVESTIGADORES EN EL ICMS
PERSONNEL OF THE OTHER LABORATORIES IN THE ICMS

IFW		
Dresden, Alemania	**Carine Rongeat**	[3 dias]
Technological University for Steel and Alloys		
Moscú, Rusia	**V. Kirykhantsev-Korneev**	[1 semana]
Universidade do Minho		
Guimaraes, Portugal	**Sandra M. Fernades Carvalho**	[1 semana]
GKSS (Forschungszentrum)		
Geesthacht, Alemania	**Ulrike Bösenberg**	[1 semana]
	José Belosta Von Colbe	[1 semana]
	Christian Bonatto Minella	[2 semanas]
INSA-Lyon		
Lyon, Francia	**Philippe Steyer**	[2 semanas]
Institute of General and Inorganic Chemistry. Bulgarian Academy of Sciences		
Sofia, Bulgaria	**Mihail Mihaylov**	[2 semanas]
	Elena Ivanova	[2 semanas]
Universidad de Antioquia		
Medellín, Colombia	**Juan Miguel Marín Sepúlveda**	[2 semanas]
	Gloria Restrepo Vásquez	[2 semanas]
	Biviana A. Llano Agudelo	[4 meses]
Université de Lille		
Lille, Francia	**Laurent Delevoye**	[1 mes]
Universidad Nacional		
Bogotá, Colombia	**Andrea Álvarez Moreno**	[1 mes]
CIDIA. Universidad de Las Palmas de Gran Canaria		
Las Palmas de Gran Canarias	**Elisenda Pulio Melián**	[2 meses]
Università degli Studi di Cagliari		
Cagliari, Italia	**Donatella Delpiano**	[4 meses]

OTRAS ACTIVIDADES
OTHER ACTIVITIES

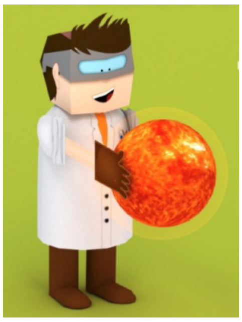
5.1. Actividades de Divulgación Científica
Activities for Dissemination of Science

MINISTERIO DE EDUCACIÓN Y CIENCIA
CSIC
FECYT
AÑO de la CIENCIA 2007

5

5.1. ACTIVIDADES DE DIVULGACIÓN CIENTÍFICA
ACTIVITIES FOR DISSEMINATION OF SCIENCE

Feria de la Ciencia / Fair of Science



La VI Feria de la Ciencia (15, 16 y 17 de mayo de 2008, 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 VI Fair of Science (15, 16, and 17 May 2008, in Seville) constituted a meeting point where many activities for spreading of science and technology were carried out. Demonstrations and experiments where presented to facilitate the understanding of scientific aspects. The Materials Science Institute of Seville presented the activity:

"Sun, Water, Hydrogen and Energy"

Coordinador/Coordinator: Dr. Juan Pedro Holgado, Dr. Gerardo Colón Ibáñez
Conferenciantes/Speakers: Dr. Gerardo Colón Ibáñez, Lda. Rosa Pereñiguez, Ldo. Yesid Hernández Enciso, Ldo. Oscar Laguna

Semana de la Ciencia y la Tecnología
Science and Technology Week

Jornadas de puertas abiertas (Semana del 10 al 23 de Noviembre de 2008, en Sevilla). La VIII 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 (10-23 November 2008). The VII Science and Technology week is open to every body. The event has an European character and is designer to demonstration in Science and Technology.

Coordinadores/Coordinators: Dr. Pedro José Sánchez Soto y Dr. Antonio Ruiz Conde

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