Book of abstracts:
Iberian Vacuum Conference, RIVA-X
8th European Topical Conference on Hard Coatings

4-6th October 2017
Bilbao, Spain

RIVA-X

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and the Portuguese Vacuum Society (SOPORVAC)
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The **Iberian Vacuum Conference, RIVA** is a join meeting of the**Spanish Vacuum Society** (ASEVA) and the **Portuguese Vacuum Society** (SOPORVAC), and follows the series started in Braga, Portugal, in 1988, changing alternatively the location between Portugal and Spain. The main goal of this conference is to cover the fields of vacuum and its applications.

It is for us a great pleasure to **welcome you to the *Bizkaia Aretoa* centre** where we celebrate the 10th edition of the RIVA conferences, Called RIVA-X. For this occasion, we have tried to accommodate a widely scoped scientific program paying especial attention to combine fundamental science and engineering. We tried our best to offer you attractive and exciting scientific talks and posters. We have received 112 abstracts, about 68% Spanish, 20% from Portugal and the rest from other countries. 60 of them have been selected as oral talks.

This edition includes important changes from previous RIVA conferences.

In particular we would like to draw your attention to the award to the **best thesis**, sponsored by **LEYBOLD** and ASEVA. The winner of this first edition will have an invited talk at the end of the conference. We have made an effort to promote the assistance of students, according a special reward to those presenting posters, also sponsored by LEYBOLD.

The **technological exhibition** of this conference is very appealing as seven firms will exhibit their products and will show us new development in the field in scientific talks. We recommend you to visit it, and interact with them.

There are three special sessions within this conference. One is the **8th European Topical Conference on Hard Coatings**, a typical satellite meeting from previous editions. We devoted a whole session to this topic.

Second, we will have a special session to make tribute to **Prof. Jose Luis de Segovia**, where his scientific career will be revisited and highlighted by reknowned colleagues and friends. Jose Luis de Segovia has been one of the main actors in previous RIVA conferences, and from the Spanish Vacuum Society we feel proud of him and we would like to offer this special tribute.

Finally, a technological session will take place, where most of the companies participating will show us their recent technological development, in a non-commercial but technical talk.

Our hope is that you will enjoy the science and technology challenges that will be shown in the conference; profit the occasion to establish links between colleagues in your field of research, approaching science to technology and viceversa, and finally that the conference may serve to increase the friendship between our close-countries.

The main organizers:

José A. Martín Gago (ASEVA, scientific committee)
Javier Barriga (TekniKer)
Enrique Ortega (UPV-EHU)
Carlos Tavares (SOPORVAC)
Miguel Manso (UAM)
Mª Francisca López (ICMM-CSIC)

ROOM DISTRIBUTION AND PRACTICAL INFORMATION

Registration: Bizkaia Aretoa, main entrance

Sala Baroja (SECOND FLOOR)

Plenary and invited sessions.

Sessions: Surf. Sci./Applied Surf. Sci. ; Thin films /Electronic materials; Biointerphases.

Opening and closing sessions; best thesis talk.

Sala Arriaga (SECOND FLOOR)

Sessions: Nanometer, Hard coatings, Technological session.

Special Session “Jose Luis de Segovia”.

Sala Laboa (SECOND FLOOR)

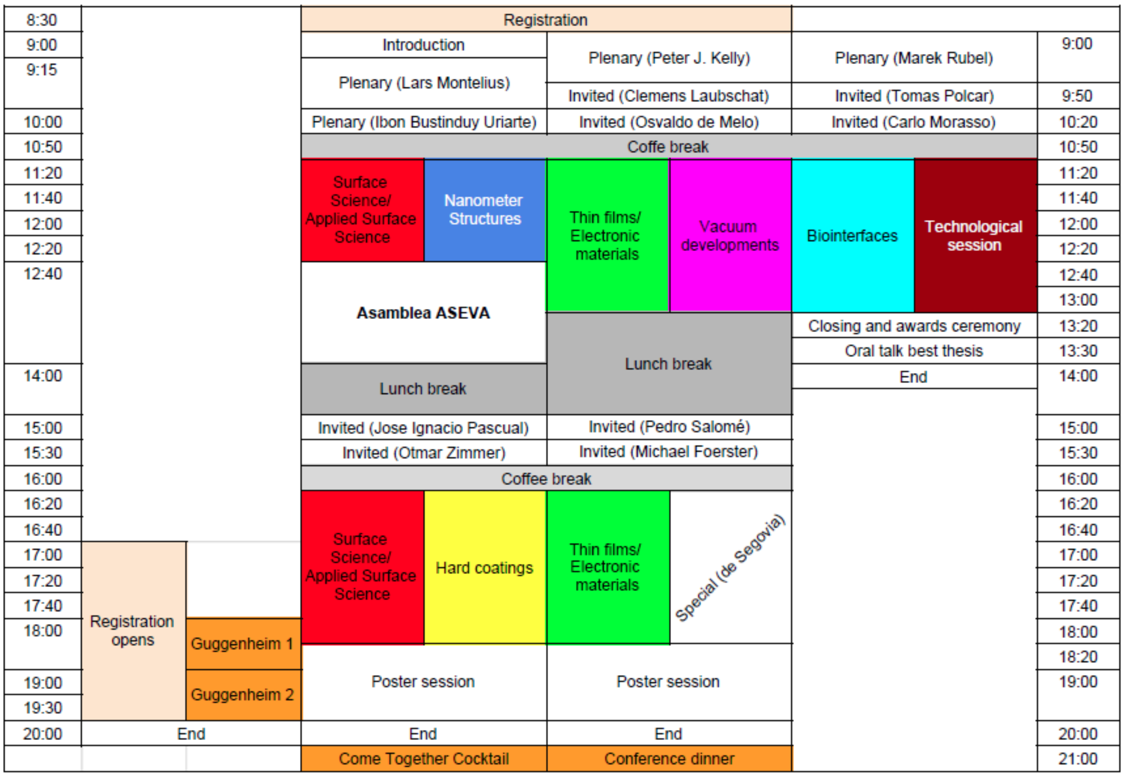
Poster session. Please use your list number. Size: 110 cm x 90 cm.

Sala Chillida (FIRST FLOOR):

Coffee and lunches.

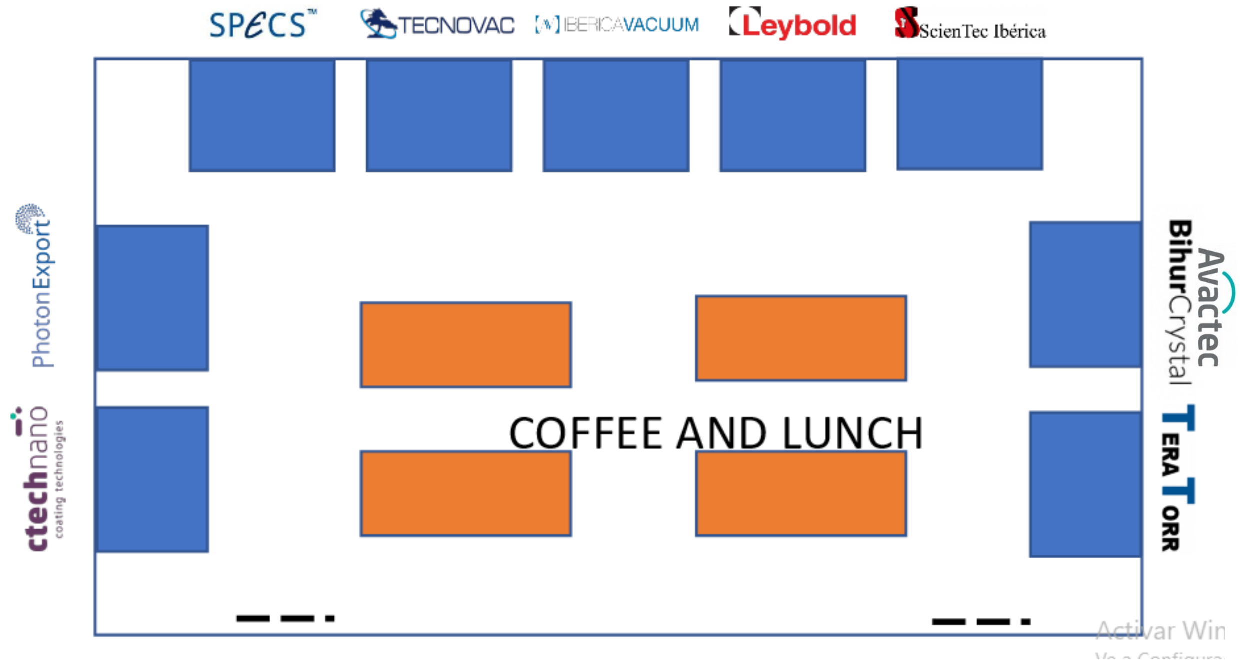
Technological exhibitions.

Overview program: Sessions



8:30			Registration						
9:00			Introduction		Plenary (Peter J. Kelly)		Plenary (Marek Rubel)		9:00
9:15			Plenary (Lars Montelius)						
					Invited (Clemens Laubschat)		Invited (Tomas Polcar)		9:50
10:00			Plenary (Ibon Bustinduy Uriarte)		Invited (Osvaldo de Melo)		Invited (Carlo Morasso)		10:20
10:50			Coffe break						10:50
11:20			Surface Science/ Applied Surface Science	Nanometer Structures	Thin films/ Electronic materials	Vacuum developments	Biointerfaces	Technological session	11:20
11:40									11:40
12:00									12:00
12:20									12:20
12:40			Asamblea ASEVA						12:40
									13:00
					Lunch break		Closing and awards ceremony		13:20
							Oral talk best thesis		13:30
14:00			Lunch break				End		14:00
15:00			Invited (Jose Ignacio Pascual)		Invited (Pedro Salomé)				15:00
15:30			Invited (Otmar Zimmer)		Invited (Michael Foerster)				15:30
16:00			Coffee break						16:00
16:20			Surface Science/ Applied Surface Science	Hard coatings	Thin films/ Electronic materials	Special (de Segovia)			16:20
16:40									16:40
17:00	Registration opens								17:00
17:20									17:20
17:40									17:40
18:00		Guggenheim 1							18:00
									18:20
19:00		Guggenheim 2	Poster session		Poster session				19:00
19:30									
20:00	End		End		End				20:00
			Come Together Cocktail		Conference dinner				21:00

Exhibitors distribution



SOCIAL EVENTS:

Come Together Cocktail: October, 4th. @ YAMIKE; c/ Esperanza 2. Bilbao → www.yamike.com

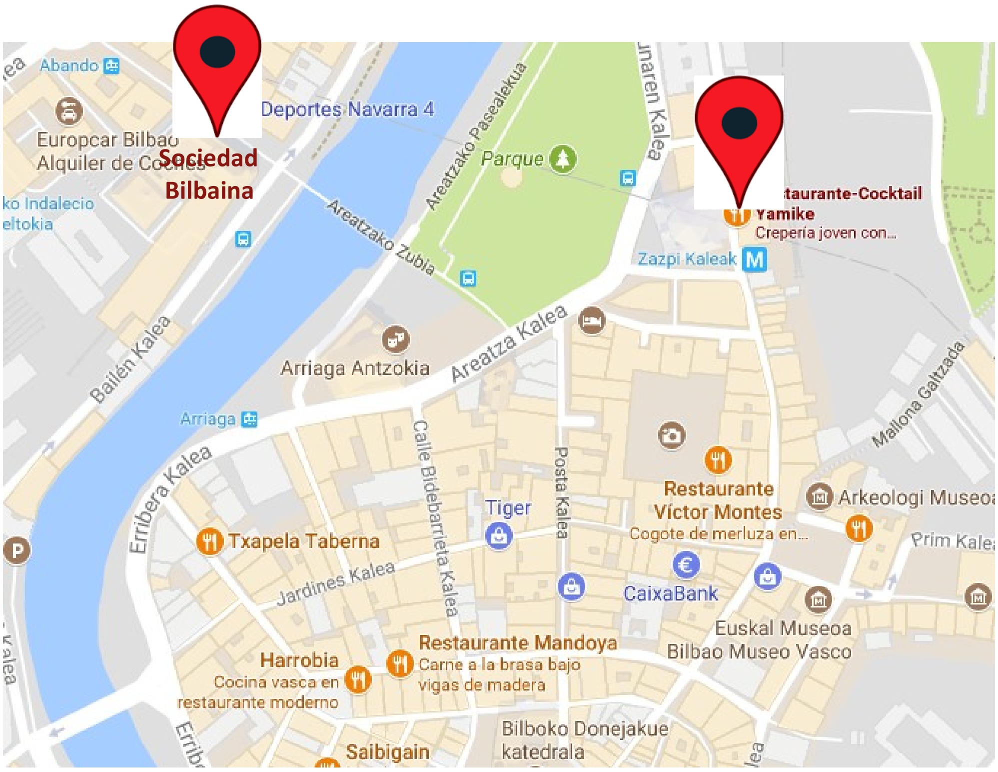
We invite you to take two drinks and 3 *pintxos* per person in one of the typical “Casco Viejo” Bars. The bar will be open for us from 21:00 to 24:00. Some vegetarian pintxos can be available on demand.

Pintxos: Bakalao crujiente sobre piperada / Foie a la plancha con frutos rojos y reduccion de Pedro Ximenez / MiniBurguer de vaca 100x100 con lechuga, tomate, queso fundido y bacon tomate

Conference Dinner: October, 5th. Sociedad Bilbaina → http://sociedadbilbaina.com

Menu 40€. Please make sure you have made your payment.

Nafarroa Kalea (c/ Navarra 1; Bilbao)



COMPILATION OF ABSTRACTS

The following abstracts are organized according to the program, in chronological order.

Every day includes the plenary and invited talks and then the rest of the contributions.

I. Wednesday 4th:
  - Surface Science and Applied Surface Science talks
  - Nanometer Structures
  - Hard Coatings

II. Thursday 5th:
  - Thin Films and Electronic Materials
  - Vacuum developments

III. Friday 6th:
  - Biointerfaces
  - Technological session

At the end, the Poster Session is also included.

ORAL CONTRIBUTIONS

Wednesday 4th

Plenary talk to open RIVA-X

Social perspective of science

Lars Montelius, DG INL

Nanotechnology is a Key Enabling Technology with promises for making solid contributions to the grand challenges of today, such as sufficient sustainable energy supply on demand, clean water to everyone, the demand for novel solutions such as e- care, e-medicine and e-health as consequences of increased elderly population as well as globalization. Solutions to these challenges demands increased transversal interdisciplinary participation. The needed changes allow disruptive innovations. The explosion of IoT-products, massive data and sharing economy services are mega-trends of today´s society. Here the direct links to Industry 4.0, Factories-of-the-Future and Added-Value-Manufacturing concepts are easy to understand. Being reductionalistic, one could argue that the demands we are now identifying are linked to the consequences of digitalization and globalisation. These major societal developments challenge society and will in turn challenge present higher education systems. Systems that still to large extents are "analogue" although several novel concepts have lately been introduced in the discussions, e.g. massive on-line courses. Higher Educational Systems are key for addressing large societal challenges. But there are needs for novel solutions and incentives in order to recruit needed trans-disciplinary engagements. Simply put, there is a need for Science 4.0.

Short Biography: Since Sept 1, 2014 Director General for INL, the International Iberian nanotechnology Laboratory located in Braga, Portugal. INL is the only by legal grounds intergovernmental organization in Nanotechnology. LM is also professor in Nanotechnology at Lund University. His nearly 30 years of research work in nanotechnology has centered around lithography and processing applied to various nanodevices. Especially in the field of Nanoimprint Lithography, he and his research group have published several seminal articles. Recent research focus on exploratory nanotechnology in the life sciences, e.g. in the neurosciences. LM has been the Director for Oresund University and Öresund Science Region, encompassing the 12 universities and five cluster organizations in Denmark and Sweden in the Oresund Region. LM is also the founder of several organizations and companies based on nanotechnology and its applications. LM is the President of IUVSTA (the International Union for Vacuum Science, Technique and Applications), an international member organization encompassing 32 countries and more than 15 000 researchers. LM is also a member of several European Technology Platforms (e.g. EuMaT, NanoFutures).

Elementary phenomena in hybrid graphene nanoribbons on metal surface

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Type of contribution: Invited

Large aromatic carbon nanostructures are cornerstone materials due to their increasingly role in functional devices, but their synthesis in solution encounters size and shape limitations. Recently, it has been shown that the production of large graphenoid nanostructures with atomic precision can be realized on a metal surface using strategies of on-surface chemistry. Chemical routes have been established allowing us to steer synthesis by properly selecting the shape of organic precursors and produce large molecular platforms with tunable intrinsic properties such as the electronic band-gap, its magnetic behavior, or its reactivity.

Our group is involved in a fruitful and Spanish-wide research project to advance in this field and create hybrid carbon-based molecular platforms with functional electronic, optical and magnetic properties. We use scanning tunnelling microscope to explore the effect of adjusting the shape and composition of the molecular precursors in the production of graphene nanoribbons. Combining high resolution imaging (Fig. 1) with local spectroscopy, we unveil the success of a reaction pathway and correlate the result with their electronic functionality.

In this presentation, I will summarize our latest results regarding the production of graphene nanoribbons and other carbon nanostructures with interesting electronic phenomenology. I will show that these ribbons behave as one-dimensional semiconductors and their band structure can be tuned by modifying their width. Doping [1] can be introduced by incorporating additional species.

Furthermore, we developed a method to create quantum dots embedded in hybrid graphene nanoribbon [2]. We found that ribbon bands are confined in them selectively, according to their symmetry. Quantum states can also be localized in extended flat platforms with cavities holding confined states. Finally, we found that it is possible to turn the ribbons magnetic by incorporating magnetic species to the reaction. In this way, we proved that the molecular spin survives in the ribbon by using spin-excitation inelastic spectroscopy

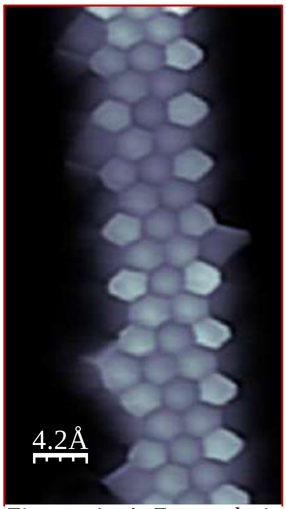

Figure 1: A 7-armchair graphene nanoribbon with CN funcional groups at the edges.

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PVD hard coatings > 20 microns, new perspectives for thin film application

Authors: **O. Zimmer**[1], F. Kaulfuss[1], T. Kruelle[1, 2]

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Session: **type of contribution**: Invited talk

PVD hard coatings have been well established in the field of wear protection of tools and machine parts. A great variety of coating materials are available now. Due to their high hardness and their chemical and thermal stability they push the performance of recent cutting tools to a very high level with respect to machining speed and cost effectiveness. Furthermore hard coatings are able to reduce friction at sliding parts with low or without lubrication.

The common thickness of all these coatings is in the range between 1… 10 microns. This is true for the following reasons:

- good film performance even at a few microns of thickness
- film structure evolution and defects at thicker films
- edge rounding at thicker films
- enormous Deposition time and costs at thicker films

In addition, thicker hard films are preferable for a lot of applications, for example for forming tools, forging tools, cutting tools or machine parts in a harsh environment.

This paper will describe how the technological challenge can be solved. Besides a high deposition rate an effective suppression of extensive growth of defects is the main pre condition for the successful deposition of PVD films in the thickness range up to 100 microns. That was done by a particular film design in combination with a deposition process based on strong plasma activation.

First results of industrial applications of these coatings are presented. Also new perspectives of PVD coatings using this new thickness range are shown and discussed.

A LEEM for the dynamical study of surfaces in Spain

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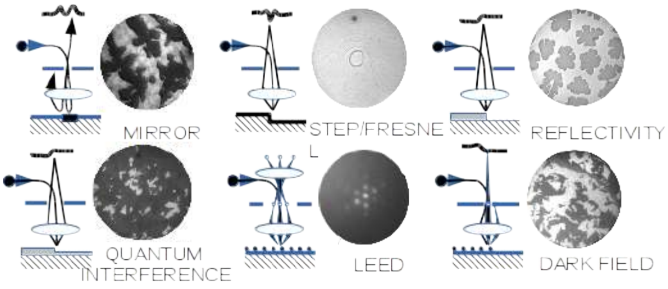
Session: LEEM/PEEM **type of contribution**: oral

Low-energy electron microscopy (LEEM [1,2]) is a technique uniquely suited to perform dynamical observations of surfaces with nanometer resolution under vacuum. A parallel beam of electrons is deflected onto a sample by a prism optic. The electrons decelerate as they approach the surface because of an electrical bias applied to the sample. Electrons backscattered from the surface are accelerated and deflected by the prism into an imaging column and finally onto an imaging detector. Apertures in the illumination and imaging columns control the size of the electron beam on the sample and the electrons that strike the detector, respectively. There are many modes of operation of the instrument, and different sources of contrast in LEEM images, as shown in the figure. For example, it can acquire electron diffraction patterns from local sample areas and form images from the zeroth order electron beam (bright field imaging) or higher order diffraction beams (dark field imaging), locate atomic steps or detect areas of a film with different thicknesses at the atomic level.



This talk emphasizes what can and cannot be done with the current generation of LEEM instruments, with suggestions to make the most of the instrument, so the spanish community can take advantage of the instrument to be installed this year at the Instituto de Química Física “Rocasolano”. We limit the scope to using electrons as the illumination source, i.e., pure LEEM. Note, though, that all LEEMs can also perform photoemission electron microscopy (PEEM) if the appropriate light source is available. In fact, Spain has a LEEM/PEEM instrument at the Alba synchrotron in Barcelona in operation since 2012 [3]. But the use of LEEM/PEEM in the limited time available at a synchrotron tends to be used to analyze ex-situ prepared samples, specially in the absence of prior experience in LEEM. However the real power of LEEM is being able to prepare materials under the carefully controlled conditions possible in an UHV-based instrument and track in real time the material's evolution. The ability to image quickly while changing temperature, annealing, exposing to gases or growing films allows for the rapid exploration of material systems. All this makes it highly desirable to have a LEEM instrument in our country that can provide such hands-on learning on the technique and its capabilities, which in turn can be complemented if necessary by the additional possibilities afforded by PEEM at Alba..

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Chiral induced spin filtering effects in organic films

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Session: Thin films **type of contribution**: Oral

Chiral surfaces open the door, from a technological point of view, to use in 2D devices different properties like chiral selectivity, enantiospecific chemical reactions [1] or the possibility to use these materials as, for instance, spin filters [2]. Chiral structures, and in particular chiral molecules, are fascinating objects in many areas: in Physics the relationship between chirality and magnetism has puzzled researchers since the 19th century, and only in the 21th century we have learn to make use of this relationship, for example using the ability of chiral layers to scatter electrons differently depending on their spin [3].

We have used surface sensitive spectroscopies based on synchrotron techniques (XAS, XPS, spin polarized UPS, XPEEM) to study the influence of the chirality on the magnetism. Thin films of pure enantiomeric diphenil ethane diamine (DPEDA) and diphenyl ethane diol (DPED) have been grown on Cu(001) and on Co/Cu(100) surface in UHV by Molecular Beam Epitaxy (MBE). Using X-ray circular natural dichroism (XNCD) measured at the C K-edge we have measured the preservation of the chiral character of these molecular thin films in the electronic structure. The effect of this chiral molecular film adsorbed on ferromagnetic cobalt has been measured though XMCD at the Co L-edges, showing a change in the magnetic moment in the cobalt atoms at the surface, with the implication of a charge transfer with spin polarization.

More indeed, we have observed macroscopic spin polarizations in electron currents photoemitted from molecular films of DPED and DPEDA adsorbed on Co/Cu(100) surfaces, showing that chiral molecules in a non-spiral geometry can filter spin electrons [2]. These measurements also show that the different enantiomers of the same molecule can produce spin polarizations oriented along different directions in space [4].

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Monitoring dynamics of different processes on rutile TiO_2(110) by following work function change

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Session: surface science **type of contribution**: oral

The (110) surface of TiO_2 rutile single crystal is probably the most studied metallic oxide surface due to the high technological impact of titania in heterogeneous catalysis, but also because this surface serves as a convenient model system for studying surface processes on metallic oxides. The surface processes on (1x1) reconstructed TiO_2 (110) rutile are mainly governed by the bridging oxygen vacancies (BOVs), which are formed upon ion and electron bombardment and sample annealing in UHV. BOVs represent adsorption sites for different molecules, including H_2O, O_2 or CO, and generally govern the surface chemistry of the system. The experimental tools used for investigation of this system are mainly restricted to Scanning Tunneling Microscopy (STM) and UV Photoeletron Spectroscopy [1], because standard surface science tools, such as X-ray Photoelectron Spectroscopy (XPS), lack the sensitivity to detect subtle changes of TiO_2(110) surfaces caused by adsorption of different species. Although Work Function study (WF) also provides enough sensitivity to monitor these changes, and can be even used to follow the adsorption dynamics [2], actual interpretation of these results were enabled only after establishing appropriate physical model [3].

In this work, we study the WF dependence of the TiO_2 (110) rutile surface on the initial concentration of BOVs due the different procedures for sample preparation, the WF time evolution due to the adsorption of H_2O, O_2 and CO molecules, the WF change due to the creation/healing of surface defects with the bombardment of electrons of different energies (electron stimulated desorption), and we measure the water adsorption temperature by following the WF vs Temperature while exposing the surface to water vapor. Both physisorption on Ti rows and dissociative chemisorption on BOVs of water molecules were identified. O_2 adsorption contributes to the increase of the work function, and partial saturation of BOVs, as obtained by subsequent O_2 and H_2O adsorptions. CO chemisorption contributes to the drop of the work function thus revealing its orientation, with carbon atom facing the vacuum. Depending on the energy of electrons bombarding the surface BOVs can be formed (WF decrease) or hydrogen atoms stemming from previously adsorbed water can be desorbed (WF increase). The obtained results can be directly correlated with the results of STM measurements and DFT calculations. In addition, this kind of measurements can potentially reveal new physical processes. For instance, it was observed that additional chemisorption sites are generated by the water adsorption on BOVs. The concentration of these sites increases with the time passed after the adsorption took place, implying their relation with the separation of hydroxyl pairs.

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Precise engineering of quantum dot array coupling through their barrier widths

J. Lobo-Checa[1], I. Piquero-Zulaica[2], A. Sadeghi[3], Z. M. Abd El-Fattah[4], C. Mitsui[5], T. Okamoto[5], R. Pawlak[6], T. Meier[6], A. Arnau[2], J. E. Ortega[2], J. Takeya[5], S. Goedecker[6], E. Meyer[6] and S. Kawai[6,7]

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Session: Surface Science **type of contribution**: Oral

Quantum dot (QD) arrays on surfaces, generated through molecular self-assembly processes, have so far provided researchers with a vast playground to study the electronic properties of new and exotic 2D materials in ultra-high-vacuum (UHV) conditions. By selecting the proper molecular constituents (tectons) and substrate, long-range ordered, periodic and robust nanoporous networks have been achieved, ranging from hydrogen-bonded to metal-organic structures. Not only do they stand out as ideal templates for nanopatterning, but also as adequate candidates for studying fundamental physical phenomena such as confinement through the scattering of two-dimensional electron gases (2DEGs). Indeed, confinement tunability has already been accomplished by varying the pore (i.e. quantum dot) dimensions, geometrical shape and molecule substrate interactions [1,2]. In addition, inter-dot coupling has been shown by photoemission through the generation of new dispersive bands [3] that can be modulated through thermodynamics [4] and the condensation of guest elements (Xe atoms) [5].

To date, 2DEGs' modification through inter-dot barrier width variations has not been experimentally demonstrated. Herein, sustained upon a combination of local scanning probes (STM/STS/AFM), angle resolved photoemission spectroscopy (ARPES) and extended model calculations, we show that we can precisely engineer the inter-dot barrier width by substitution of a single atom in a haloaromatic compound. As a result, we tune the confinement properties at each nanopore affecting the degree of QD intercoupling both on bulk and thin Ag films alike. Our findings complete the toolbox for tuning surface electronic properties, which started in the 90's with the quantum corrals.

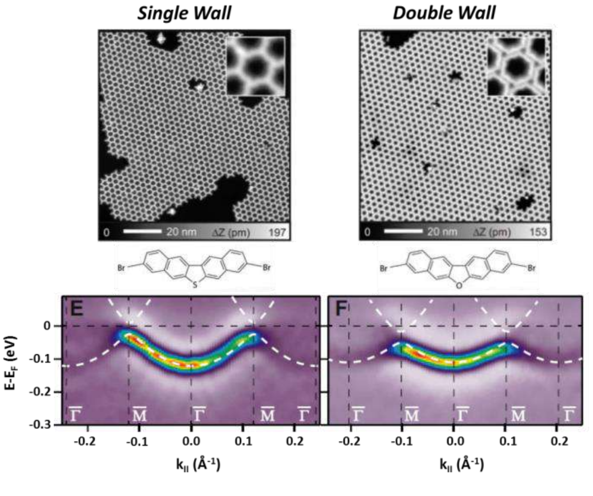

Figure 1: Inter-dot barrier width engineering: single vs double molecular walls that tunes the QD intercoupling properties.

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Organic covalent patterning of nanostructured graphene with selectivity at the atomic level

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Session: Surface Science **type of contribution**: Oral

Organic covalent functionalization of graphene has been suggested as an ideal tool to provide control over its electronic, optical, or magnetic properties. The chemical oxidation of graphene in ultrahigh vacuum (UHV) conditions has also been demonstrated [1]. The attachment of hydrogen to each atomic site of the graphene lattice to create graphane was proposed [2], resulting in a change in the hybridization of carbon atoms from sp^2 to sp^3, as well as the opening of a sizable gap at the Dirac point [3]. In these experiments, all of the atoms in the graphene lattice exhibit very similar reactivity, and the only way to get an atomically well-defined long-range order is to saturate all the atomic sites, creating a completely new material, e.g., graphane or graphene oxide. This lack of selectivity is a major drawback if the objective of the covalent modification is to modulate the electronic properties of graphene but also remarkably challenging.

In this work we describe a method for the covalent modification of graphene with strict spatial periodicity at the nanometer scale [4]. The periodic landscape is provided by a single monolayer of graphene grown on Ru(0001) that presents a moiré pattern due to the mismatch between the carbon and ruthenium hexagonal lattices. The moiré contains periodically arranged areas where the graphene−ruthenium interaction is enhanced and shows higher chemical reactivity. This phenomenon is demonstrated by the attachment of cyanomethyl radicals ($CH_2CN^\bullet$) produced by homolytic breaking of acetonitrile (CH_3CN), which is shown to present a nearly complete selectivity (>98%) binding covalently to graphene on specific atomic sites as measured by means of scanning tunneling microscope (STM) (See Figure 1). This method can be extended to other organic nitriles, paving the way for the attachment of functional molecules.

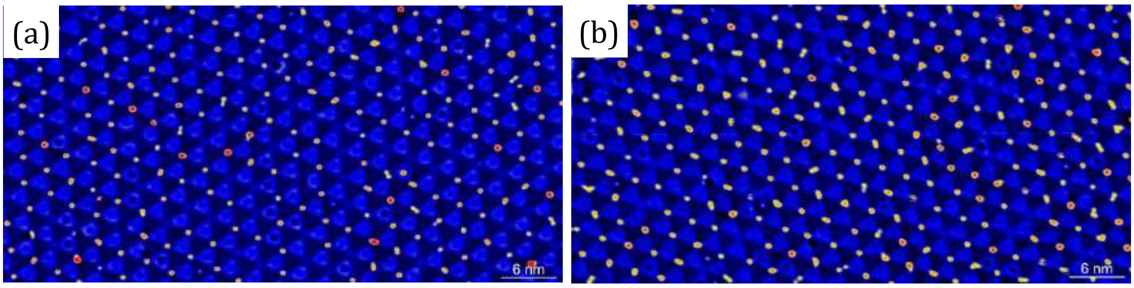

Figure 1: (a) STM image (81 × 40 nm^2, V_b = +1.7 V, I_t = 10 pA) acquired after exposing the sample at 374 K to 720L of CH_3CN. (b) STM image (73 × 32 nm^2, V_b = +1.7 V, I_t = 15 pA) acquired after exposing the sample at 374K to 1080 L of CH_3CN. All images acquired at 78K.

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On-surface synthesis: a new route towards azines

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Session: Surface science **type of contribution**: Oral

Surface science is becoming a frame of reference for the development and study of the synthesis of nanomaterials of different dimensionalities. On one hand, catalytic surfaces are able to induce some chemical reactions that sometimes are not available under conventional routes [1]. On the other hand, the technological advances and the UHV environment allow us to work with high precision and control, following the processes step by step, at nanometre scale. [2].

In this work, using p-aminophenol (PAP) as a precursor we are able to induce by a simple thermal activated process a cyclohexanone-azine (BHC) compound via Cu (110). The use of different surface investigation techniques in UHV combined with DFT calculations allows to figure out the mechanism of BHC formation. We will discuss the BHC formation through three different phases at different temperatures, which are a low temperature phase (LT) made of pristine molecules, a room temperature phase (RT) where a self-assembly monolayer is formed by dehydrogenation of hydroxyl group, and a high temperature phase (HT) where the BHC species are formed. High resolution images of STM/NC-AFM at the HT phase shows that a condensation reaction between two PAP molecules is induced leading to the synthesis of highly organized rows rotated 40°with respect to the[110] main crystallographic direction of Cu [Fig.1]. XPS measurements evidence that the HT phase is produced by an oxidative reaction yielding the total dehydrogenation of OH and NH_2 and that PAP molecules are bonded through nitrogen. In order to gain more insight into the structure of the nitrogen bond, NEXAFS experiments were carried out. Thus, we could discriminate between an azo or azine character. Furthermore, NEXAFS reveals that BHC are presented in a flat geometry configuration.

In summary, we present a powerful new route for azine formation on Cu (110), which transforms PAP into azine by a thermal on-surface process. This strategy has not been yet reported by other methods.

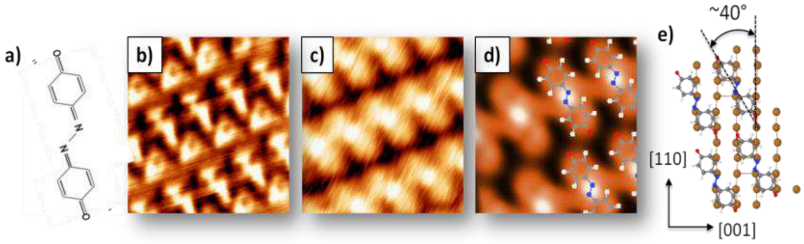

Fig. 1: a) Cyclohexanone-azine (BHC) structure. b) Frequency shift image acquired by a LT nc-AFM/STM with a CO-functionalized tip at 4K. c) STM experimental image at RT of HT phase: V_{bias} = +1350 mV and I_{tunnel} =0.031 nA(1.5nm^2) d) Computed Keldish-Green STM image under the same conditions than experiment. e) Molecular self-assembling optimized geometry of BHC scheme.

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Energy level alignment and selective synthesis of armchair-oriented graphene nanoribbons on gold surfaces.

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Session: surface science **type of contribution**: oral

Graphene nanoribbons (GNRs) have attracted enormous interest due to their widely tunable electronic properties, , which can vary from a gapless band structure with correlated low-dimensional magnetism as for zigzag GNRs (zGNRs), to a strongly gapped semiconductor behaviour for armchair GNRs (aGNRs), with their gap scaling inversely to their width. A recently established bottom-up synthesis method based on the use of molecular precursors as building blocks allows for the synthesis of GNRs with atomic precision [1].

Here, using the same molecular precursor-based methodology, we report on the energy level alignment evolution of valence and conduction bands of armchair-oriented graphene nanoribbons as their band gap shrinks with increasing width. We use 4,4''-dibromo-*para*-terphenyl (DBTP) as molecular precursor on Au(111) to form extended poly-*para*-phenylene (PPP) nanowires, which can be fused laterally to form atomically precise aGNRs of varying width [2]. We measure the frontier bands by means of Scanning Tunnelling Spectroscopy (STS), corroborating that the nanoribbon's band gap is inversely proportional to their width as was theoretically predicted. Interestingly, valence bands are found to show Fermi level pinning, further confirmed by density functional theory (DFT) calculations. Such behavior is generally expected for weakly interacting metal-organic interfaces and is of critical importance to understand the properties of potential contacts in GNR-based devices. Our measurements further reveal a relatively unique system for studying Fermi level pinning by modifying the adsorbate´s band gap while maintaining an almost unchanged interface chemistry defined by substrate and adsorbate. Furthermore, we show how the proper selection of a substrate can provide selectivity to this synthetic process by limiting the lateral fusion of PPP nanowires along the homogenous distribution of well-defined terraces as in a vicinal surface like Au(322). This substrate-mediated synthesis led to the exclusive formation of highly aligned 6-aGNRs along the Au(322) step orientation what allows to characterize their valence band by angle-resolved photoemission spectroscopy (ARPES).

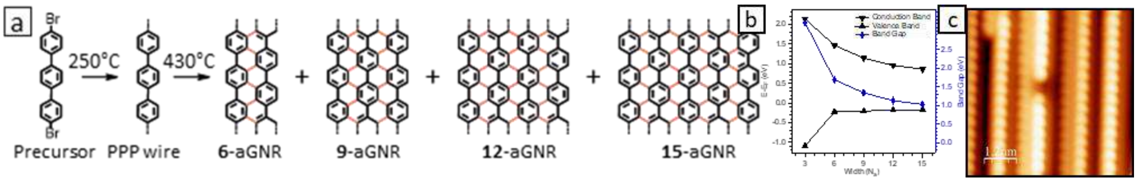

Figure: (a) Synthesis of varying-width armchair graphene nanoribbons from DBTP molecular precursor and **(b)** overall results obtained by STS for valence and conduction bands (in black), and the width-dependent band gap (in blue) in aGNRs on Au(111). **(c)** Topography STM images of PPP nanowires and 6-aGNRs in Au(322).

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Contacting magnetic porphyrines with graphene nanoribbons

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Session: nanometer structures **type of contribution**: Oral

Wiring single molecules into circuites requires precise control on the interface between molecules and electrodes. The use of metal as electrodes is hampered by the lack of well-defined molecule-electrode contacts with high transparency and reproducibility[1]. Alternatively, graphene and graphene nanoribbons[2,3] are good candidates for transport and contacting[4]. They have extraordinary electric and thermal conductivity, and especially that, atomically precise contacts between single molecules and graphene nanoribbons can be produced using strategies of on-surface synthesis such as Ulmann reaction. Here we construct a hybrid device composed of a magnetic Fe Tetraphenylporphyrin bounded to graphene nanoribbons, and investigate the nature of the contact and their magnetic and electronic properties with atomic resolution. We find that the Fe TPP fuses perfectly into the graphene nanoribbons and can be connected to mutiple channels. Its spin and magnetic anisotropy survives even if their structure may become partially modified. The graphene nanoribbons also present unperturbed bands in the proximity of the porphyrine, proving that they are ideal leads to contact a single molecule.

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Transparent ZnO:Ga,Bi and TiO_2:Nb thin film electrodes with thermoelectric properties:

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Session: Applied Surface Science **type of contribution**: oral+poster

One of the biggest challenges to face in the near future will be to meet the energy demand (+35% by 2030) in an economically, efficient, and environmentally responsible way [1]. Beyond the materials for photovoltaic systems, there is another class of materials under intense investigation, the thermoelectric [2]. These can convert thermal differences into electrical energy, or reciprocally, cool down. Recent research has demonstrated the effectiveness of ZnO-based coatings for thermoelectric applications [4-5]. In this work, ZnO:Ga,Bi and TiO_2:Nb thin film electrodes were developed with the objective to enhance the efficiency of photovoltaic systems [3]. For this purpose, besides having good electric and thermoelectric properties, these thin films are need to be optically transparent. To do so, it is necessary to study and understand the inherent physical properties, such as, the electrical conductivity, transport properties (carrier concentration and mobility), and optical transmittance in the visible region, and establish the relation between these properties and the chemical composition, crystal structure and microstructure. Besides the theoretical considerations of the problem, it is described the production method and charge transport properties of several Ga-doped ZnO thin films with different concentrations of Bi, and TiO_2 doped with Nb, deposited by magnetron sputtering. Furthermore, these results are correlated in view of XPS and ToF-SIMS characterization.

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Strontium hexaferrite: from single crystal to thin films

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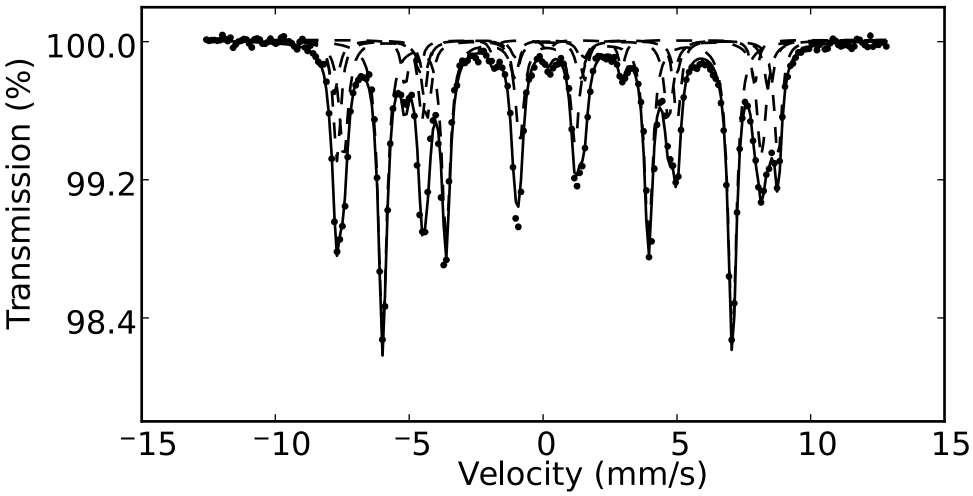
Session: applied surface science **type of contribution**:oral

The M-type ferrites are isostructural to magnetoplumbite, and have a large magnetocrystalline anisotropy. They are used in the bulk of ferrite-based commercial magnets [1]. One of the best examples of such ferrites is strontium ferrite, $SrFe_{12}O_{19}$, first manufactured in 1960's by Phillips. The crystal structure of strontium ferrite is composed of alternating spinel and hexagonal blocks, the latter housing the Sr cations. In $SrFe_{12}O_{19}$, the magnetic easy axis lies in the c-plane, which in combination with its tendency to grow in the A-B planes and form platelets, makes it an appealing candidate for out-of-plane magnetized insulating oxide thin-films.



In this work we characterize the structure and composition of both films and micrometer sized single-crystals by means of Mössbauer spectroscopy (see Figure), x-ray photoemission microscopy, Raman microscopy, atomic force microscopy and x-ray diffraction. The single crystals are obtained from a commercial supplier, and are analyzed before and after annealing at high temperature to increase the grain size. The films are grown by magnetron sputtering. The vector magnetization is determined with nanometer resolution in remanence by x-ray magnetic circular dichroism (XMCD) in photoemission electron microscopy (PEEM). Strategies and conditions that lead to out-of-plane magnetization will be presented.

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Influence of Mo-doping on the optical, electrical and tribological properties of BCN coatings

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Session: Hard coatings **type of contribution**: indiferent

A series of MoBCN coatings with Mo contents between 1- 10 at.% and a broad variation of B:C:N ratios, from carbon-rich to boron-rich, were grown by Ion Beam Assisted Deposition (IBAD), by using simultaneously two electron beam evaporators and a broad beam ion gun. The first e-beam evaporator was fed with different mixtures of C:Mo, the second one with the stoichiometric B_4C compound, and the ion gun with N_2 gas. In this way, the atomic and ionic fluxes of Mo, B, C and N condense as thin films of MoBCN with composition dependent on the substrate location. The method is optimized to produce up to 20 different coatings in a single run.

The thickness of the coatings was measured by profilometry, the composition by EDX in a SEM electron microscope, and both results are compared with the expected results from the independent calibration of the different sources.

Characterization of the bonding structure was performed by FTIR, Raman and NEXAFS spectroscopies. Information on the optical properties was obtained by transmission in the UV-vis-NIR range. The electrical conductivity was determined by 4-point measurements. The tribological properties of the coatings were measured by pin-on-disk tests

A general discussion is presented on the growth method, the effect of Mo incorporation on the BCN structure and how the physical properties of BCN coatings are affected.

Magnetic nanowires with chemical notches for spintronics applications

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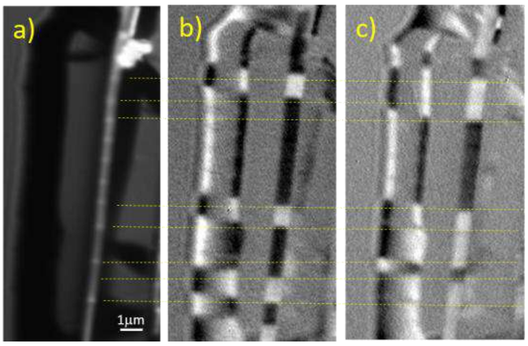
Session: nanometer structures **type of contribution**: oral

Future magnetic storage technology might rely on the movement of magnetic domain walls using spin polarized currents [1]. When not in motion, the magnetic domain walls which define the bits should be pinned in artificially created notches along magnetic wires [2]. It has been shown recently that the depinning of a domain wall from these notches has an intrinsic stochastic component which complicates the application of the proposed scheme in real devices [3]. New types of notches are needed to overcome those limits. In this work we have introduced local changes in composition along permalloy nanowires. These chemical boundaries may act as local pinning sites (chemical notches).

To study the behaviour of magnetic domain walls in these nanowires with chemical pinning sites, it is mandatory to use a technique that combines magnetic and chemical information at submicrometer spatial resolution: an electron microscope (to localize the nanowires) with the possibility of chemical analysis to identify the chemical notches and with magnetic contrast to measure the type and position of the magnetic domains and the magnetic domain walls. The LEEM-PEEM microscope in the CIRCE beamline at ALBA synchrotron fulfils all these requirements. The LEEM microscope has enough resolution to search for the individual nanowires in the substrate. We have used XAS-PEEM to obtain images with chemical contrast (see Fig. 1a) and XMCD-PEEM to get magnetic contrast (Fig 1b). From these figures we correlate composition and magnetic properties of the nanowires. We have proven that chemical notches act as pinning sites for the domain walls. After applying a magnetic field, the domain walls move and pin to a different notch (see Fig 1c). These results open the possibility of using these chemically modulated nanowires as storage elements in race-track memories.



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Nanoparticle formation using an adjustable multi-magnetron gas aggregation source

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Session: Nanometer structures **type of contribution**: Oral

Gas aggregation sources are undoubtedly of attracting interest as an alternative route for nanoparticle fabrication. This is mainly due to the fact that it is a technique able to fabricate nanoparticles with controlled size and composition in clean environment (high or ultra-high vacuum). Among different types of gas aggregation sources, the ones based on sputtering are the most popular mainly due to the important proportion of ionized nanoparticles produced, which allows mass/charge selection by using a quadrupole. In the framework of the European project ERC Synergy Grant "Gas and dust from stars to the laboratory: Exploring the NANOCOSMOS", we are building the Stardust machine, designed to simulate in the laboratory the formation of nanoparticles, small clusters and molecules in the photosphere of a red-giant star. The first part of Stardust, is an implementation of a sputtering gas aggregation source called Multiple Ion Custer Source (MICS). The MICS consists in three completely independent magnetrons inside an aggregation zone. With it, it is possible to fabricate nanoparticles of controlled size, composition and structure in ultra-high vacuum. Previous works demonstrated that with this equipment it is possible to fabricate nanoparticles of a single element, alloyed nanoparticles with controlled stoichiometry [1], as well as core@shell nanoparticles [2,3]. Furthermore, nanoparticles that were only predicted theoretically were fabricated for the first time with this equipment [4]. For the Stardust machine, the size of the magnetrons and the aggregation zone were scaled up in order to be able to fabricate nanoparticles of bigger sizes in larger quantities (high flux). The aggregation zone includes new entrances that will enable to perform new fundamental research. We will present the experiments carried out during the commissioning of Stardust in order to test some of the capabilities of the equipment, focusing on the generation of nanoparticles but also presenting some in-situ processing and analysis.

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Enhancement of optoelectronic properties on indium tin oxide layers by co – sputtering of silver nanoparticles

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Session: Thin Films **type of contribution**: Oral

Transparent conducting oxides (TCO), acting as transparent electrodes, are essential components in the basic structure of a large number of electronic devices as flat panel displays, touch screens, photovoltaic cells, lighting emitting diodes or electrochromic systems. The trade-off between transparency and conductivity in these materials is a major bottleneck towards higher device performance. Indium tin oxide (ITO) is the most established transparent conductive film in the market as currently presents the best optoelectronic properties. The current solution to further improve conductive properties of these materials is to deposit some metallic grids or nanowires on surface of the TCOs but transparency is always decreased and different manufacturing processes are combined. In this work, Ag nanoparticles deposited by gas aggregation sources has been incorporated into ITO layers deposited by DC pulse magnetron sputtering improving the conductivity of the layers while keeping transmission values by a simple one step process. The study of the composite optoelectronic properties has been carried out as a function of the process parameters to correlate those properties with the composition and morphology of the layers. The influence of the nanoparticles density has been carried out to optimise optoelectronic properties. This hybrid electrode is demonstrated to have a 5 times smaller sheet resistance compare to a single TCO layer, while maintaining high light transmission in a wide wavelength range.

On the reactive element effect of yttrium in the oxidation behavior of multilayered CrAlYN coatings

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Session: hard coatings or surface engineering or applied surface science **Type of contribution:** Oral

Multilayered $Cr_{0.50}Al_{0.50}N$ and $Cr_{0.51}Al_{0.46}Y_{0.03}N$ coatings (c.f. Figure 1) were deposited on M2 and 316 steel substrates and heated to 1000 ºC in air for 2 h to study their oxidation mechanism and thermal stability. X-ray diffraction, glow-discharge optical emission spectroscopy and transmission electron microscopy coupled with spatially resolved microanalysis techniques are used to investigate the nanostructure, constituent phases and chemical elemental distribution of the as-prepared and oxidized samples. The incorporation of Y in low contents (< 4 at.%) in metallic nitride coatings has been demonstrated to increase the thermal stability and oxidation resistance above 900ºC but less is known about the action mechanisms. In this work, we confirm the reactive element effect of Y but displaying a different pattern from the typical observed in metallic alloys. The interdiffusion of substrate elements plays an important role in the oxidation process influencing the corrosion products. The presence of yttrium retards the iron outward diffusion by forming oxides in M2 and yttrium nitride in 316 steels. The microstructural analysis determined that yttrium migrates to the grains and interface of the oxide scale and to the nitride column boundaries.

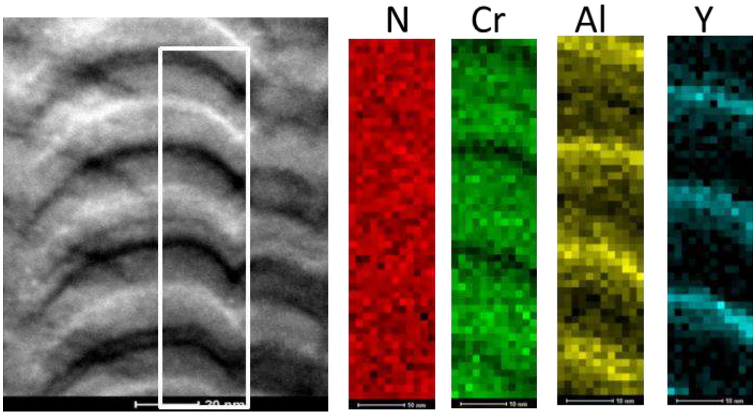

Fig. 1. HAADF-STEM image of the CrAlYN coating and X-EDS elemental maps

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DLC coatings for piston rings deposited by Deep oscillation magnetron sputtering

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Session: Hard coatings **type of contribution**: oral

Diamond-like carbon coatings (DLC) make up the largest proportion of coating solutions applied in the automotive industry, in particular in the piston rings. DLC combine high hardness with low friction coefficient, chemical inertness, high thermal conductivity and high refractive index. In order to comply with the current trends of rising operating temperatures and lower viscosity oils, component manufacturer are currently seeking to develop a new generation of DLCs coatings, with improved properties. The main limitations of the existing DLC solutions stem from high internal stresses and limited thermal stability. The stresses, often in excess of 10 GPa, limit the maximum achievable thickness of hard DLCs due to adhesion problems. The main objective of this work is to develop a new generation of significantly improved DLC coatings. DLC films were deposited by deep oscillation magnetron sputtering, a variant of high power impulse magnetron sputtering. The bombardment energy was controlled by changing the substrate bias. In order to improve the film's adhesion an interlayer was deposited. In this work, the microstructure and mechanical properties of the films were characterized using scanning electron microscopy, Raman spectroscopy, X-ray reflectivity, nanoindentation.

Enhanced adhesion of hard DLC coatings on steel substrates with HIPIMS metal etch.

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Session: hard coatings **type of contribution**: oral

Diamond-Like Carbon (DLC) coatings have been recognized as one of the most valuable engineering materials for various industrial applications including manufacturing, transportation, biomedical and microelectronics. Among its properties, DLC has good frictional behaviour combined with high surface hardness, offering an elevated protection against abrasive wear. As the industrial success of DLC films in tribological contacts is strongly dependent on their adhesion properties, a HIPIMS metal etching step was used to enhance DLC coating adhesion onto steel metallic.

HiPIMS metal ion etching and implantation with both Ti and Cr plasmas was used to pre-treat the M2-HSS metallic substrates, obtaining Rockwell HF1 values and critical loads in the macro-scratch tests above 100N .

Micromechanics of TiN/CrN coatings

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Session: hard coatings **type of contribution**: Oral

In recent years TiN/CrN multilayered PVC coatings are well known for their unique properties like high hardness and good wear resistance. Large number of studies has been reported, mainly focused on tribology characterization as well as detailed transmission electron microscopy analysis of interfaces. On the other hand, information on the contact damage and fracture is rather scarce. A deeper knowledge is crucial to improve the performance of these materials and to enhance the lifetime of coated systems.

The present work aims to conduct a systematic micro- and nanomechanical study of the mechanical integrity of three multilayer TiN/CrN systems with different bilayer period (8, 19 and 25 nm). In doing so, nanoindentation and nanoscratch techniques are implemented and corresponding deformation/damage mechanisms are also investigated. Work includes the use of different indenter tip geometries to induce distinct stress fields. In general, three different approached for each multilayer TiN/CrN system are followed to accomplish the main goal of this investigation:

(i) Assessment of the micromechanical properties (hardness and elastic modulus) and the main deformation mechanisms,
(ii) Evaluation of the fracture toughness as well as observe the damage mechanisms induced during the cantilever deflection (Figure 1) as a function of the bilayer period through ex-situ tests by FIB-milling microcantilevers, and
(iii) Evaluation the adhesive/cohesive damage at the interface by combining micro- and nanoscratch tests.

It is found that the multilayer approach is quite effective on promoting crack growth resistance mechanisms. Finally, through ex-situ microcantiliver deflection is quite effective approach on promoting crack growth resistance mechanisms. Within all of these observations, thus, damage tolerance if these systems is clearly enhanced, as compared to the one exhibited by the single layer ones.

Figure 1. Fracture surface observed by FESEM of TiN/CrN specimen with a bilayer period of 25 nm. Zig-zag crack paths, corresponding to small scale deflections are clearly discerned [1].

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Influence of Ag additions on the structure, thermal and tribological properties of Cr-O films deposited by HiPIMS

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Session: Hard coatings **type of contribution**: oral

SUMMARY:

Solid lubricant coatings are potential candidates for providing green solutions to problems associated with liquid lubricants. However, these coatings degrade at high temperatures and fail to provide controlled release of lubricant material. Combination of Cr-O and Ag can be a potential solution if the controlled release of silver through Cr-O matrix is achieved. Cr-O has excellent high temperature oxidation resistance and anti-diffusion properties[1]. While, silver is an excellent lubricant due to its high ductility, plastic shearing effect and oxidation resistance [2]. The prime objective of this research is to investigate the influence of Ag additions on the microstructure, mechanical, thermal and tribological properties of Cr-O coatings. The coatings were deposited by sputtering using two targets and two power sources (HiPIMS and DC). HiPIMS power supply was connected to the Cr target to promote a higher ionization level of the deposited species, while the DC source was connected to the Ag target. The chemical composition, crystal structure and mechanical properties of the films wwere analyzed by EDS, X-ray diffraction, nanoindentation and dynamic indentation, respectively. Temperature effect on the structure of the Ag rich coatings was characterized in open air in-situ by hot-XRD device in the range of 500 °C to 1000 °C. Oxidation of films was assessed by thermogravimetric analysis (TGA) using industrial air (99.99% purity). After oxidation tests, the surface morphology of the specimens was examined by scanning electron microscopy with energy dispersive X-ray spectroscopy (SEM–EDS) and their structure was evaluated by XRD diffraction. The oxide products on the surface were characterized by Raman spectroscopy. Tribological experiments were performed in a pin-on-disc tribometer at RT, using Al2O3 balls as counterpart. The friction coefficient was continuously recorded and the wear rate of the coatings calculated from the crater of the worn surface of the ball using a 3D optical profilometer. All the films displayed a compact morphology independently of the Ag content on the films. However coatings displayed an amorphous structure and consequently low hardness values. Oxidation resistance of films was extremely high and independent of the Ag content on the film. Ag has a beneficial influence on the tribological performance of films.

Keywords: Cr-O-Ag Self-Lubricating Coatings, Control Release of Silver, Annealing, Hot-XRD, Crystal structure, Tribology

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CrAlN based hard coatings for high demanding cutting operations

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Session: HARD COATINGS **type of contribution**: Oral

In difficult to cut materials, like aerospace alloys (i.e. Inconel alloys), the temperature at the cutting edge can exceed 1000 C. Consequently, the applied protective coatings must be capable of withstanding these extreme conditions. CrAlN protective films show high hardness, good thermal stability and excellent oxidation resistance behaviour. These properties depend on chemical composition and microstructure and when optimized, excellent performance in cutting tests can be obtained. . CrAlN coatings are more suitable than TiAlN coatings when they need to face high temperature conditions. In this study, Cr_xAl_yN films have been deposited by combined high power pulsed magnetron sputtering (HPPMS) and conventional pulsed DC magnetron sputtering techniques under different sputtering process parameters. The Cr_xAl_yN films performance in terms of composition is analysed under high temperature tribological testing. Write the session in which your abstract better fit between the followings: Applied surface science, electronic materials and processing, biointerfaces, nanometer structures, Plasma science, surface engineering, surface science, thin films, vacuum science and technology, technological session, hard-coatings workshop.

ORAL CONTRIBUTIONS

Thursday 5th

The production of photocatalytic materials by magnetron sputtering techniques

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Abstract

Semiconductor photocatalysis is attracting increasing interest as an efficient and sustainable solution to environmental problems, including decontamination of air and water and reducing microbial contamination on hygienic surfaces. Titanium dioxide is the most widely studied photocatalyst and, along with the majority of other photocatalytic materials, it is commonly produced by various chemical techniques, including hydrothermal synthesis, sol-gel, chemical vapour deposition, etc. The characteristics of each process has a major bearing on material properties, such as grain size, crystallinity, surface area, lattice defects and, therefore, the photocatalytic performance of the material is inextricably linked to the choice of production process. Magnetron sputtering represents a relatively simple, versatile and readily scalable method for the deposition of thin functional films onto a variety of substrates. Furthermore, magnetron sputtering offers precise compositional control and makes use of non-hazardous sputtering targets, with no toxic waste products.

It is well-known that titanium dioxide has two major drawbacks limiting its practical application, namely a lack of visible light photocatalytic activity and low quantum efficiency. The use of magnetron sputtering techniques for the deposition of photocatalytic coatings offers the potential to address the main issues associated with use of $TiO_{2,}$ by either the production of doped titania coatings or the deposition of less studied narrow band gap semiconductor coatings as alternatives to titanium dioxide.

This paper will summarise recent achievements in the use of magnetron sputtering techniques for production of photocatalytic materials, including deposition of pure and doped (both metallic and non-metallic dopants) titanium dioxide coatings onto a range of planar and particulate substrates, the use of novel semiconductors as efficient visible light-activated photocatalysts, as well as the modification of existing commercial photocatalytic materials to enhance the photocatalytic performance. The influence of deposition parameters on crystallographic, structural and optical properties of the materials is discussed. The assessment of photocatalytic activity includes a number of techniques, including dye degradation, VOC degradation, inactivation of microorganisms and photoinduced hydrophilicity measurements.

Functionalization of graphene layers on transition-metal substrates

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Session: Thin films **Type of contribution**: Invited

Graphene is an allotrope of carbon and forms a two-dimensional hexagonal lattice which is the basic structural element of graphite but may also be synthesized by chemical vapour deposition (CVD) in form of monolayers on closely packed transition metal surfaces or insulating substrates like SiC(0001). Originally observed in 1962 the material was rediscovered in 2004 by A. Geim and K. Novoselov who were awarded with the Nobel Prize in 2010 for their research work. Apart from high chemical stability graphene reveals several unusual mechanical, thermodynamical, electrical, and optical properties. As a transparent and flexible conductor graphene holds e. g. promise for several applications in electronic devices and may be used for surface passivation or as electrode material in galvanic cells and batteries.

Most of its unusual properties are related to its peculiar electronic structure: Free-standing graphene is characterized by linear dispersive valence bands in form of Dirac-cones intersected by the Fermi energy only at the K-points of the hexagonal Brillouin zone. Adsorbed on surfaces, however, the chemical potential is usually shifted in energy with respect to the apices of the cones due to charge transfer with the substrate and the linear dispersion of the cones is frequently heavily disturbed by hybridization with substrate bands [1].

These interferences may be suppressed by intercalation, i. e. selective embedment of foreign atoms or molecules in between the graphene layer and the substrate [2]. Experimentally this may be achieved by low temperature adsorption or deposition of foreign atoms on the graphene surface followed by moderate annealing of the system. While at room temperature and below the substrate surface is usually fully passivated by the graphene overlayer even against reactive media like oxygen foreign atoms become intercalated at elevated temperatures without affecting the structures of the graphene layer and the substrate. Only at rather high temperatures interdiffusion takes place and the graphene overlayer becomes destroyed.

Alternatively, effects of charge transfer between graphene layer and substrate may be compensated by doping, i. e. replacing carbon atoms of the overlayer by B, N, or S [3]. This may be achieved during graphen preparation by adding B, N, or S containing molecules to the hydrocarbons used in the CVD process. Depending on the concentration of the dopands the position of the Fermi energy may properly be adjusted. The talk gives an overview of respective intercalation and doping studies performed with scanning tunnel microscopy (STM), (angle-resolved) photoemission (ARPES) and near-edge x-ray absorption spectroscopy (NEXAFS).

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Vapor phase growth and phase stability of bidimensional tellurides MoTe2 and Bi2Te3

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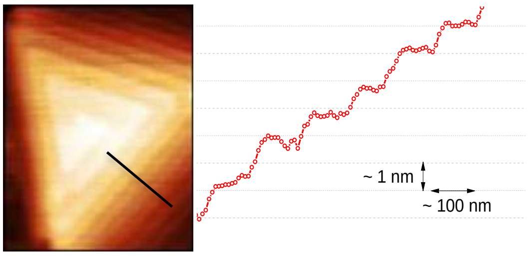
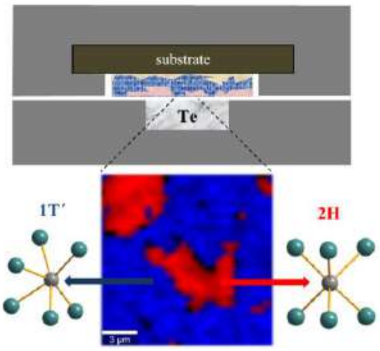
Session: thin films **type of contribution**: oral or invited

Layered chalcogen-based materials are important members of two relevant materials groups that have received a lot of research efforts in recent years: transition metal dichalcogenides (TMDs) [1] and topological insulators (TIs) [2]. In particular, one structural modifications of TMDs have been found to have finite band gap energies which make them compatible with the semiconductor industry. On the other hand, the unique properties of TIs (protected conducting surface states) promise several interesting applications in quantum computer or spintronic, for example. The preparation of these materials with the desired crystalline phase and good structural quality for desired applications demands a reliable control of the growth process. Here, we present results on the growth of Bi_2Te_3 and $MoTe_2$ films using vapor phase techniques.



For the growth of Bi_2Te_3 nano-crystals, a novel procedure is presented. The crystals are obtained by physical vapor transport using Bi and Te sources. The influence of different substrates, carrier gas flux or vacuum environment, and sources temperatures was studied by means of scanning electron microscopy, x-ray diffraction, Raman spectroscopy and atomic force microscopy. In all cases, Bi_2Te_3 platelets were preferentially oriented with the (00L) planes parallel to the substrate surface. When sapphire substrates were used the films grew with an epitaxial character following a spiral growth mechanism as shown in the AFM image and height profile (along the black line), with 1 nm steps (the thickness of the quintuple layer) and 100 nm terraces.



In the case of $MoTe_2$, we used isothermal close space (ICS) Te annealings in pure H_2 atmosphere for the tellurization of Mo oxide thin films. $MoTe_2$ can exist in two distinct stable modifications, namely hexagonal (2H) with semiconductor behavior and distorted octahedral (1T′) with metallic properties. We used a relatively low temperature of 500 °C and observed that, in all cases, Mo oxide initially transformed to 1T′ before reaching the equilibrium 2H phase. Highly oriented $MoTe_2$ films with the [001] direction perpendicular to the surface were obtained in all samples. The obtained phase, morphology, chemical composition and binding energies were characterized by X-ray diffraction, scanning electron microscopy, Raman spectroscopy, energy dispersive and x-rays photoelectron spectroscopies. Then, the stability of the two different phases is discussed in relation with the growth parameters.

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[2] Y. L. Chen et al. Science 2009, 325, 178

Thin film solar cells: vacuum processes and application of nanotechnology

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Session: Invited – thin films **type of contribution**: invited presentation

Thin film solar cells based on the semiconductor Cu(In,Ga)Se_2 (CIGS) achieve power conversion efficiency numbers already higher than any other polycrystalline technology, including even multi-crystalline silicon (22.6 % vs 21.9%) [1]. A small introduction to thin film solar cells will be performed. In the past decades CIGS technology development has been focused on the improvement of material quality itself and research and development on novel architectures has not improved significantly. There is a vast room for improvement by optimizing the solar cell structure, namely with regards to interface passivation. Some of the most important developments in silicon solar cell manufacturing was the development, know-how and implementation of solar cell structures that allowed for minimal interface recombination. With the same motivation, we are developing new CIGS solar cell structures with higher manufacturability and decreased interface recombination. In this talk we will show two steps given with such objective. The first one is a study how the now chemically-processed CdS buffer layer can be replaced by a $Zn_xSn_yO_z$ layer deposited by atomic layer deposition achieving lower front interface recombination [2]. Special emphasis is given into the diffusion of elements at the CIGS surface, using transmission electron microscopy (TEM) and to the optoelectronical properties of the devices. The second study, is by incorporating a nanopatterned Al_2O_3 layer at the rear contact can lead to lower rear interface recombination and allow for significant material savings due to the use of ultrathin absorber layers [3]. A transmission electron microscopy (TEM) image of the device cross-section is shown in figure 1. The image shows the Al_2O_3 layer in-between the rear contact (Mo), and the absorber layer (CIGS), with 18 nm. Since the Al_2O_3 layer has insulating properties, the electrical contacts are made by the nanopatterned holes seen in the figure. They are produced by e-beam lithography by etching trough the Al_2O_3 layer a square array of 400 nm diameter circles. Such approach can lead to gains in power conversion efficiency close to 3 % (in absolute numbers) compared with reference devices.

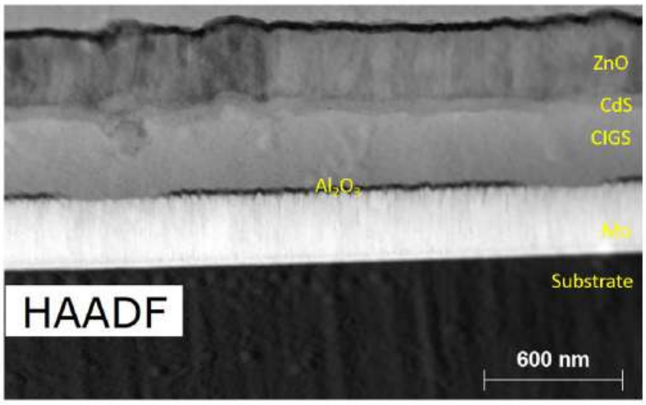

Fig1: TEM HAADF image of the cross-section of the passivated solar cell. The dark layer in-between the Mo layer and the CIGS layer, is the Al2O3 passivation layer. The observed openings on this Al2O3 layer are the nanopatterned point contacts

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Magnetism catches the wave

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Surface Acoustic Waves (SAWs) are propagating Raleigh waves in the upper micrometric layer of a crystal, which propagate large distances and can be generated in piezoelectric materials by applying RF electric fields to transducer electrodes on the surface. We have shown that it is possible to image such waves in $LiNbO_3$ by X-ray PhotoEmission Electron Microscopy (XPEEM), since it is sensitive to the piezoelectric part of the SAW. Thus, the effect of fast strain changes on structures grown on $LiNbO_3$ can be studied with temporal resolution below 100 ps and up to 50 nm spatial resolution, offering a novel approach for studies of systems under dynamic strain.

The application to the study of dynamic magneto-elastic effects in Ni microstructures will be presented. The magneto-elastic effect or inverse magnetostriction (i.e., the change of magnetic properties caused by an elastic deformation) has attracted much interest due to its potential to write small magnetic elements by an electric voltage rather than current, avoiding energy losses. However, so far practical demonstrations were realized on timescales far too slow for most applications. Combining XPEEM with XMCD magnetic contrast we have imaged the Ni magnetic states at the different phases of the SAW, demonstrating that the strain-driven magnetic anisotropy changes on the sub-nanosecond timescale are as efficient as for the static strain case. Different delays (100-300 ps) of the magnetic response to the strain wave were measured, depending on the magnetic configuration. The delays are related to the intrinsic magnetization dynamics of the Ni patterns. Thus it is shown that while the magneto-elastic effect itself is very fast, for the speed of a potential device the magnetization state has to be properly designed.

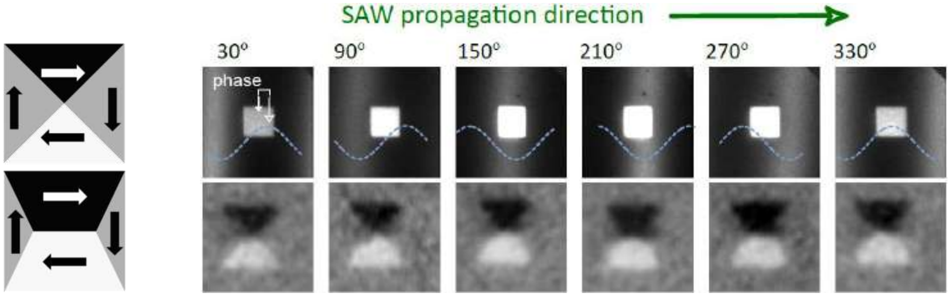

Figure 1: *Left, top: Scheme of magnetic domains in a Ni square without net anisotropy, forming a Landau flux closure state (arrows indicate magnetic directions and gray color contrast in XMCD-PEEM). Left, bottom: domain configuration if an additional uniaxial magnetic anisotropy is induced, favoring horizontal magnetization (black and white domains). Right, top: Series of direct images taken with different respective positions of the strain wave and a Ni square (2 um side). The square is in the maximum of the strain wave (white zone) between the images of 150°and 210° and in the minimum between 330° and 30°. Right, bottom: Corresponding images with XMCD magnetic contrast showing the magnetic domains in the Ni square.*

[1] M. Foerster *et al.*, arXiv:1611.02847

Utilization of atomic layer deposition (ALD) for vapor phase infiltration and doping of conducting polymers

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Session: Thin Films **type of contribution**: Oral

Vapor phase infiltration is a top-down strategy that is based on the ALD process and allows fabrication of organic-inorganic hybrid materials by incorporation of metal organic precursors into polymeric substrates. The growth of inorganic clusters or particles in the subsurface area of a polymer allows modifying some of the physical properties of the polymer greatly. While related earlier work investigated the improvement of mechanical properties of polymers applying the infiltration route, here we describe a novel approach, namely a single precursor infiltration process to dope polyaniline (PANI) or the polythiophene P3HT. The infiltration was performed with various precursors typically used in ALD processes. The conductivities were assessed with four-point probe measurements and showed significant enhancement by up to 6 orders of magnitude, confirming the efficiency of the infiltration process. Furthermore, we found that the thermal and temporal stability of the thus doped polymers were significantly enhanced in comparison to their traditionally wet-chemically doped counterparts. For example, conductivities of infiltration-doped PANI outperform the conductivity of HCl-doped PANI if exposed to elevated temperatures (150 °C) in vacuum. In the case of P3HT, the infiltration-doped polymer maintains the gained conductivity even after exposure to ambient conditions for more than 30 days. The chemical changes resulting from the infiltration of the two polymers were characterized by FTIR and Raman spectroscopy and will be discussed. SEM micrographs showed that the morphologies of the samples did not alter after the infiltration process, being one of the most important arguments for doping conductive polymers in the presented way.

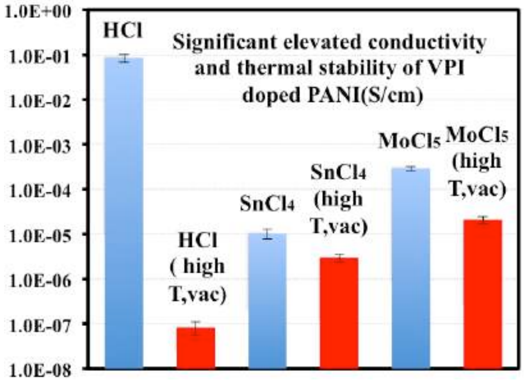

Figure 1. Conductivity comparison of PANI/1M HCl, PANI/$SnCl_4$ (60 cycles) and PANI/$MoCl_5$ (100 cycles) as prepared, and after storage at 150 °C in vacuum for 100 min.

Optically active porous 1D Bragg Microcavities prepared by evaporation at oblique angles as optofluidic sensor of glucose

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Session: Nanometer structures **type of contribution**: Poster

In this work we report the use of polarization active porous 1D Bragg microcavities (BM) prepared by physical vapor deposition at oblique angles for the optofluidic sensing of glucose solutions. These photonic structures consist of the stacking of highly porous layers of two materials with different refractive indices and, depending on preparation conditions, high birefringence. Their operational principle implies filling the pores of the multilayer stack with the analyzed liquid while monitoring the associated changes in optical response as a function of the solution refractive index. In the case of the BM presenting optical activity, the analysis can be made much simpler and robust using linearly polarized light and a polarizer to determine the variation of retarder behaviour of the system. The response of both polarization active and inactive BMs as optofluidic chips for the determination of glucose concentration in water solutions has been systematically compared. Different methods of detection, including monitoring the BM wave retarder behaviour, are critically compared for both low and high glucose concentrations. Data are taken in transmission and reflection modes, this latter compatible with its use as optical fiber sensor for liquid monitoring and different options explored to prove the incorporation of these transducers into microfluidic systems. The advantages and limitations of the developed transducer chips for the optofluidic analysis of liquids are discussed.

New advancements in material characterization using Mechanically Stimulated Gas Emission Mass-Spectrometry

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Session: Applied Surface Science **type of contribution**: oral

Mechanically Stimulated Gas Emission (MSGE) is a complex phenomenon that involves various processes on the solid surface and in the deformed subsurface layer leading to gas emanation from a solid under applied mechanical deformation, rubbing, rolling, scratching, or other types of mechanical activation. Under mild conditions (low normal load and speed) and for miniature contacts frictional heating is by far insufficient to activate any significant gas emission. Therefore, the gas emission relies on plastic deformation and fracture that trigger various physical and chemical reactions including gas diffusion in the bulk, transport of interstitials by dislocation, opening of nano- and microvoids, tribochemical decomposition and synthesis among others. When the amount of gases adsorbed on the surface can be neglected, e.g. in vacuum or under inert atmosphere, the main sources of gas emission are the gases contained in the material bulk and those instantaneously generated due to tribochemical reactions. Measurement of MSGE can provide valuable information on both of these sources.

A new technique – MSGE Mass-Spectrometry (MSGE-MS) - was developed for quantitative characterization of MSGE rate and composition of emitted gases. It is composed of a mass-spectrometer coupled to a device for surface mechanical activation and a dynamic gas expansion system in high vacuum. Special procedure relied on behavioural analysis was developed for the analysis of transient pressure time series. MSGE-MS was further modified coupling it with the analysis of the volume of deformed material to develop a new technique of analysis of the gas content in the materials and surface coatings. The combination of the features of the latter technique – TriDes - is unique since it has nanometre resolution in depth coupled with high sensitivity (<0.5 ppm). It can be applied for any kind of solid materials.

In this work two applications of the techniques are described. MSGE-MS was used to measure the composition and kinetics of the gas emission from shale and concrete in order to figure out the possible sources of atmosphere contamination during construction of transport infrastructure, whereas TriDes was applied in the study of extrinsic sources of hydrogen absorption in low alloy high-strength steel used for mooring of oil and gas platforms. A mooring steel grade R4 was analysed before and after immersion in isotopically marked (deuterium) synthetic sea water. The effects of the surface roughness and immersion duration were analysed. It was found that the amount of hydrogen contained in the microstructure first increased due to hydrogen uptake from the environment, but later on decreased that was ascribed to the dissolving of the topmost surface layer rich in surface defects, which trap hydrogen atoms.

This work was supported by the Ministry of Economy and Competitiveness of Spain through the projects IPT-2012-1167-120000 with contribution from the European Regional Development Fund of the European Union (FEDER) and BIA2016-79582. Authors also thank the partners from IK4-Azterlan, IK4-Tekniker and Vicinay Marine Innovación for their collaboration.

Mo–Si–N Hybrid System for Absorbers in Solar Selective Coatings

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Session: Thin Films **type of contribution**: Oral

The design of solar selective coatings (SSC) for concentrated solar power (CSP) applications requires a precise knowledge of the whole stack optical behaviour. Moreover, the study of its chemical stability becomes essential for their use at high temperatures. In this communication, we report on properties of SSCs prepared with absorbers based on novel cermets from the Mo–Si–N system.

As required from an adequate balance between cost and efficiency, the studied SSC stacks are formed by: (i) an IR-mirror metal, (ii) a double cermet layer and (iii) an antireflective dielectric cover.

The optical reflectance in the whole visible – infrared range is simulated from the complex dielectric permittivity of the components. Such a simulation allows the optimization of the optical characteristics by changing the double cermet and the antireflective dielectric layers thickness, as well as the metallic volume fraction in the cermet (cermet filling factor).

The precise control of thickness and composition of sputtering–deposited SSC stacks based on Mo-Si_3N_4 cermets or $MoSi_2$-Si_3N_4 hybrid composites absorbers leads to high solar absorptivity and low thermal emissivity values [1,2]. On the other hand, its thermal stability seems to indicate its use at temperatures near 600 ºC. For this purpose, the specific Inconel\\$MoSi_2$-$Si_3N_4$\\$Si_3N_4$\\$Al_2O_3$ architecture has been proposed for high temperature air operation [3].

The aim of using such kind of SSCs at high temperature without degradation in vacuum or at the air makes particularly helpful the fundamental research of chemistry taking place inside the coating. In this report, the SSC functional optical stability at high temperatures is correlated with the study of the short-range order around Mo by extended X-ray absorption fine structure (EXAFS) and X-ray absorption near edge structure (XANES) spectroscopies.

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Abstracts are brief summaries of the overall goal of the research, showing the specific ideas or concepts that will be presented, including outcomes and implications for practice. Please use cambria 10 as Font and size.

Write the session in which your abstract better fit between the followings: Applied surface science, electronic materials and processing, biointerfaces, nanometer structures, Plasma science, surface engineering, surface science, thin films, vacuum science and technology, technological session, hard-coatings workshop.

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Include **maximum 2 images** with your abstract (500 x 500 px max). **References are optional but encouraged**. Please limit references to the 5 most pertinent citations at the end of the document. Refer to them with a number between brackets. Notification of acceptance will be done to the presenting author email address.

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Early stages of growth of ZnO on graphene/Cu: graphene decoupled from Cu

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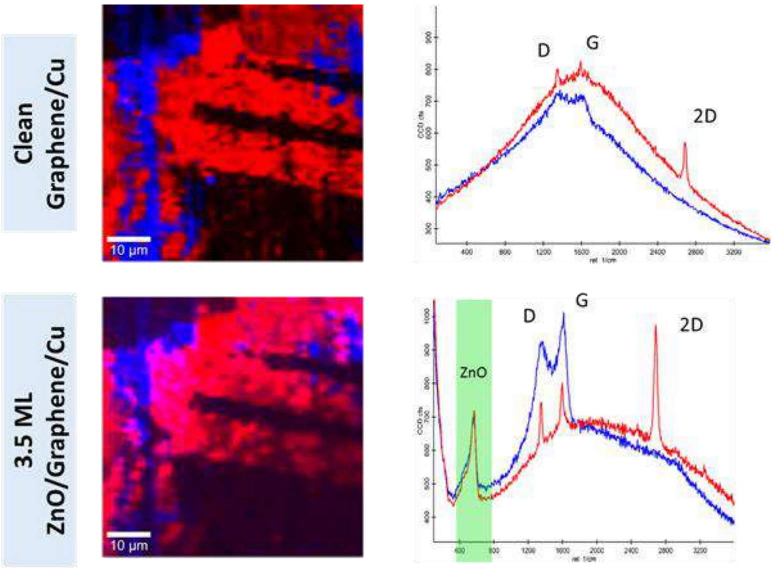
Session: Thin Films **Type of contribution**: Oral

ZnO has been grown on graphene/Cu polycrystalline by reactive evaporation of metallic zinc in an oxygen atmosphere at 1.5 x 10-3 mbar. In situ characterization of the growth has been done by successive evaporation steps followed by X-ray Photoemission Spectroscopy (XPS) measurements. Factor Analysis has been applied on the Zn LMM Auger photoemission to characterize the chemical changes on Zn during the growth [1]. Then, an inelastic peak shape analysis using the QUASES software [2] has been performed from the XPS survey spectra in order to get morphological information from the surface. The characterization was completed ex situ for a series of samples with representative growth steps by Atomic Force Microscope (AFM) and Raman spectroscopy.

Raman spectroscopy mapping over the clean graphene/Cu [3] substrate shows an important inhomogeneous graphene distribution with different qualities. ZnO growth reflects the initial graphene distribution, growing preferably on it. The graphene Raman signal improves after the deposition of ZnO, what might suggest that graphene decouples from Cu.



Mean Raman spectra associated with the corresponding color areas in the mapping

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New Strategy for Graphene Growth: a MBE Carbon-source

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Session: electronic materials and processing (or surface science) **type of contribution**: Oral

Graphene is nowadays recognized as an outstanding material from the point of view of its applications [1]. Since it was first produced by mechanical exfoliation of graphite by Geim and Novoselov, many different methods have been investigated: from chemical oxidation to chemical vapour depositions. Many of these methods require complicated and delicate transfer protocols for translating the graphene as-grown layer to a technologically useful substrate, sometimes distorting the properties or quality of the graphene.

In our group, we have investigated several strategies for growing graphene. First of all, we have used the decomposition of organic molecules (as fullerenes) in UHV conditions [2]. However, this method requires the use of substrates (platinum, copper or iridium) with catalytic properties for transforming the molecules in a carbon layer.

In this work, we present another method for growing graphene on more common substrates. With this purpose, we have used a carbon source base on a glassy carbon filament. By this strategy we reproduce the growth of graphene on metallic substrates as Pt(111) and Au(111) [3], and we demonstrate the formation of graphene patches on diamond surfaces using Raman, STM, EELS and other surface characterization techniques [4].

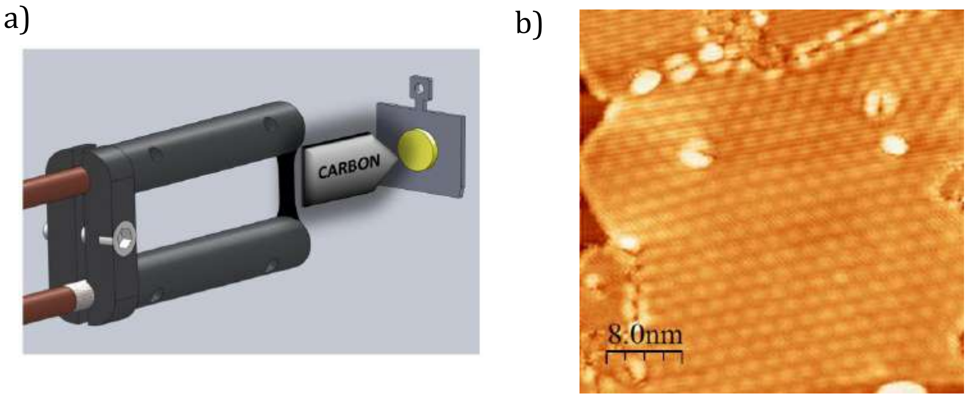

Figure: a) Carbon source based on a glassy carbon filament. b) STM image of graphene grown on Pt(111) using a MBE carbon-source.

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Band gap and film structure control by H_2 addition to Ar discharge gas in Cu_2ZnSnS_4 thin film deposition by reflector-wall sputtering

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Session: Thin Films **type of contribution**: oral

Cu_2ZnSnS_4 (CZTS) has been considered as one of the most promising materials for non-toxic solar cell absorber. To enhance the engineering feasibility for the deposition onto wide-area and low-temperature substrates, sputter-deposition is most advantageous among coating techniques. It has been demonstrated that the use of the reflector wall, which is positioned between the target and the substrate in an rf-sputtering system improved the film stoichiometry, crystallinity, and optical and electrical properties1). However, the band gap of the thin films ranged between 1.7 and 1.9 eV, possibly due to the formation of Cu_2ZnSnO_4 (CZTO), the band gap of which was >2.5 eV2). In this study, to control the band gap, H_2 was added to the Ar discharge gas in reflector-wall sputter-deposition of Cu_2ZnSnS_4 thin films from a sintered quaternary target. The rf power (13.56 MHz) applied to the 75 mm dia. target was 50 W. Substrate temperature was changed from 70°C to 400 °C. Thin film structure was evaluated by X-ray diffractometry (XRD) and Raman spectroscopy and composition was evaluated by X-ray photoelectron spectroscopy (XPS). Optical band gap was estimated from Tauc plots obtained from optical absorption measurements. The electrical resistivity and Hall effect measurements were carried out by using the van der Pauw method. It was shown by XPS measurements that the contents of O in CZTS thin films were reduced by the addition of H_2. XRD and Raman shift measurements showed that thin films were kesterite type CZTS. The lattice spacing was increased from 311-312 nm to 313 - 315 nm for (112) by the addition of H_2, in particular for a substrate temperature of < 100 °C (Fig. 1). The crystalline diameter was also increased from < 18 nm to about 22 nm. In addition, the band gap was narrowed from 1.7- 2.0 eV to 1.4 - 1.5 eV (Fig. 2). The resistivity of thin films deposited with an Ar-H_2 mixture ranged from 1 to 10 Ωcm. The carrier concentration was 10^{17} to 10^{19} $cm^{-3}$and the mobility was 0.1 to 10 $cm^2V^{-1}s^{-1}$. The increase in the (112) lattice spacing suggests the suppression of the formation of CZTO. The change in the lattice spacing well correlates to the change in band gap, indicating that the suppression of the O incorporation results in the decrease in the band gap width. It is concluded that the reflector-wall sputtering using an Ar-H_2 gas mixture from a quaternary CZTS target has an advantage to fabricate a solar cell consisting of CZTS absorber with an appropriate band gap.

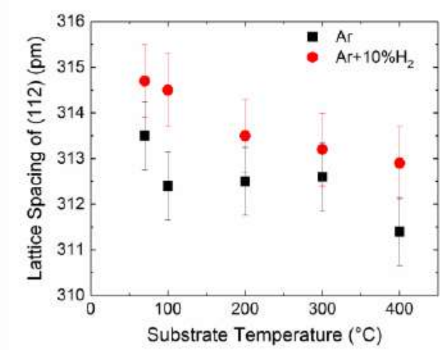

Fig. 1 Lattice spacing of (112) plane of CZTS thin films deposited in Ar and in Ar-10%H_2 mixture. Error bars indicate one standard deviation of uncertainty.

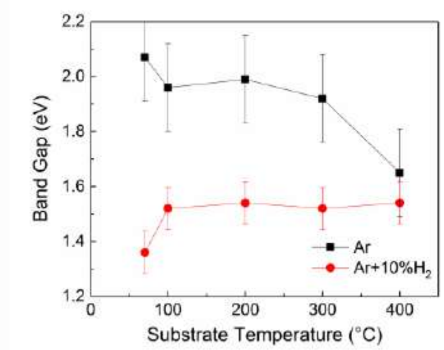

Fig. 2 Optical band gap evaluated from the Tauc plots for CZTS thin films deposited in Ar and in Ar-10%H_2 mixture. Error bars indicate one standard deviation of uncertainty.

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N-H recombination enhancement in nitrogen-hydrogen Glow-Discharge plasmas induced by energetic helium bombardment on the tungsten surrounding surfaces

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Session: Hard-coatings workshop **type of contribution**: Oral presentation

In the routine operation of divertor configured fusion devices with metal walls, the injection of nitrogen as seeded plasma impurity has become necessary to induce plasma divertor detachment [1] and achieve good performance. During this impurity seeding operation, the nitrogen molecule acts as a radiative cooler in the plasma edge, reducing the sputtering of divertor materials (tungsten) and improving the confinement [2]. However, its use leads to a significant ammonia formation on the in-vessel surface that has been reported in relevant tokamaks [3, 4]. In the future ITER (International Thermonuclear Experimental Reactor) active phase with deuterium-tritium fuelling, the presence of (generated) tritiated ammonia that increases the tritium inventory and the deleterious effects of ammonia corrosion on the vacuum system, cryopump panels and pumping lines would limit the ITER operational cycle due to the necessary regeneration of the gas exhaust modules and safety issues related with the radioactive hazards associated to tritium retention in the reactor. This problematic supposes an important issue for the magnetic fusion community and its study has been given priority for the future ITER research roadmap [5]. Despite the recent studies on this topic, the effects of a fusion reactor environment with the presence of helium as an intrinsic plasma impurity, on the ammonia formation is uncertain. Under such scenario, the comprehension of the induced effects by the reactor conditions on ammonia formation is clearly necessary in order to estimate and try to mitigate its generation. In this research, direct current N_2-H_2 Glow Discharge plasmas (dc-GD plasmas) have been used to simulate the plasma-surface processes in diverted N_2 seeded plasmas that determine the ammonia formation on tungsten walls. The ammonia formation yields have been measured by using differentially pumped mass spectrometry on the residual gas obtained from the dc-GD discharge. The effects of a fusion reactor environment, with the presence of energetic helium in the plasma, on the ammonia formation yields have been investigated, showing that the seeding of helium increases the ammonia formation up to a 45%. Furthermore, optical emission spectroscopy analyses have been performed to estimate the electron temperature of the plasma as important factor for the ionization/dissociation (plasma-gas phase) processes. These reactions provide the necessary neutrals and radicals for the surface N-H recombination that complete the underlying mechanism of the ammonia formation. After an exhaustive analysis of the plasma phase parameters and surface processes, the modification of the surface chemistry (N-H recombination) induced by the bombardment with energetic helium projectiles (E~300 eV) together with changes in the surface roughness (that leads into an increase in the active tungsten recombination area) seems to be reason that explain the enhanced ammonia formation.

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Liquid metal (Li, SnLi) thin film protection of metal surfaces: fusion applications

E. Oyarzabal[1], F.L.Tabares[1], D. Tafalla[1], A. B. Martin-Rojo[1], A de Castro[1] and the TJ-II Team

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Session: Thin films **type of contribution**: Oral presentation

Covering and protection of metal surfaces by liquid metal (LM) thin films can provide several advantages with respect to the sole solid materials. In particular, for the case of fusion applications they offer some unique properties; they are basically free from permanent damage by neutron and plasma irradiation and can be re-circulated and regenerated for lifetime and particle and heat exhaust issues [1]. The expected advantages for the power exhaust issues, mainly arising at the divertor target at power densities of 10– 20 MWm−2, relay on the self-healing properties of liquid surfaces as well as the ability to in situ replacement of the surfaces exposed to the plasma by the effect of capillary forces that appear in the Capillary Porous Systems (CPS)[2] envisioned for their use as divertor materials. The main LM candidates presently considered for the development of an alternative solution to the Power Exhaust Handling in a future Fusion Reactor are Li, Sn and tin lithium alloys. The later ones offer unique properties in terms of evaporation, fuel retention and plasma compatibility. This is the reason why this particular LM was chosen as main candidate in the US APEX project [3]. Very recently, LiSn (20-30:80-70at.%) alloys have been exposed to ISTTOK and TJ-II and very promising results on D retention and surface segregation of Li were obtained [4,5].

Motivated by these results a full campaign of comparative Li/ LiSn testing in TJ-II plasmas has been initiated. Liquid metal wetted CPS heatable electrodes have been manufactured in the Plasma Wall Interaction laboratory at CIEMAT and later exposed to TJII plasmas at different temperatures. For both solid and liquid states a negligible perturbation of the plasma has been recorded in the Li and LiSn cases, even when stellarator plasmas are particularly sensitive to high Z elements due to the tendency to central impurity accumulation. The surface temperature of the liquid metal/CPS electrodes (made of a Tungsten mesh impregnated in Li or SnLi) has been measured during the plasma pulse with ms resolution by pyrometry and the thermal balance during heating and cooling has been used to obtain the thermal parameters of the LM/CPS arrangements as well as to calculate the thickness of the film interacting with the plasma. Temperatures as high as 1100K during TJ-II plasma exposure were observed for the LiSn case and hints of sputtering-enhanced evaporation were deduced from the temperature dependence of the lithium fluxes entering the plasma.

Furthermore, laboratory experiments showing a much lower hydrogen retention of SnLi compared to Li (as expected) and a secondary emission coefficient (SEE) closer to pure Li have been undertaken in order to further study the relevant properties of tin lithium alloys for their possible use as PFC in a future reactor.

This research was partially financed by the Spanish “Ministry of Economy and Competitivity” under project ENE2014-58918-R.

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http://dx.doi.org/10.1016/j.nme.2016.11.026

Black gold obtained by sputtering glancing angle deposition

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Session: Thin films **type of contribution**: Oral presentation

Black metal coatings are metallic coatings that exhibit high absorption in a certain region of the electromagnetic spectra. They are of interest in a wide range of applications [1] such as radiative heat exchangers, solar energy absorbers, photovoltaic cells electrodes, separators to avoid cross effects in optical devices, thermal light emitters, or biosensors electrodes, to name a few. In particular, gold is frequently used due to its high resistance to oxidation. As the spectrum of the solar radiation exhibits maximum irradiance in the visible range, finding a suitable method to produce black-metal coatings in that range is of fundamental importance.

In the last few years, we have followed a low-cost approach to fabricate nanostructured coatings: glancing angle deposition with sputtering. It is energetically efficient, since it takes place at room temperature in one single step and no chemicals are involved (i.e. no recycling problems). Any kind of flat substrate can be used, and with feasible modifications, it can be scaled up to large surfaces. Up to now, we have studied the growth regimes of the nanostructured coatings [2, 3], as well as the antibacterial properties of nanocolumnar films made of titanium [4].

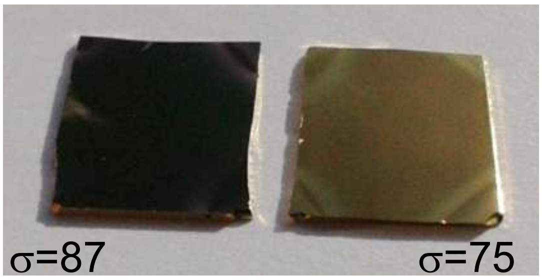

Figure: Photograph of two Au samples prepared by sputtering glancing angle deposition onto Si substrates with deposition angles 87º (left) and 75º (right). Notice the black color of the left sample.

Recently, we have obtained black gold coatings in the visible range with this fabrication technique by rotating the substrate [5]. As it can be seen in the figure, high tilt angle is needed in the deposition to obtain the black behavior. In this work, we will present the optical properties of the black gold films, with reflectivities below 10% in the 400-700 nm range for Au films deposited on Si. We will also analyze the morphological differences between the two obtained optical regimes in order to understand the main features responsible of this black behavior.

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Effect of pulling rate on redox state and crystallization of Fe-Si-O glass ceramic prepared by laser floating zone

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Session: Electronic Materials and Processing **type of contribution**: Oral Presentation

Abstract

Silica-based glasses have gained increasing attention due to wide variety of emerging applications in industry and research and becausse of their unique physical and chemical properties, including chemical durability, abrasion resistance, specific electrical transport features and biocompatibility. Moreover, silica glasses show reasonably high ionic mobility along with high concentration of weakly-bonded mobile ions.

The addition of transition metal oxide ions like iron to the silica glasses is expected to improve their electrical, dielectric and magnetic features. Regardless of the original oxidation state of the iron in the starting glass batch, the final glass contains Fe^{3+} (in both tetrahedral and octahedral coordination environments) and Fe^{2+} ions in octahedral coordination.

Laser Floating Zone (LFZ) method shows good prospects for studying the crystallization mechanisms in silica based glasses with additions of redox-active cations, by providing flexibility in tuning their oxidation state and crystalline/amorphous nature.

This work focuses on the behavior of silica glass system, containing 10 mol% iron oxide, under various pulling rates during the LFZ process. The selected amount of iron implies that it will be rather incorporated into the glass as a network modifier. The prepared samples were characterized by structural, morphological, electrical and magnetic measurements in order to assess the effects of the pulling rate on redox properties of iron oxide in silica glasses.

The XRD and SEM results showed the crystallization and heterogeneity improve as the pulling rate increases, respectively. Using Raman spectra, we concluded that Fe^{+2}/Fe_{total} ratio increases with the growth rate. The pulling rate dependence of AC conductivity could be explained in terms of the polaron hopping between iron ions, the crystallization of microcrystallites, induced by high Fe^{2+}/Fe_{total} ratio and also the amount of inclusion α-Fe_2O_3 phase in the fibers. The ZFC-FC curves of the fibers showed a superparamagnetic-like behavior, characterized by a T_P (the blocking temperature) near to the Verwey transition and T_{irr} (the bifurcation temperature) ranged from 200 to 250K. The increase in magnetization with the pulling rate can be correlated to the sharp increase of the Fe^{2+}/Fe_{total} ratio. The temperature-dependence of saturation magnetization and coercivity has been fitted by a modified Bloch's law and a modified Kneller´s law, respectively.

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Benefits of the multilayer design in the oxidation resistance of cathodic arc evaporated nitride coatings in the energy industry

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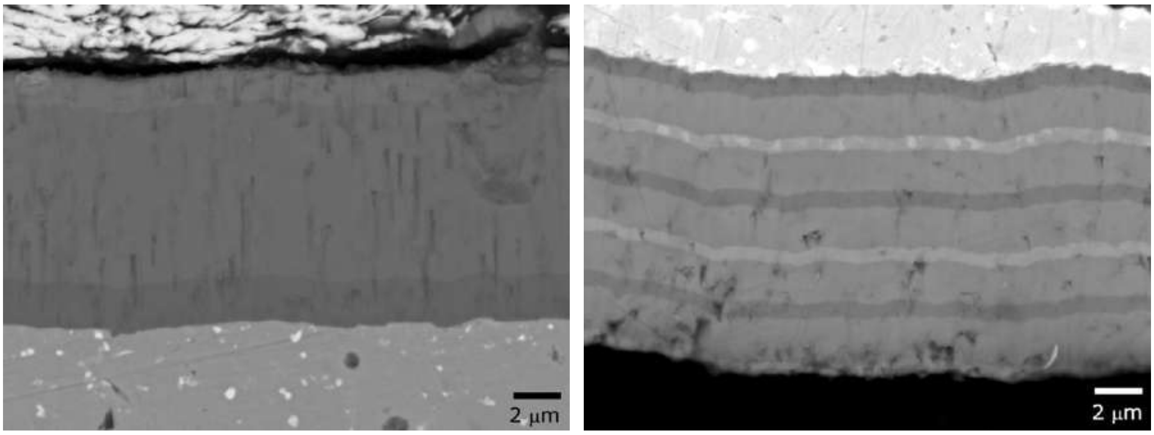
Session: Surface Engineering **Type of contribution**: oral

There is a permanent interest in exploring new protecting coatings to improve the performance of the materials employed in power plants. Traditional hard coatings have attracted the attention in this sector due to their good mechanical properties, thermal stability and corrosion resistance. Finding suitable hard coatings for high temperature applications would extend the multifuntionality of these outstanding materials. Therefore, in this work nitride-based coatings with alternating layers of CrN and TiN have been investigated in the working conditions of supercritical turbines (Figure 1). Previous findings showed the convenience of using nitride monolayered coatings as protection on steel enhancing oxidation resistance in similar conditions [1]. The study has been developed by means of thermogravimetric analysis, scanning electron microscopy (SEM), electron probe microanalysis (EPMA) and glow discharge optical emission spectroscopy (GDOES). The behaviour of the coatings on a ferritic-martensitic steel has shown the important role of the multilayer design in the oxidation resistance tested up to 2000h.



a) b)

Figure 1. SEM micrographs of the cross section of a) CrN/CrTiN/TiN three layered coating and, b) cross section of a CrN/CrTiN/TiN multilayered coating, oxidized to 2000h at 650ºC in 100% steam atmosphere.

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Simulating the life of cosmic dust in the laboratory

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Session: Vacuum Science and Technology **type of contribution**: oral

Laboratory astrochemistry plays a key role in elucidating the mechanisms underlying the complex chemistry of the interstellar medium (ISM). The large molecular complexity found in the ISM cannot be solely explained by gas-phase chemistry; therefore the catalytic processes on the surface of cosmic dust grains are believed to strongly contribute to the richness of molecular species observed in the ISM. However, much remains unknown on cosmic dust formation and evolution in the ISM.

In this context, we present the STARDUST machine, an innovative experimental station devoted to the simulation of cosmic dust formation and its evolution in space. In particular, we focus on investigating the catalytic reactions taking place on the surface of small dust grains present in the universe. Analogues of small dust grains are created using a Multiple Ion Cluster Source (MICS). The versatility of the MICS enables us to create a wide variety of clusters and nanoparticles (NP), allowing for the simulation of dust expelled by both C-rich and O-rich stars.

In Stardust, clusters/NP are provided in-flight in the gas phase where most relevant physical parameters and environments, such as temperature, speed, and background gasses can be controlled. This versatility allows to simulate processes, for instance, at conditions mimicking that faced by cosmic dust particles in spatial environments. Furthermore, these dust analogues after being deposited on a surface can be covered with astrophysically relevant ices, in order to study grain-ice boundary processes.

Besides the outstanding possibilities of STARDUST for fabricating and processing interstellar dust analogues and ices, analysis modules have been constructed to allow for the *in-situ* analysis of both the analogues and the processes that simulate dust formation, growth, accretion and chemistry therein. Thus, X-Ray Photoemission Spectroscopy, Infra-red Spectroscopy or thermal induced mass spectrometry can be performed *in-situ* to avoid contamination of the produced analogues.

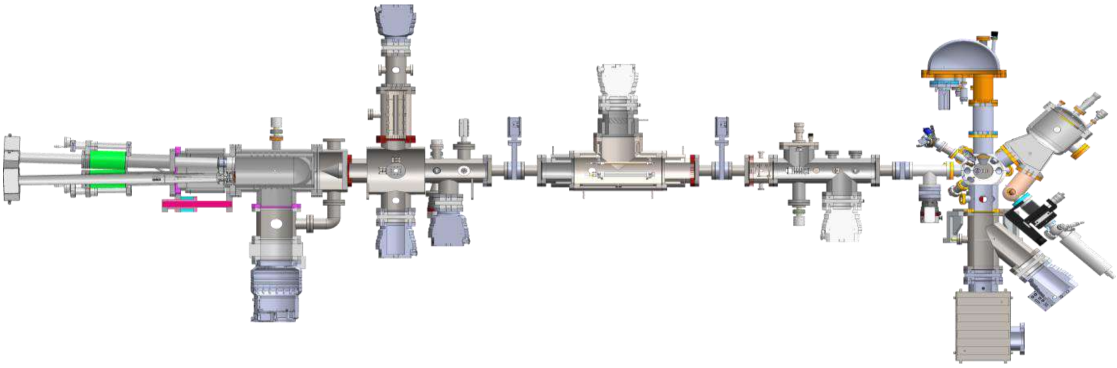

Figure 1: Schematic overview of the STARDUST machine.

Acknowledgements: This work is supported by the European Research Council (ERC-2013-SyG NANOCOSMOS).

Hyperloop UPV: a concept for the future of transportation

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Session: vacuum science and technology **type of contribution**:

Hyperloop is a transport system based on high-speed and low energy consumption, currently proposed by Elon Musk. Nevertheless, the concept of this transport system had already been proposed at the beginning of the XXth century by several authors. Basically, the system consists in a train (pod) levitating inside a tube whose air had been previously evacuated. Thus, when the pod would move inside the tube, the friction force with the air would be avoided (thanks to the low-pressure atmosphere inside the tube), as well as the rolling resistance (due to levitation). This would allow for zero energy consumption to keep the speed constant, only needing energy during accelerations. However, the development of this promising concept of transport system was stopped in the past and was revised several times to determine its feasibility. Currently, several consortiums are trying to popularize this transport system and to analyse its feasibility considering today's technology. The Hyperloop Makers UPV proposes different solutions to tackle these challenges in the following report.

The final proposed pod has a cruise speed of 276 m/s, consuming as low as 26 W•h/(pass•km). It weighs around 20t and has capacity for 30 passengers or 3600 kg of payload in a 19 m total length.

Experimental characterization of a 1 kW HPT

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Session: write your session here **type of contribution**: Oral presentation

A Helicon Plasma Thruster prototype [1], HTP05 hereafter, has been designed and built by SENER and EP2-UC3M in 2015. The first test campaign (ignition test) was carried out successfully on October 2015 at the Electric Propulsion Lab facilities at ESTEC, ESA. The current work is devoted to explore and assess the thruster performances by means of plasma diagnosis. All results presented here have been obtained during the in the experimental campaigns performed at the recently inaugurated UC3M-EP2 facilities in Madrid, Spain.

The UC3M-EP2 LAB main vacuum chamber consists of a 3.5 m long and 1.5 m diameter stainless steel vessel, with three cryopanels and two turbomoleculars pumps with a total pumping speed about 37,000 l/s. This facility allows performing tests with up to 1.5 mg/s of Argon or Xenon keeping a background pressures below $2.6 \cdot 10^{-5}$ mbar. The employed intrusive plasma diagnostics include: a Langmuir probe (LP), a radio frequency compensated LP (RFCLP), a Faraday probe and an emissive probe. These probes are mounted on a 3 DoF positioning system that allows scans of the whole plume, 0-1500 mm downstream from the thruster exit, and -400 mm to 400 mm on both transversal and vertical direction.

Plasma density and potential, electron temperature, the electron energy distribution function, the ion energy distribution function, plume divergence (Example in Fig 1a), and the total ion beam current (Example in Fig 2) are measured at different positions in the magnetized plume of the HPT05. All these plasma properties are obtained for several magnetic topologies and magnetic intensities, RF power levels, and mass flow rates. The main objective is to identify these parameters that optimize the HPT05 thrust capabilities. Different plasma operational modes,(inductive, helicon mode, etc.) are identified and the mode variation conditions are assessed as well. Experimental results could be compared with those obtained from analytical and numerical models for the Helicon Plasma Thruster [2] and Magnetic Nozzle [3] developed by EP2 during last years.

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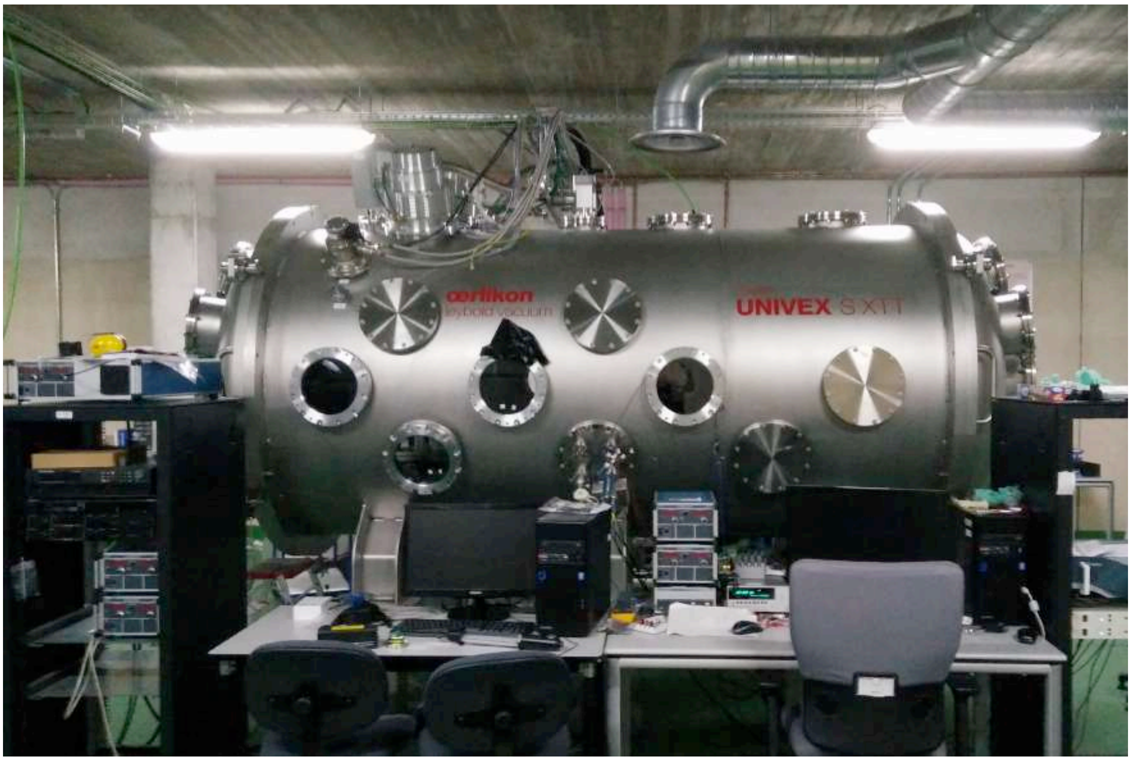

Figure 1. EP2-Lab main vacuum chamber

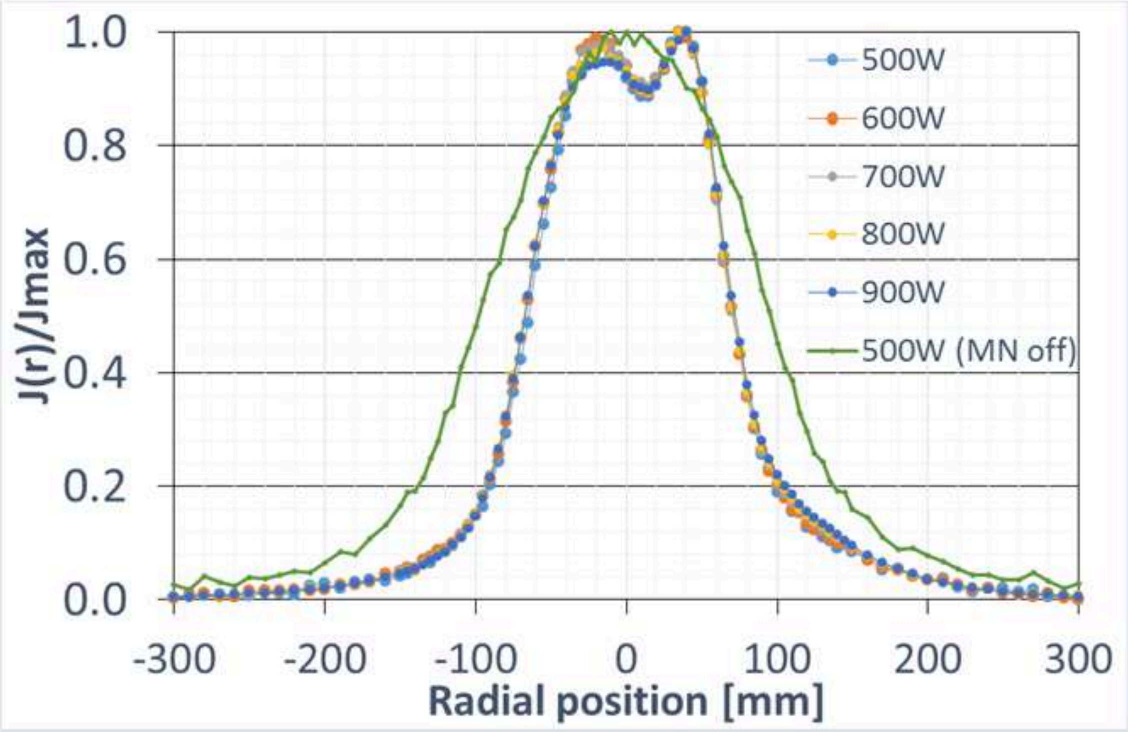

Figure 2. Normalized ion flux on a transversal plane at z = 200mm from the HPT exhaust section, for several levels of RF transmitted power. Each curve is normalized with its maximum measured flux. This proves that plume divergence does not depend on the RF power coupled to the plasma, but on the magnetic field strength at the MN stage (green case is obtained with the MN coil turned off).

Development of a Sputtering System for in-situ fabrication of $Cu(in,Ga)Se_2$ thin-film solar cells: STAR

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Session: vacuum science and technology **type of contribution**: Oral

Photovoltaic (PV) technology is dominated today by crystalline silicon (c-Si) technology. Thin-film technology based on $Cu(In,Ga)Se_2$ (CIGS) absorbers is currently the most-efficient polycrystalline alternative [1]. PV modules with CIGS are very effective in converting light directly into electricity, and, at the same time, can be produced on flexible and lightweight supports. CIGS can be used also in tandem devices that will enable impressive efficiency values well beyond 30%.

In order to fully push the limits of CIGS thin-film materials, a new **S**pu**t**tering for **A**dvanced **R**esearch (**STAR**) system has been designed and constructed at IMM, CNM-CSIC in collaboration with the INL, Portugal under Spanish National Program AIC-2011-0806. The final objective of the collaboration is to share a novel laboratory-scale fabrication tool capable to integrate all basic steps to fabricate high-quality semiconductor thin film cells at low deposition temperature, with a high control of the stoichiometry through operation of a newly developed Pulsed Reactive Hybrid Sputtering of Selenides using a specially designed pulsed Se source. This novel tool, based on our MBE experience with III-V [2] and chalcogenide materials [3], will allow to develop in the laboratory all decisive sputtering processes that are fully scalable to in-line industrial production of large-area thin-film solar cells.

Among other capabilities of the STAR system (Fig. 1 a and b) we can highlight: compact design, small footprint, full ultra-clean UHV technology, full in-situ structure deposition, high throughput by means of a sample parking, reliable transfer mechanism between growth chambers, flexible control software, and modular chamber architecture.

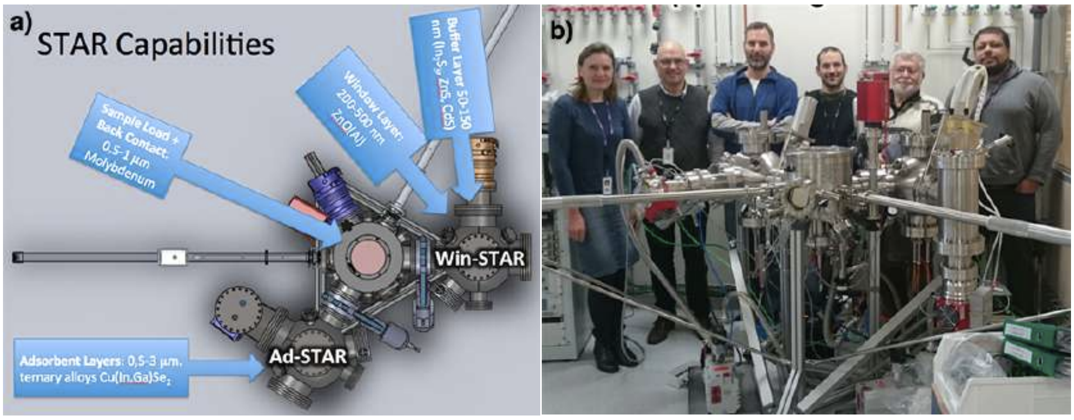

Figure 1: a) Top view scheme of STAR. b) System deployed at INL.

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Innovative Solutions for the Machining of Composite-Ti alloys stacks for the aeronautic sector

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Session: Hard coatings **type of contribution**: Oral presentation

The need for more efficient aircrafts, consuming less fuel and increasing the flying capabilities either in comfort, eco-efficiency and range of operation, became a priority on the last decades for the airplane manufacturers, non-regarding the size and type of market they envisage. Manufacturers were led to take advantage of the weight-to-strength ratio, with more efficient solution that necessarily comprehend the use of lighter and stronger materials, which allow them to step forward decisively and not marginally every time they launch a new apparatus. Over the last years, materials like steel, Al and Ti conventional alloys, have been replaced in many cases by the increasing appearance of composite structures, either composed by these materials or being mixed with new alloys to produce near net shape parts, decreasing the amount of machining operations needed and giving rise to new opportunities in concept and design. Many other materials are nowadays being introduced in this manufacturing landscape, like Al-Li alloys, Ni alloys for specific applications and ceramic matrix composites [1], but the ability to resist heat and corrosion of Ti-alloys has quickly started to replace aluminium parts, being now widely used in fastening elements, airframe and landing gear of airplanes. The applications for Ti-alloys are not limited to the aircraft structural parts, since high strength and low density of titanium gives the engine manufactures the high levels of performance they desire. Especially, on parts like blades, shafts, casings for the front fan and to the rear end of the engine, where temperatures of 600 degrees Celsius can be achieved, being the high temperature performance of titanium ideal for such request.

One of the drawbacks of Ti-alloys is their poor machinability, the high-chemical reactivity of titanium alloys causes the chip to weld the tool, leading to cratering and premature failure. The low thermal conductivity of these materials, prevent the heat to dissipate from the tool edge, causing high tool tip temperatures and excessive tool deformation and wear. On other hand, composites offer completely different difficulties when machined, especially due to the absence of defects of reinforcement fibres and abrasive behaviour caused on the tools by the mix of thermoset resins and high mechanical properties of the reinforcements. These characteristics raise completely different problems when both materials are brought together in the same part, building a stack of bi-material, needing machining operations.

The challenges on machining Ti-alloys, together with composite materials, bring a huge amount of space for improvement, by the development of new tool geometries as well as coatings and machining strategies that can make a big difference in the reduction of production costs.

The objective of this research work, addresses the strengthening of the competitiveness of the Ti-alloys, composites and Bi-materials for the transportation field through the improvement of the efficiency of the cutting process.

The aim is to develop new solutions for the cutting processes, based on the optimization of the tools geometry and modification of their surface by deposition of thin films able to resist wear conditions and having self-lubrication capabilities. It is aimed to increase production rates, to improve the tools lifetime and to decrease or remove the liquid lubrication during the cutting process.

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Development, Calification and Application of a Thermal Protection PVD coating Designed for the Solar Orbiter Project

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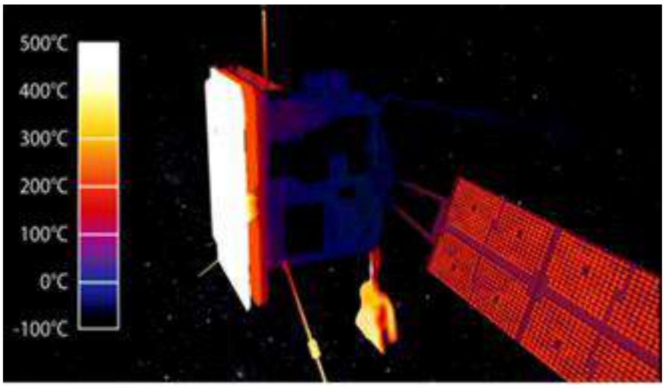
A novel PVD coating was developed to be applied on critical parts that need thermal protection in the Solar Orbiter space probe. This probe will be located in an orbit close to the Sun that will involve extreme temperature and radiation during its service life. The developed coating was designed to achieve optimal thermo optical properties being also able to withstand the harsh conditions of up to 500 ºC and the incoming radiation from the Sun. The calification of the coating involved tests for evaluating UV, radiation, aging resistance, adhesion tests and electrical conductivity. The good values obtained for the developed coating resulted in its approval for applying on the Solar Orbiter probe.



ORAL CONTRIBUTIONS

Friday 6th

The Role of Surface Analysis in Studies of Plasma-Wall Interactions in Controlled Fusion Devices

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The ultimate goal of research on controlled thermonuclear fusion is to construct and operate an efficient energy generating system. Under terrestrial conditions hydrogen isotopes must by confined either by strong magnetic fields or intense laser beams. Plasma must be surrounded by walls of a vacuum vessel. This contribution is focused on studies of materials originating from toroidal systems for magnetic confinement fusion, such as tokamaks or stellarators.

First wall material in fusion devices undergo serious modification by several physical and chemical processes arising from plasma–wall interactions (PWI). Materials eroded from the wall are ionised, transported along the magnetic field lines in the vacuum vessel of a tokamak and then re-deposited in another location than the place of origin. This leads to the formation of mixed-material layers which contain both eroded species and hydrogen isotopes, i.e. fuel atoms such as deuterium and tritium [1,2]. Consequently, the list of isotopes of interest encompasses a broad spectrum of masses from low-Z species (H,D,T), via He, light wall materials (Li, Be, C) to medium (steel) and heavy metals such as W and Re. The effectiveness of material migration studies is enhanced by tracer techniques based either on the exposure marker PFC tiles or injection of a rare isotope gas (e.g. $^{15}N_2$, $^{13}CD_4$) or a volatile compound of a high-Z metal, e.g hexafluorides (MoF_6, WF_6). As a result, conclusive characterisation of PFC requires application of a large number of material research tools among which surface analysis techniques play a prominent role [3,4]. Over the years, more than forty different methods have been used to get a comprehensive insight into the structure and composition of the outermost and near-surface region of wall materials. Various ion beam analysis (IBA) and high-resolution microscopy methods are particularly important.

The aim of this contribution is to provide an overview of experimental procedures and results obtained in surface analyses of materials from the JET and TEXTOR tokamaks and from the TJ-II stellarator. The role of ^{3}He-based NRA, RBS, PIXE (standard and micro-size beam) and HIERDA in fuel retention and material migration studies is presented. Examples are given on the application of tracer techniques with rare isotopes (e.g. ^{13}C, ^{15}N, ^{18}O), marker layers on wall materials and optical diagnostic components such as mirrors. Development of equipment to enhance research capabilities and issues in handling of contaminated materials are addressed.

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Recent advances of solid lubricants prepared by vacuum-related processes

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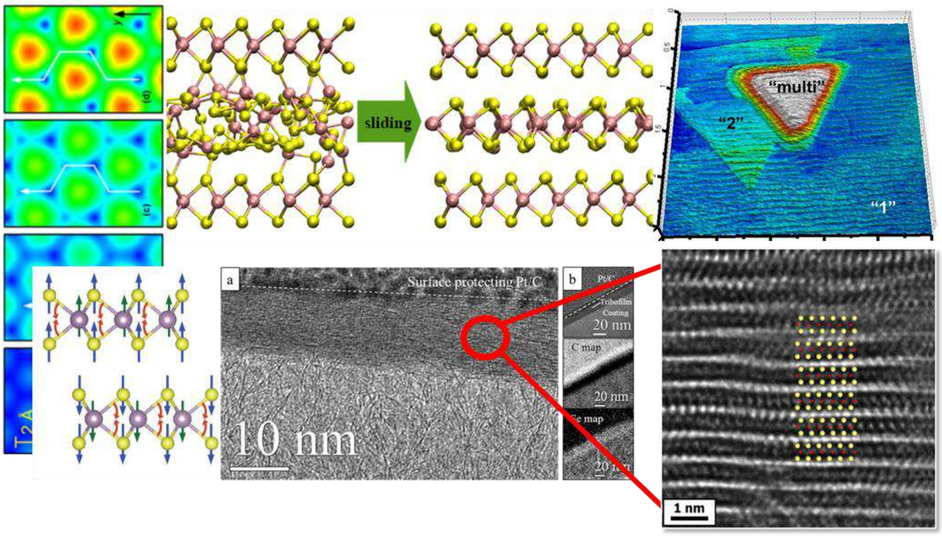
Session: n.a. **type of contribution**: Invited

The friction of solids is an extremely complex and multiscale problem. Simulations of friction at the atomic scale have just started and still have to unravel their full potential; moreover, experimental validation is an ongoing challenge. Recent advances in 2D materials, such as graphene or transition metal dichalcogenides, opens, perhaps for the first time, the possibility for bottom-up design of frictionless material.

2D materials may readily be used as lubricants in nanoscale contacts, but their applicability as externally supplied lubricants in mainstream engineering applications is questionable. Preferably, low dimensional materials minimizing friction should be produced continuously during the sliding process. We show our recent results on solid lubricant coatings with self-adaptive nanostructure. Our ultimate ambition is to prepare thin films, which will produce an ultra-low friction interface based on optimised low-dimensional structures in situ, i.e. during sliding

We try to establish links between fundamental properties of selected 2D materials obtained by ab initio methods (electronic structure, covalency, etc. [1,2]), molecular dynamics and measured friction [3]. These results, together with nanoscale experiments, form a base of design of novel sputtered solid lubricant coatings.



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Surface Enhanced Raman Scattering as tool for the improved detection of biomarkers

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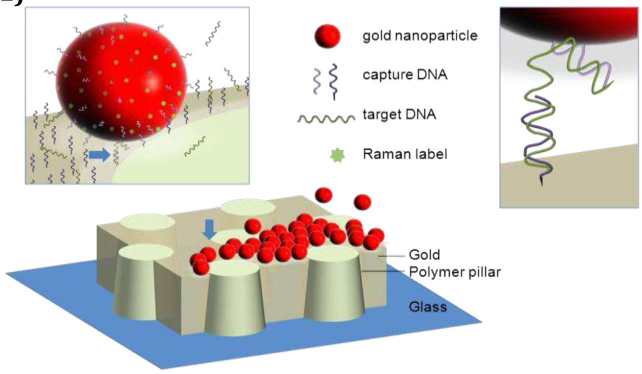
Session: write Biointerfaces **type of contribution**: Invited Talk

Raman spectroscopy is a vibrational spectroscopy which provides detailed information on the molecular composition of the analyte with an high level of specificity and virtually without sample preparation. Raman however is a weak process and its sensitivity is not sufficient for a clinical exploitation. When Raman spectroscopy is performed on the surface of suitable metallic nanostructured materials, a particular enhancement of the signals (SERS) arises. Thanks to the SERS enhancement Raman spectroscopy could become the basis of the next generation of diagnostic tests [1]. In the present talk we will describe some examples of how SERS could be used for the detection of biomarkers relative to cancer and to neurodegenerative diseases by using some Raman label (labelled approach) or by the direct measure of the signals from the biomarker of interest (label free approach).

In a first study, we will describe the development of a SERS substrate made of a 2D crystal structure of polymeric pillars embedded in a gold layer to be used for the detection of multiple genetic sequences relevant for the diagnosis of Acute Myeloid Leukemia with low picomolar sensitivity [2-3]. In the second part we will focus on the use of SERS for the study of the small metabolites present in human blood applied to the diagnosis of Alzheimer's disease a neurological disorders in desperate need for new diagnostic test based on the analysis of biofluids easy to access such as plasma or serum.

1)



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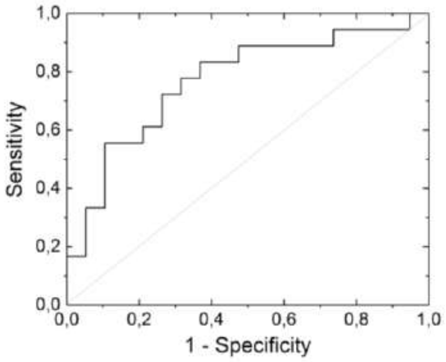

Figure 1: Schematic representation of the SERS based biosensor developed by using the nanostructured surface. Figure 2: ROC curve of the SERS analysis of human serum for the diagnosis of Alzheimer's disease

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Water on viral surfaces

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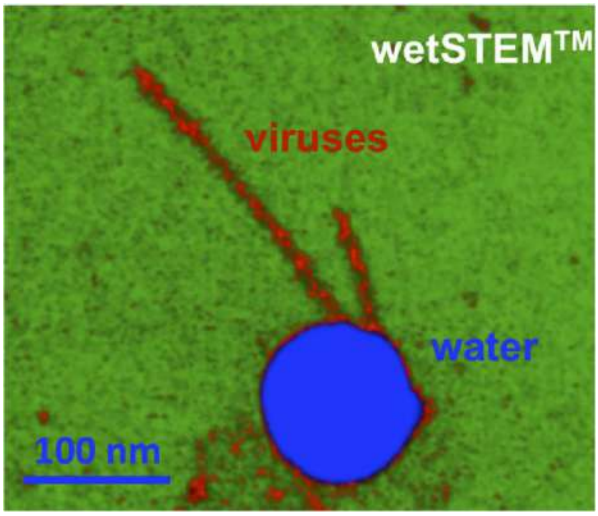
Session: biointerfaces **type of contribution**: oral

The interaction of water with the coat proteins of viruses influences the transmission. We started our investigations with a textbook virus example, Tobacco Mosaic Virus (TMV) [1-3]. Its highly regular helical coat was as yet probed by methods that average over many particles at very high humidity (X-ray diffraction, cryo-electron microscopy) [1]. We achieved local probing of single virus particles, without averaging, by multifrequency AFM [4] and low voltage SEM. TMV in the dry state shows unexpected nanoscale surface features at irregular axial spacings.

The stepwise and reversible wetting by water can be studied by AFM in a humidity chamber, and by environmental electron microscopy in up to 10 mbar water. We observed scenarios such as wet wedges (around TMV), layers (on TMV), and water pools (confined by TMV) [5]. Possibly such features play major roles in the transmission of human viruses.



Environmental electron microscopy of virus particles at a water nanodroplet on a thin carbon film

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Irreversible humidity indicators based on Zinc Nitride and water vapor effects

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Session: Biointerfaces **type of contribution**: Oral Presentation

Zinc nitride (Zn_3N_2) is a semimetal with a band gap energy of 1.23 eV, high mobilities (~100 $cm^2/V\cdot s$), high carrier densities (10^{18}-10^{20} cm^{-3}), and low resistivities (10^{-2}-10^{-3} $\Omega\cdot cm$) [1]. It has a black colour and it tends to form polycrystalline films when it is deposited by magnetron sputtering at low temperatures ($T < 500$ K) using reactive N_2 plasma. Despite the reported fabrication of electronic devices from those films [2,3], Zn_3N_2 is still poorly developed due to the transformation into ZnO at normal ambient conditions [4]. The transformation starts at the top surface and propagates vertically up to reaching the interface with the substrate. As a result of the transformation, the material becomes insulating and transparent in appearance.

In this work, we focus on the properties of electronic sensors made of thin films of this material and how the transformation of Zn_3N_2 into ZnO affects their electrical properties. Our studies reveal that humidity plays a crucial role in the process, so a good correlation between the relative humidity and the transformation time is found [5], opening the possibility for the development of low-cost irreversible humidity indicators based on this material. Furthermore, the devices are exposed to the vapour of aqueous solutions with different pH in order to compare the signal recorded during the adsorption of the different molecules. Generally, the signal shows two different behaviours depending on how large the gas flow is. Thus, at low gas flows, the conductivity of the layers increases whereas, at high gas flows, condensation occurs so the transformation of Zn_3N_2 into ZnO speeds up. The influence of pH in both operation ranges is analysed in detail.

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Ex-vivo studies on friction behaviour of urethral stent coated with Ag clusters incorporated DLC matrix

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Session: write your session here **type of contribution**: Oral presentation

Coated urethral stents must be placed in the human body without hurting the body tissue and, simultaneously, support the application without degrading the top active layer. Therefore, improvement of the frictional performance of the coating is required. Diamond-like carbon (DLC) coatings are largely used as wear protective coating, owing to their low friction coefficient and high hardness; moreover, these coatings are biocompatible and chemically inert, presenting outstanding corrosion resistance. All these characteristics made carbon based coating suitable for biomedical devices. Also, the incorporation of different metal atoms (e.g. Ti, Zr, W, Cu, Ag, among others) enables to optimize the functional properties of DLC coatings, specially, the toughness and residual stress.

Silver nanoparticles have been used as antimicrobial agents in many different biomedical applications. Alloying DLCs with Ag nanoparticles has been a solution for fixing the nanoparticles and allowing silver ions release along the time. The size, shape and conditions of incorporation of Ag nanoparticles are important to control the ions release.

In this sense, in this work Ag clusters were produced by plasma gas condensation process consisting in a gas aggregation cluster source connected to a main deposition chamber of a magnetron sputtering equipment and the working pressure in the main chamber and the cluster gun were studied as deposition parameters. Then, the friction behaviour of Ag-alloyed DLC coated urethral stents have been investigated by means of a homemade ex-vivo model using porcine liver as counterbody material and saline solution as lubricant. In the developed tribotest rig which has simulated the in-vivo condition for the urethral stents, the friction coefficient of the coatings and the uncoated reference were determined and show comparable results.

Study of colloidal crystalline monolayers for a versatile nanofabrication process

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Session: Biointerfaces **type of contribution**: Oral

Nanomaterials are particularly interesting for the development of advanced biosensing platforms based on surface plasmon resonance, which can provide multiplexing, enhanced sensitivity and low detection limits [1]. In addition to the classical fabrication approaches, the development of hybrid top-down/bottom-up techniques allows a fast, parallel and cost-effective fabrication of large area surface patterns [2], such as in the case of fabrication techniques based on a combination of colloidal lithography and plasma processes. Among others, the Langmuir-Blodgett technique is an efficient method for a repeatable and controllable formation of high quality crystalline monolayers of colloidal particles [3], which can be transferred on different solid substrates by vertical dipping and used as sacrificial etching mask to obtain a nanostructured surface.

In this work, we investigated the assembly of Langmuir-Blodgett monolayers (made of polystyrene and silica beads) by combining different suspension-related parameters and then the peculiar effect of varying subphase-related parameters to improve the microcrystalline structure of the transferred colloidal films. These monolayers were then used as sacrificial mask and conditioned through different reactive ion etching processes to nanostructure the underlying substrate. The sequential gold deposition and particle lift off provided a plasmonic surface made of gold cavities. The versatility of our fabrication method allowed us to tailor the spectral response of the surface by easily tuning the nanostructure features, leading to a wide range of selection of plasmonic surfaces, especially in terms of shape, diameter and periodicity. The optimized surfaces were efficiently tested as efficient platforms for biosensing in SPR and SERS experiments.

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Reduced Graphene Oxide sensor formed by dielectrophoresis across AZO electrodes

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Session: Biointerfaces **type of contribution**: Oral Presentation

Graphene oxide (GO) shows useful properties for many devices applications due to the presence of functional groups provide an opportunity to modify its chemical functionalities as well as its electrical and optical properties. In particular, GO is considered to be an ideal candidate for the fabrication of gas sensors and biosensors due to its excellent capabilities for direct wiring with different molecules.

This study reports on the precise positioning of graphene oxide flakes across sputtered aluminium-doped ZnO (AZO) electrodes on both glass substrate and transparency film using a positive dielectrophoretic (DEP) force for the future development of a gas sensor. AZO films were deposited at room temperature wit RF power of 150 W. The gap size between each AZO electrode is between 2 and 6 µm. Assembly was optimized by controlling the DEP parameters such as the applied frequency, applied peak-to-peak voltage (V_{pp}), and processing time. The presence and arrangement of the GO flakes aligned between the AZO electrodes are characterized by atomic force microscope (AFM) (Figure 1). A Chemical reduction using Sodium Borohydride ($NaBH_4$) was used to restore the structure and properties of graphene and therefore, enhancing the conductivity of the device several orders of magnitude. In order to investigate the impact of the reduced GO (RGO) on the device properties, the current-voltage (I-V) characteristics of both GO and RGO-based devices are studied. Figure 2 shows I-V for GO and RGO-based devices fabricated on glass substrate under the DEP conditions of a Vpp of 20 V and at fixed 500 kHz for 1 min, for a gap size of 5.6 µm. It was found that the conductivity of the device raised dramatically demonstrating the effectiveness of reducing treatment. In addition, a stable electrical connection as time passed is observed.

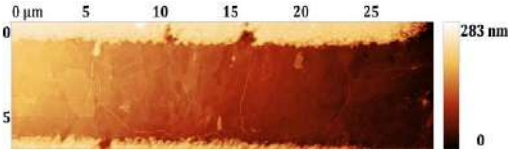

Figure 1. Tapping-mode AFM of rGO device assembled via DEP. At the edges of the photo, view of a pair of AZO electrodes with a gap smaller than 6 µm.

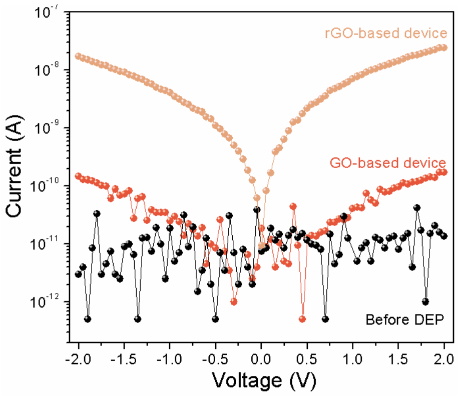

Figure 2. Current–voltage characteristics of GO and RGO devices on glass substrate at 500 kHz and 20 V.

Impedance biosensor interface based on nanostructured porous silicon

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Session: biointerfaces **type of contribution**: oral

Biosensing technology is a rapidly advancing field that benefits from the possibility to use the properties of functional advanced materials to analyse biological systems. Electrical biosensors, and in particular impedance biosensors, have potential for simple, rapid, label-free and low-cost detection of biomolecules [1]. On the other hand, among all the functional materials, porous silicon (PS) constitutes an ideal substrate for developing new chemistries owing to its biocompatibility, well-established fabrication methods and large adsorption surface, which allows an enhanced sensitivity [2].

In the present work, we use PS as a conductive and biocompatible platform in order to fabricate an impedance biosensor. The first step involves the formation of a conductive PS structure. For that, two parallel slots created by ion etching and filled with metal by sputtering are formed on the PS surface. The second step consists of the formation of a biorecognition interface. Indeed, after modification of the surface by a self-assembled monolayer to trigger its sensitivity and allow a molecular selectivity and a control of the biomolecular interactions, the surface of the functionalized material is biologically activated for the detection of specific genomic or proteomic species. Indeed, we perform a sandwich assay in which the biomarker is first recognized by a surface-anchored antibody and then by an antibody in solution that identifies a free region of the captured biomarker. This second antibody is tethered to a gold nanoparticle. Finally, the changes in the interfacial impedance upon analyte binding are detected. The gold nanoparticles act as a mass-electric label and allow increasing the impedance changes and consequently the sensitivity of the detection.

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Atomic and Molecular Layer Deposition of Hybrid Nanostructured Materials

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Session: Technological Session **type of contribution**: Oral presentation

Different from chemical vapour deposition (CVD) and physical vapour deposition (PVD), atomic layer deposition (ALD) is based on saturated surface reactions. In this case, the thin films are grown in a layer-by-layer fashion allowing sub-nanometer thickness control, low temperature depositions, good uniformity and superior step coverage on high specific surface area components compared to CVD and PVD.

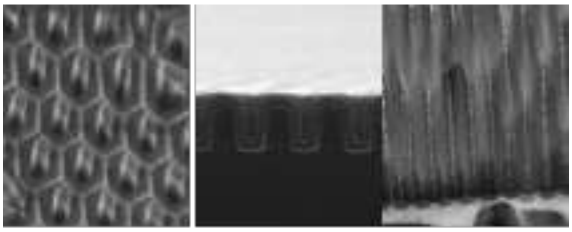
These advantages of ALD over other thin film deposition processes have been conventionally applied mainly in semiconductor electronic industry on the preparation of layers of outstanding High-K dielectric materials.

But, due to the advances in tool design and recipe development, the importance of ALD is rapidly expanding for producing innovative nanoscale materials.

ALD new applications are highly multidisciplinar. It has an emerging potential on photo-voltaic cells, flexible electronics, enhanced performance glass, paper and textiles, new generation transistors, sensors, and advanced energy materials technology. Innovations brought by nanotechnology to biosciences and biosensors are also proving to be good candidates to benefit from these potentialities and its surface functionalization possibilities.

Some of these advanced applications require the deposition of hybrid materials that could combine the beneficial aspects of both inorganic and organic phases.

Molecular layer deposition (MLD) methods extend the ALD strategy to include organic and hybrid organic–inorganic polymeric materials, so a combination of both techniques opens the door to the creating of highly at-tractive nanostructural frameworks.



Images courtesy of Mato Knez research group

Figure 1: Figure illustrating several structures that could be prepared by this technique, emphasising the high surface-area porous structures that could be deposited at low temperature, providing good uniformity and superior step coverage.

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The novel hemispherical energy analyser in the advance surface science research

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Session: surface science **type of contribution**: oral

The complexity and the range of materials and their surfaces studied will be expanded across a wide range of topics, including surface science, semiconductors research, catalysis, corrosion, photoelectrochemical energy conversion, battery technology, or energy-saving technologies [1-5]. An unique and exceedingly flexible analysis cluster with a detection system is needed for these fundamental and applied research. Here a new energy and angle resolved spectrometer for photoelectron spectroscopy will be presented. The analyser has a hemisphere shape with a mean radius of 150 mm and is based on combining an advanced focusing electron lens system, which can be operated in different modes, transmission, spatial resolution or angular resolution. An angular resolution of better than 0.1° and spatial resolution 50 μm can be obtained. The spectrometer includes highly stable 6 kV power supply, where each independent voltage module achieves temperature stability below 0.5 ppm of the voltage span per degrees Celsius. The modern 2-D low noise CCD-MCP assembly with a noise level of < 0.01 cps/channel and a 90 fps fast camera are used. Fully automation and environmental software system make it a user-friendly tool for the conducted researches. The combination of the new generation hemispherical energy analyser with a modular PREVAC surface analysis system as part of multi-technique surface analysis systems will be presented, in order to permit complete characterization of the surface structure via XPS, UPS, ISS and APRES mapping. We will report on the results of the metallic semiconductors, and topological insulator, photovoltaic materials, graphene, or self-assembled organic monolayers of organic molecules. studied by means of ARPES and XPS techniques, using analyser and induced by UV/X sources. This analyser opens up new possibilities for angular/spatial resolved electron spectroscopy, band-mapping and other applications.

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A Short Review of Outgassing

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ABSTRACT

There are several contributions to the gas load of a system of which often the most important is outgassing. Adsorption occurs via two main processes; physi-sorption and chemi-sorption, and can be described using five classifying isotherms. Outgassing is the result of desorption of previously adsorbed molecules, but also bulk diffusion, permeation and vapourisation. Analysing the desorption rate, pumping speed and re-adsorption will give the net outgassing of the system. There is significant variation in outgassing rates between *different* materials but also between published rates for the *same* materials, in part due to the number of different methods used to measure outgassing. This subject is historically dense and this paper aims to review the outgassing process, rates, measurement techniques and methods that can be used to mitigate or reduce the outgassing of a system.

*This talk will be based on that first presented at OLAV-V workshop, Hamburg, May 2017

POSTER SESSION

(Wednesday & Thursday)

Poster list

1. Abad, J. *Surface self-assembly of heteroacenestructures driven by hydrogen bonding*
2. Sanchez-Sanchez, C. *H-induced etching of the rutile TiO2 (110)-(1x1) surface*
3. Schiller, F. *Electronic and magnetic properties of metal phtalocyanine molecules on monolayer thick magnetic rare-earth noble-metal substrates*
4. Schiller, F. *Spatial variation of the active phases during the catalytic oxidation of CO measured on a curved Pd(111) surface*
5. Azpeitia, J. *New method to synthesize graphene by using C60 as carbon source*
6. Costa, J. *Advanced processes for coated plungers used on glass industry*
7. Ribeiro, J. *TiO2:Nb Thermoelectric Thin Films for Touch Displays*
8. Merino-Diez, N. *Electronic structure characterization of atomically-precise chiral graphene nanoribbons on gold surfaces*
9. Bueno, R.A. *Controlled covalent organic functionalization of epitaxial graphene*
10. Ramadan, R. *Realization of Titanium- doped Zinc oxide planar and photolithographed structures treated by MW plasma for biomedical applications*
11. Monteiro, R. *New concepts and materials for glass containers moulds, to increase production efficiency*
12. García, S. *Functional coatings of nanoparticles applying atomic layer deposition in a fluidized bed reactor*
13. Esteban, D. *Ultraflat hexagonal boron nitride films with hexagonal and amorphous surface termination*
14. Santos Louro, C. *Are W-based coatings a surface alternative to the adverse Ni release in orthodontic applications?*
15. Conde Garrido, J.M. *AgGeSe thin films deposited by PLD under vacuum conditions*
16. Conde Garrido, J.M. *Low cost cold trap for vacuum systems. Design and fabrication*
17. da Silva Oliveira, C.I. *Thermal properties and oxidation resistance of Zr-O-N(:Ti) coatings deposited by magnetron sputtering*
18. da Silva Oliveira, C.I. *Decorative Zr-O-N coatings deposited by magnetron sputtering: strategies to avoid the chemical and color confinement*
19. Dominguez-Meister, S. *Comparative tribological behaviour of MoS2 and WSe2 –based nanocomposite coatings*
20. Alcalá, G. *Atomic transport of sputtered species in a plasma and nanostructural development of SiO2 thin films grown by magnetron sputtering*
21. Gonzalez-Elipe, A.R. *Propagation of the microstructure during magnetron sputtering deposition of multilayer thin films*
22. Santoro, G. *The STARDUST machine: an UHV station for simulating cosmic dust formation and processing*
23.
24.
25. Herrero, V.J. *Structure and energetic processing of interstellar hydrocarbon dust analogs formed by plasma deposition*
26. Albella, J.M. *Optical and structural properties of ZnO:Ti thin films grown by reactive magnetron co-sputtering*
27. Sobrado, J.M. *Liquids in vacuum. Coexistence and emergence*
28. Olano, L. *Secondary emission yield in rough dielectric surfaces*
29. Fernandez, L. *Growth and vibrational properties of ultra-thin TiOPc films on Ag(111)*
30. Niño, M.A. *Surface reactivity of iron monosulfide (FeS) films*
31. Manso Silvan, M. *Multiscale patterning of cell guides and traps through fs laser writing*

32. Manso Silvan, M. *Sol-gel tailoring of surface chemistry towards controlled adsorption of icosahedral P22 virus capsids*
33. Salvador, P. *ZnO:Al,Bi thin film electrodes for perovskite solar cells*
34. Sanchez Lopez, J.C. *Oxidation resistance of CrAlYN protective hard coatings for high temperature applications: Influence of Al and Y content*
35. Torres-Costa, V. *Laser carbonization of porous silicon for locally tuning the surface wettability*
36. Fernandez-Martinez, I. *The industrialization of HIPIMS: High Power Impulse Magnetron Sputtering*
37. Zubizarreta, C. *The influence of target erosion grade in the optoelectronic properties of AZO coatings growth by magnetron sputtering*
38. Fonseca, A.L. *Pressure evolution inside cork cells*
39. Martínez, L. *High-quality, one-step production of Au@TiO2 nanoparticles by gas-phase synthesis*
40. Merino, P. *Real-Space Atomic-Scale Imaging Circumstellar Carbon Cluster Analogues*
41. dos Santos, M.P. *Optimization of dye-sensitized TiO2 nanorod solar cells*
42. Palacio, I. *Chemistry Below Graphene: Decoupling Graphene From Metals By Electrochemical Oxidation*
43. Sanchez-Lopez, J.C. *On the reactive element effect of yttrium in the oxidation behavior of multilayered CrAlYN coatings*
44. Garcia, J.M. *Carbon evaporator for Molecular Beam Epitaxy graphene growth*
45. Azpitarte, I. *Improving the thermal and UV stability of Kevlar through Atomic Layer Deposition*
46. Yubero, J. *Energy-Sensitive Ion-and Cathode-Luminescent Radiation-BeamMonitors Based on Multilayer Thin-Film Design*
47. Sik, O. *Low Energy Ion Scattering as a Depth Profiling Tool for Thin Layers*
48. Palomares, F.J. *Ordered arrays of Si-based nanocrystal pyramids achieved by electron-beam lithography and MBE growth on Si(001)*
49. Janke, D. *In situ RBS and Raman study of nickel-catalyzed amorphous carbon graphitization*
50. Krause, M. *Central receiver coatings for high-temperature concentrated solar power studied in situ by RBS, Raman spectroscopy and spectroscopic ellipsometry*

Surface self-assembly of heteroacene structures driven by hydrogen bonding

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Session: Surface Science **type of contribution**: Poster

The development of organic semiconductor materials represents a growing area of research, with many applications in the manufacture of electronic devices (OLEDs, OFETs, Organic Solar Cells, etc.) based on the use of organic materials [1]. The advantages of the organic materials lies in its great potential for very cost effective production of large area devices (solar cells and large displays) as well as the very flexible manufacture of low cost electronics (so called ''printed electronics'').

An extended π-conjugated system and close intermolecular stacking are generally considered to be a prerequisite for good charge transport and, consequently, a good performance in organic devices. Nevertheless, the weak non-covalent interactions that govern the solid state packing of organic molecules result in inherently disordered materials. Since charge transport is conditioned by the arrangement of molecules, highly organised materials can contribute to enhance the performance of organic semiconductors. To achieve this issue strong intermolecular interactions via hydrogen bonds would promote better crystalline ordering and π-stacking. In addition, another important factor to be taken into account is the 2D-chirality or "surface chirality" of some small molecules when they are deposited on a surface. Therefore the self-assembly of the molecules can be affected by two competing effects: the hydrogen bonding interaction and the "surface chirality" of the adsorbed molecules.

In this work, derived from preliminary results that showed the semiconducting properties of indolocarbazole [2,3] and carbazolocarbazol [4] type structures, we have introduced a slight structural modification that, based on the properties of the unit 7-azaindole to establish intermolecular interactions by hydrogen bonds. This could favour the self-assembly of molecules promoting greater ordering of the solid structure. Preliminary Auger electron spectroscopy (AES) and low energy electron diffraction (LEED) results show ordered structures at low molecule coverage and room temperature on Au substrates. Therefore, we use scanning tunnel microscopy (STM) to confirm the ability of this new series of compounds to self-assemble on different surfaces (HOPG, Si, Au).

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H-induced etching of the rutile TiO2 (110)-(1x1) surface

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Session: surface science **type of contribution**: poster

Titanium dioxide is an important catalytic substrate commonly employed in heterogeneous catalysis and photocatalysis [1]. The highly oxidative character of the bridging oxygen vacancies is known to induce hydrolysis, i.e., the dissociation of water into hydroxyl radicals and hydrogen. It can also photocatalytically oxidize NO or NO_2. However, its interaction with molecular hydrogen is weak, leading to no molecular adsorption at room temperature. On the other hand, atomic H can strongly adsorb on bridging oxygen atoms, remaining even at temperatures as high as 730 °C [2]. Additionally, there are evidences of TiO2 reduction when annealed in a molecular hydrogen atmosphere. However, so far, little is known about the interaction of atomic hydrogen and TiO_2 at elevated temperatures. Given the reductive character of hydrogen and the presence of oxygen in the substrate, a reduction of TiO_2 surface can be expected.

In this communication, we report on the study of the interaction of atomic hydrogen and rutile TiO_2 (110)-(1x1) surface. We observe a progressive etching of the surface upon annealing the substrate above 500K while exposed to atomic hydrogen. Effect of annealing temperature and H dose is studied by means of scanning tunneling microscopy (STM) and x-ray photoelectron spectroscopy (XPS). Experimental results are complemented with theoretical simulations, thus allowing us to propose a model for the H-induced etching of the rutile TiO_2 (110)-(1x1) surface.

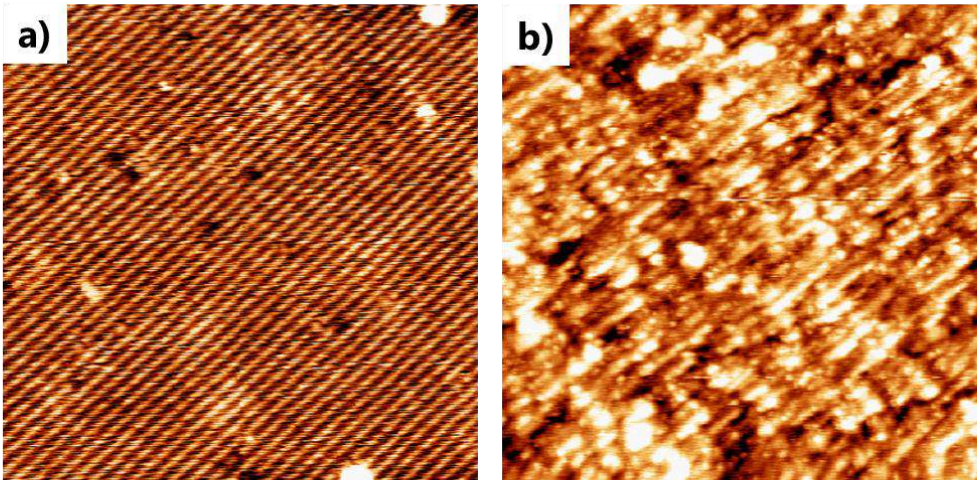

Figure.- STM images of the rutile TiO_2 (110)-(1x1) surface before (a) and after (b) exposure to H at elevated temperatures.

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Electronic and magnetic properties of metal phtalocyanine molecules on monolayer thick magnetic rare-earth noble-metal substrates

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Session: surface science **type of contribution**: poster

Fundamental research on new states of matter, e.g., on Majorana fermions [1] as well as many potential nanotechnology applications on spintronics [2] rely, to a great extent, on the ability to interface magnetic materials with superconductors, topological insulators, and organic or inorganic semiconductors. To this end, tailoring magnetic properties on structurally robust substrates is crucial. The survival of the long-range magnetic order upon interface formation is a basic requirement for one application type that intent to maintain the substrate magnetism and that is the reason why, besides structural stability and chemical inertness, substrate materials with strong ferromagnetism, i.e., high Curie temperatures T_C are sought. For the survival of the magnetism of single molecular magnets, however, strong substrate ferromagnetism supresses all the desired properties of the molecules and there, a different type of magnetic substrates is needed. Rare-earth/noble metal monolayer alloys, grown on noble metal surfaces, possess a big potential as nanostructured magnetic templates with structural stability. Different elements of the lanthanide series have been observed to form surface-confined alloys in Au(111) and Ag(111) [3], characterized by a high crystal quality and nanoscale periodic corrugation. In the case of the Gd-Au combination, by varying the Gd coverage, Moiré or trigon patterns can be tuned, which have been shown to drive the self-organized growth of ferromagnetic Co nanodot arrays. Notably, the Gd-Au templates remain structurally stable upon Co growth, allowing to trigger magnetic coupling of the Co nanodot array with the supporting Gd alloy [4].

Given the variety of REs and their exotic magnetism, the observations made on $GdAu_2$ encouraged a thorough search combining different RE elements and noble metals. In this sense, a remarkable high $T_c = 85$ K in $GdAg_2$ compared to $T_c = 19$ K in $GdAu_2$ was recently observed [3]. It was show by photoemission experiments and by Density Functional Theory that magnetic coupling is effectively mediated by a noble metal-Gd hybrid s,p-d band giving rise to such a strong increase in T_c. On the other hand, our results of the magnetic properties in $SmAu_2$ reveal completely different behaviour with respect to $GdAu_2$, namely zero magnetic moment in the hard axis, while maintaining a ferromagnetic loop along the in-plane easy axis with a much lower T_c compared to the $GdAu_2$.

Here we will present experimental evidence based on photoemission and X-ray magnetic dichroism experiments that magnetic properties of the substrate and the magnetic molecules are influenced by each other depending on the strength of the magnetic moment of each contributor.

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New method to synthesize graphene by using C60 as carbon source

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Session: Surface Science **type of contribution**: poster

The synthesis of large area high-quality graphene has been one of the main interests of the scientific community after the discovery of this exceptional material. Many different experimental protocols have been followed with the aim of achieving a controlled, scalable and low-cost production of this carbon allotrope [1]. To date, most of the works have been focussed on growing graphene from hydrocarbon gaseous or liquid precursors. In this work, we describe a new protocol to grow high-quality graphene by physical vapour deposition (PVD) using C60 molecules evaporated in ultra high vacuum conditions (UHV) on Cu foils substrates. The use of low carbon solubility Cu substrates is really appealing for graphene growth due to its inexpensiveness and the possibility of post-growth graphene transfer on arbitrary substrates [2].

The quality of the resulting graphene layer has been assessed by the combination of complementary surface characterization techniques After growth, in-situ LEED images exhibit a polycrystalline graphene pattern. Ex-situ AFM and Raman spectroscopy (Figure) were used to determine the quality of the graphene layer. XPS experiments showed the C1s XPS core level signature of high quality graphene layers. ARPES measurements unveil the linear behaviour of electrons near Dirac point and show a clear n-doping of 0.7 eV consequence of the interaction between graphene and substrate. Finally, DFT calculations allow to understand the mechanisms that determine this interaction. This work reveals that the use of C60 as precursor molecules is an alternative route for growing high-quality large area graphene layers on Cu foil substrates [3]. The advantages of this PVD method lie in the use of a lower synthesis temperature as compared to that of conventional CVD methods, a low amount of oxygen-containing species in the surface due to the clean UHV environment and the formation of single graphene layer due to the singularity of being a self-limiting process.

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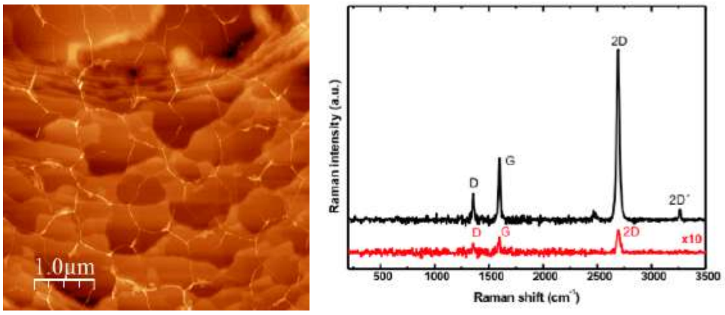

Figure. Left: AFM topographic image of graphene on Cu foil. Right: Raman spectra of as-grown graphene (red spectrum) and aged graphene (black spectrum) on Cu foil.

Advanced processes for coated plungers used on glass industry

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Session: hard-coatings workshop **type of contribution**: Poster

One of the main problems in the glass industry is the fast wear and degradation of the surface of molding tools used in the glass manufacturing processwhich, in direct contact with the melted glass, are subjected to severe conditions of abrasion, corrosion and fatigue at high temperatures. The wear occurring in these components (plungers, molds, mouthpieces, etc.) has led, in the last years, to efforts to develop surface engineering solutions to overcome this problem. Having not yet reached the desired success, these solutions would allow reducing the wear, the cracking problems and increase the lifetime of the tools, thus, making the whole process more efficient, by reducing the number of rejected parts and the maintenance time/costs, as well as bydecreasing the production cycle duration and improving the process efficiency from the energetic perspective.

This study is focused on the development of surface engineering solutions based on sputtering technology – PVD, for the deposition of thin films with good mechanical properties at high temperature, whichcould support the harsh conditions of use and increased durability relative to the state-of-the-art solutions. Nitride-based hard coatings have proved their capability to increase tool lifetime when exposed to abrasiveand corrosive environments at high temperature.

Within the frame of this work, two types of hard coatings were studied: Cr-Al-Ti-Si-N and Ti-Al-C-N, produced by DC magnetron sputtering. Both coatings wereused to protect the surface of the plungers and were subject to industrial tests in a glass company. Firstly, the plungers were only tested for 20 minutes for initial quality assessment, After the first stage, they entered the machine for a normal production cycle until the end of the tool lifetime.The evaluation was performed in the *Hot Zone* during IS Machine production through the Analysis of Thermal Distribution, Cooling of the Plunger and Section Efficiency and in the *Cold Zone* after production in IS Machine through a set of tests (Internal Pressure Test, Vertical Load Testing, Destructive Impact, Dimensional Analysis).

The coated plungers presented failures with occurrence of coating loss at the end. It has, however, been found that Ti-Al-C-N coating have made it possible to reduce the cooling cycle which is normally used to cool the plungers, reducing at the same time the energy consumption of the process. This may allow the process of bottles production to become more efficient, thus achieving two main objectives, reducing the cost of production and increasing the energy efficiency due to carbon footprint reduction.

$TiO2:Nb$ Thermoelectric Thin Films for Touch Displays

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Session: Applied surface science **type of contribution**: Poster

Nanoporous thin films have recently been widely studied for applications in thermoelectrics, as materials are able to convert thermal differences into electrical energy and vice-versa. The interesting structural, optical, electronic and photocatalytic properties of TiO_2 have been extensively documented in the literature. More recently, it was referred that a cationic doping of the films can improve their electrical conductivity properties [1]–[4]. In this work, thin films are developed for a specific application: touch displays. For this purpose, and in order to enhance the thermoelectric figure of merit, the films must not only be optically transparent to visible light, but also possess a high Seebeck coefficient, high electrical conductivity and low thermal conductivity. This is difficult to obtain, as it requires very specific deposition conditions. Magnetron sputtering has become a preferred method for the deposition of thin films due to its good reproducible surface morphology, good film adhesion onto the substrate and long-term stability [1], [5]. In this work it is reported the production of several TiO_2:Nb (Titanium Dioxide doped with Niobium) thin films (~100 nm), deposited on glass and Si substrates by magnetron sputtering in vacuum. This is achieved by adjusting the deposition parameters such as gas flux (reactive and work), pressure, temperature and target current density. The effect of these parameters on the development of these thin films is correlated with the optical properties, morphology, structure, composition, electric, thermal and thermoelectric properties.

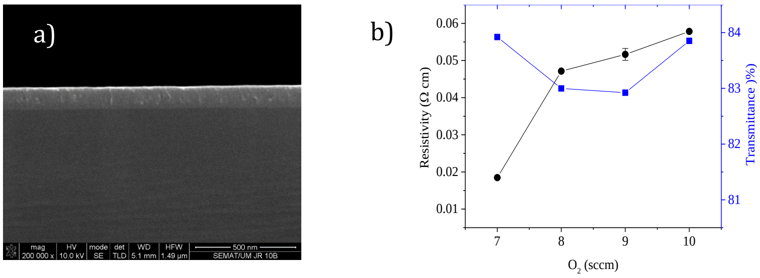

Figure 1 – a) SEM image of a TiO_2:Nb thin film; **b)** Comparison of electric resistivity with optical transmittance of the films as a function of the reactive gas O_2 (sccm) during film deposition.

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Electronic structure characterization of atomically-precise chiral graphene nanoribbons on gold surfaces.

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Session: nanometer structures **type of contribution**: poster

Graphene nanoribbons (GNRs) are narrow 2D stripes of graphene that have attracted great attention because of their interest for both fundamental physics and promising applications. While sharing many of the appealing properties of their predecessor material i.e. graphene, such as high mobility charge-carriers and high specific surface area, they overcome some of its limitations as is the lack of a band gap. These nanostructures can display different edge orientations with respect to graphene´s lattice vectors that largely determine their main properties. Therefore three types of ribbons can be synthesized: armchair (aGNRs) zigzag (zGNRs) or chiral (cGNRs) graphene nanoribbons, the latter ones presenting a periodic combination of both armchair- and zigzag-like segments. However, the limited experimental results on these structures are mostly focused on the electronic structure of armchair and, to a lesser extent, on zigzag GNRs, thus letting chiral GNRs hardly explored. The growth of these ribbons on different noble metals was recently reported [2], hence we focus on the electronic structure of these nanomaterials.

Here, we access to the electronic structure of (3,1)-cGNRs on Au(111) by (Fourier Transformed-) Scanning Tunneling Spectroscopy. Moreover, the use of Au(322) vicinal substrate as template promotes the aligned growth of these ribbons along the terrace length thus enabling us to characterize the valence band by means of angle-resolved photoemission spectroscopy (ARPES). Our results reveal a semiconducting bandgap on these chiral nanoribbons therefore confirming its potential applications for future nanoelectronics devices.

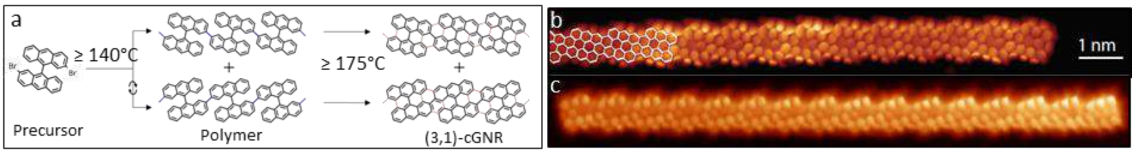

Figure 1. (a) Synthetic scheme and **(b,c)** CO-functionalized-tip images of (3,1)-cGNRs.

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Controlled covalent organic functionalization of epitaxial graphene

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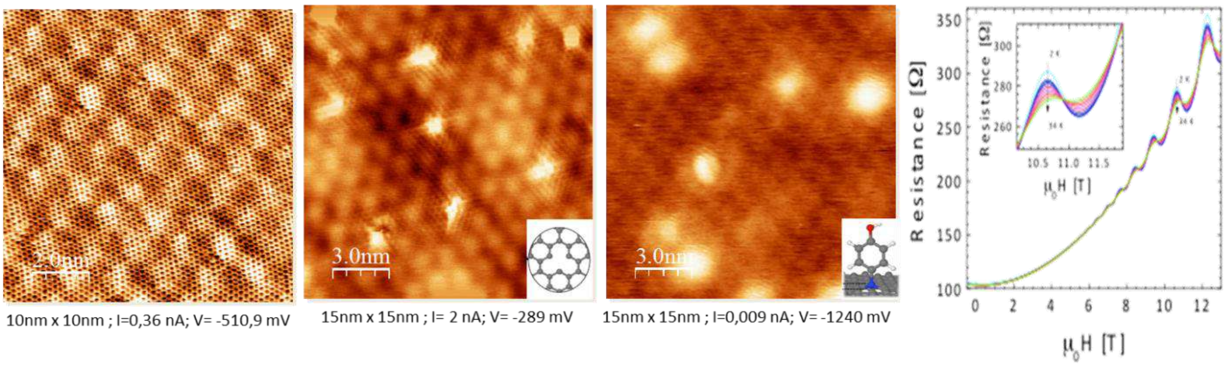
Session: electronic materials and processing **type of contribution**: Poster

Due to the high chemical inertness of graphene makes fundamental the development of controlled and selective covalent functionalization for the development of graphene-based materials with tailored electronic properties.
Most of the works performed up to the date report electrostatic molecular adsorption or unruly functionalization. We show hereafter an unprecedented reported mechanism for promoting highly specific covalent bonding of any amino-terminated molecule and a description of the operating processes. We show, by different experimental techniques and theoretical methods, that the excess of charge at carbon dangling-bonds formed on single-atomic vacancies at the graphene surface induces enhanced reactivity towards a selective oxidation of the amino group and subsequent integration of the nitrogen within the graphene network.
Remarkably, functionalized surfaces retain the electronic properties of pristine graphene. This study opens the door for development of graphene-based interfaces, as nano-bio-hybrid composites, fabrication of dielectrics, plasmonics or spintronics.



10nm x 10nm ; I=0,36 nA; V= -510,9 mV

15nm x 15nm ; I= 2 nA; V= -289 mV

15nm x 15nm ; I=0,009 nA; V= -1240 mV

Fig. 1. Atomic resolved STM images of the different steps in the functionalization process. The functionalized graphene surface does not degrade its electrical properties and Shubnikov-de Haas oscillations are seen after molecular functionalization.

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Realization of Titanium- doped Zinc oxide planar and photolithographed structures treated by MW plasma for biomedical applications

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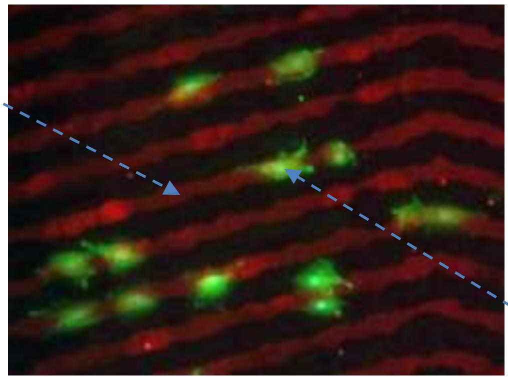
Session: Biointerfaces **type of contribution**: Poster

ZnO is an outstanding optoelectronic material with attractive composition for biomedical applications. However, the ionic character of this compound prevents its use, due to intrinsic solubility in alkaline buffers and body fluids. This compromises the lifetime and stability of ZnO devices oriented towards biomolecular detection and induces Zn^{2+} toxicity in cellular systems. This study proposes the modification of ZnO thin films with different Ti concentrations by combining wet chemical synthesis with physical activation processes. ZnO sol was prepared from zinc acetate in ethanol after stabilization under reflux in presence of ethanolamine. Different Ti concentrations were incorporated from a titanium isopropoxide solution in ethanol. This sol was spin casted on Si substrates to induce the xerogel transition. We propose a comparative study of the properties of xerogel films condensed by alternative MW plasma and thermal annealing. From the point of view of surface finishing, we show that Ar plasma annealed samples present considerably smaller roughness than thermally annealed samples. However, its microstructure consists of short range ordered nanocrystals as supported by vibrational spectroscopies, with a thermal annealing equivalent of circa 300ºC. However, hydrophilic character as indicated from water contact angle, optical indices (as studied by ellipsometry) and electrical characteristics, as derived from impedance spectroscopy, denote particular advantages for the MW plasma annealed samples. Pointing to their application in cell adhesion studies, their biocompatibility was assayed by culturing mesenchymal stem cells on planar and photolitographed structures (see image below). In overall, the Ti doped samples show more confluent adhesion than un-doped ZnO, allow preparing transparent electrodes and can be processed on polymer structures, which supports the added value of Ti doping and processing route towards particular biomedical applications.



Ti:ZnO Micropatternes

Mesenchymal Stem Cells

New concepts and materials for glass containers moulds, to increase production efficiency

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Session: Hard-coatings workshop **type of contribution**: Poster

In order to attain market needs in glass industry and to be able to produce glass containers at competitive prices, high manufacturing rates at competitive costs are required. As a consequence, moulds are being submitted to shorter and shorter thermal cycles leading to higher mechanical stresses and, in some cases, to plastic deformation. Therefore, fatigue, oxidation, corrosion, cracking, wear and demoulding problems are often occurring, inducing premature failure and accelerated wear of the moulds during service. Furthermore, these problems are responsible for the instability of the production process, the compromised quality of the manufactured parts and the increase of the maintenance costs. In order to prevent the premature occurrence of such problems, moulds have been: (i) manufactured with high thermal conductivity materials, further improved by channels and fins cooled by compressed air; (ii) coated with high temperature thermal and mechanical resistant materials and, (iii) lubricated (with liquid lubricants) to allow the easy demoulding operation. Although successful improvements have been achieved in the lifetime and production rates of the moulds, the above described problems are constantly updated due to either the increasing mechanical loading, to which moulds and coatings are submitted, or the use of liquid lubricants inducing moulding corrosion and leading to a deficient demoulding and defective parts with incorporated debris.

Thus, the project addresses the selection and development of a new range of materials which will allow to overcome moulds problems in glass industry, promoted by either harsh service conditions and liquid lubricants use. The objectives are focused on the simultaneous increase of the lifetime and production rates, as well as on the decrease of the maintenance and operation costs. Three research lines were defined to accomplish these objectives:

(i) replacement of the high thermal conductivity alloys, presently used in moulds manufacturing, by state of the art ones with better mechanical and thermal properties;

(ii) a new mould concept based on bulk materials with better mechanical and thermal properties, associating self-lubrication, will be developed. The purpose is to develop composite materials, to be applied as a shell on the mould body, manufactured with the alloys studied in the previous research line;

(iii) the third line of research is focused on the application of a new class of hard coatings with high temperature self-lubricant properties, sputter deposited onto the surfaces of the moulds manufactured with the alloys previously developed.

The first solution is to have outputs in the short term whereas the other two show a radical innovation change which can contribute to significantly improve the performance of the industrial partners, not only at short but at medium and long terms. The industrial success of the application of these materials allows forecasting important productivity and agility gains which are fundamental for the improvement of the companies' international competitiveness, either on the production of glass containers and on the manufacturing of moulds for the glass industry.

Functional coatings of nanoparticles applying atomic layer deposition in a fluidized bed reactor

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Session: Surface engineering **Type of contribution**: Poster

Coating technologies are important for adding or improving functionalities of diverse materials. The use of atomic layer deposition (ALD) as a deposition technology allows generating very precise and homogeneous coatings on top of various substrates. Nanoparticles (e.g. TiO_2, ZnO, MgO, Al_2O_3 and Fe_2O_3) are playing an increasingly important role for numerous applications, but their chemical and physical properties often still need to be improved or stabilized. ALD has proven to be a viable option to apply conformal, pinhole-free films with Ångstrom-level control to the surfaces of ultrafine primary particles [1]. Such films will increase the stability and durability and will add value to the functionalities of nanoparticles without seriously altering their weight or size. However, a coating of particles in a traditional chamber type reactor without agitation or mobility of the particles will induce non-conformality of the coatings wherever the particles are in touch with each other. To overcome such issues, the use of a fluidized bed reactor (FBR) was proposed. A fluidization of the particles allows creating a dynamic environment with the particles being in steady motion, while a parallel coating process enables a conformal coating of those. The objective of this research is to design a fluidized bed reactor in which variety of parameters can be optimized for obtaining functional coatings of nanoparticles for an anticipated use in energy storage applications. Figure 1 shows the setup of a fluidized bed reactor. Nitrogen is used as an inert carrier gas, which facilitates the fluidization of the bed as well as the transport and purging of precursors to and from the reactor column [2]. After the coating process, nanoparticles are characterized using various techniques including, X-Ray diffraction (XRD), Environmental Scanning-Electron Microscopy (E-SEM), Energy Dispersive X-Ray analysis (EDX) and the analysis of the specific surface area.

Figure 1. The fluidized bed reactor (FBR) configuration for coating nanoparticles using ALD.

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Ultraflat hexagonal boron nitride films with hexagonal and amorphous surface termination

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Session: Applied Surface Science **type of contribution**: indiferent

Hexagonal boron nitride (h-BN) is the preferred substrate for graphene growth, because of the similar structure and its electrical insulating behavior. However, h-BN grown in thin film form by CVD and PVD methods shows a surface roughness much larger than expected for a 2 dimensional material, which deteriorates the quality of graphene layers grown on top, as monitored through the electron mobility in the graphene layer. The roughness of the h-BN film seems to be related to the clash and lift at grain boundaries formed by the coalescence of the original h-BN nuclei.

In this work, a series of h-BN films with different thickness, texture, grain size and defect ratio were grown by Ion Beam Assisted Deposition (IBAD), by boron evaporation concurrent to the bombardment with nitrogen ions, using different ion energies and growth temperatures. In this way, we can control the order of the surface layer in the film.

As a general trend, the films with an amorphous surface layer are extremely flat, with an rms roughness of about 0.1 nm. On the other hand, the films with hexagonal order at the surface show a larger roughness of the order of 1-10 nm.

A discussion of the surface roughness compared to h-BN growth parameters and details of film characteristics will be presented, together with a description of the development of the surface roughness with the film thickness.

Are W-based coatings a surface alternative to the adverse Ni release in orthodontic applications?

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Session: Applied Surface Science or Biointerfaces **type of contribution**: poster

Abstract:

It is well recognized that bio metallic alloys (BMA´s), mainly stainless steels, Co and Ti alloys, regarding the suitable mechanical properties, the biocompatibility and the spontaneously passivation, release metal ions into tissues, blood and others biological solutions with imminent risks of irreversible effects on human health.

Special attention should be given to those classified as inactive ions, such as Ni and Cu ions, which once formed do not immediately interact with water molecules and/or inorganic anions. This subsistence increases the probability to react with biomolecules, revealing metal toxicity. Moreover, since 1990, that Ni is classified as carcinogenic to humans, according to the International Agency for Research on Cancer (IARC) [1].

Tungsten, as a surface material, shows important prospective for biomedical applications, owing to its excellent biocompatibility, high mechanical strength and hardness as well as high adhesion to metal substrates. In addition, the formation of metal tungstates proceeds according to: WO_4^{2-} (aq) + M^{2+} (aq) → MWO_4(s), where M denotes bivalent ions as Fe^{2+}, Co^{2+}, Mg^{2+}, Mn^{2+}, Cr^{2+}, Ca^{2+}, Zn^{2+}, Cu^{2+} and also Ni^{2+}.

Previous research work [2] showed that in dry aggressive environments it is possible to obtain an external passive layer of $NiWO_4$ spinel-type phase if metallic alloys were previously functionalized by hard W-based coatings. Based on those results for mechanical application, it is now important to make bridges for biomedical applications.

Selecting the oral cavity, which is an adverse aqueous environment, where different factors as pH, salivary conditions, enzymatic and microbiological activity and mechanical loads are present simultaneously, at this time, a full answer can´t yet be given. Although the results of W and W-N films, with thickness of 1 to 6μm, produced by DC magnetron sputtering on austenitic stainless steel (AISI 316L) incubated at 37ºC during 30 days into artificial saliva will be presented. The quantitative Ni^{2+} data, acquired by X-Ray Fluorescence Spectrometry (XRF) will be discussed as a function of the coatings characteristics, such as chemical composition, surface morphology and topography, structural properties and microstructure.

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AgGeSe thin films deposited by PLD under vacuum conditions

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Session: Thin films **type of contribution**: Poster

Pulsed laser deposition (PLD) is a technique for fabricating thin films that, because of its simplicity, offers great experimental versatility. It allows the stequiometric transfer of mass from the target to the substrate and the physical properties of the films are, in many cases, superior to those obtained by other techniques.

The main limit for the application of PLD in micro/nano-devices is the presence of particulate at the surface of -and sometimes even inside- the films.

In this work, we deposited thin films by PLD under vacuum conditions of the AgGeSe system on Si wafers. We tested various deposition parameters (including deposition time, target-substrate distance, and fluence) and studied the films through SEM. We present the dependence of the number of particulates and their sizes on the deposition parameters.

We examined the targets after ablation and found that the largest particulates originate from the tips of the cones that form at the target's surface during the ablation.

Low cost cold trap for vacuum systems. Design and fabrication.

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Session: Vacuum Science and Technology **type of contribution**: Poster

In many high vacuum applications, the ongoing process generates gasses that need to be continuously evacuated. This is the case, for example, of thin films deposited by pulsed laser deposition in vacuum.

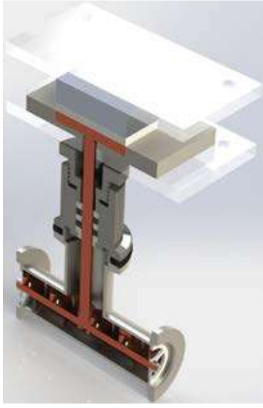
During the continuous pumping, these gases -sometimes hazardous- contaminate the interior surfaces (and liquids) of the vacuum pipes and pumps. This situation imposes a frequent maintenance schedule.

To minimize this, cold traps are used. A cold trap is simply a cold piece of surface that is placed in the way of the particles as they travel down the vacuum pipes. Particles are continuously hitting the surfaces of the pipes and being reemitted from them. However, when they hit a very cold surface, the low thermal energy they are left with is not enough to overcome the binding force and they remain “stuck” to the surface.

Traditional cold traps are, basically, hollow buckets filled with liquid nitrogen. They cost over 1,000 US dollars and require a supply of liquid nitrogen.

In this work, we have designed and fabricated a cold trap that is much cheaper and does not require liquid nitrogen since the cooling is done by means of a thermoelectric cooler (TEC, a.k.a: peltier module). On the downside, this cold trap does not provide temperatures as cold as liquid nitrogen, so it is not as efficient as the traditional cold trap.

The cold trap consists of a TEC that is placed on the atmosphere side. The heat is dissipated by a water block with water continuously circulating at ambient temperature. The cold side of the TEC is connected to a copper block with a copper rod in the middle. This rod enters the vacuum system with two o’rings pressing against the rod and the walls of a custom-made vacuum connector (made out of stainless steel). The rod is screwed into the middle of another copper rod. Along this second rod, a copper foil is soldered with the form of a helix. This design, forces the gases flowing down the vacuum pipes to circle along the helix, and thus providing a very low conductance and a very large surface of interaction kept at low temperatures.



Thermal properties and oxidation resistance of Zr-O-N(:Ti) coatings deposited by magnetron sputtering:

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Session: thin films **type of contribution**: Poster

Transition metal oxynitrides are very interesting technological materials due to the possibility of easily tuning among metallic, nitride and oxide behaviours. This modification of the bonding allows to obtain a wide range of materials with different properties within the same system, e.g. conductors, semiconductors or isolators. Other properties (e.g. optical, thermal) can be tuned in the same way.

In this work, zirconium oxynitride coatings with different composition have been prepared by DC reactive magnetron sputtering of a Zr target in a controlled mixture of N_2 and O_2. Samples with different characteristics have been obtained, such as Zr-rich (metallic grey), nitride (golden), oxynitride (semi-transparent) and oxide (transparent). The inclusion of Ti was carried out by partial coverage of the target racetrack with a Ti ribbon.

The thermal stability and oxidation resistance of the films has been evaluated through 'in situ' and 'ex situ' X-ray diffraction under different heating atmospheres (vacuum, He, and a mixture of H_2/He) up to 1000ºC. The measurement of thermal diffusivity of the films was performed using Modulated IR Radiometry, and the results have been analysed with the so-called Extremum method [1]. Three different substrates (Si, glass and steel), and four different deposition times (on the same deposition batch) were used for three selected films with different characteristics. This approach constituted a 4x4x3 matrix that allows evaluating the impact of the three relevant parameters of such theoretical model, i.e. the thickness and thermal properties of the film and the substrate.

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Decorative Zr-O-N coatings deposited by magnetron sputtering: strategies to avoid the chemical and color confinement

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Session: thin films **type of contribution**: Oral

Zirconium oxynitride coatings are an interesting choice for aesthetic purposes, due to the combination of chemical stability, biocompatibility, good mechanical properties and a nice palette of achievable colors. Additionally, its preparation by reactive magnetron sputtering is relatively easy and simple. Nevertheless, a revision of the literature has shown that the chemical composition of the films lays in a significantly restricted area of the Zr-N-O ternary diagram. Such 'chemical confinement' is probably one the main reasons behind the limited palette of the observed colors.

In this contribution, the results from previous studies will be summarized in a comprehensive manner, in particular a critical evaluation of the detected Zr-N-O crystalline phases, and the above mentioned chemical and color confinement. Afterwards, various experimental strategies followed to avoid both restrictions (exploration of the parameter space, doping with different elements) will be presented. The chemical and phase composition and structure of the films are evaluated by EDX, RBS, XRD and SEM, respectively, and correlated with the synthesis conditions. Finally, the color of the coatings is measured by spectrophotometry and interpreted in terms of the characteristics of the films.

Comparative tribological behaviour of MoS_2 and WSe_2 – based nanocomposite coatings

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Session: Surface engineering or applied surface science **type of contribution**: Poster

Tribological coatings made of MoS_2 and WSe_2 phases and their corresponding combination with WC were prepared by non-reactive magnetron sputtering of individual targets of similar composition. A comparative tribological analysis of these multiphase coatings was done both in ambient air (30-40% RH) and dry nitrogen (RH<7%) environments using the same tribometer and testing conditions. A particular nanostructural study of the initial coatings by advanced transmission electron microscopy and examination post-test of the friction counterfaces by different analytical tools enabled to determine the tribological behavior for each type of environment. Rightful conclusions about the influence of coating microstructure and composition on the tribological response were inferred. The best performance obtained with a WSe_x film (specific wear rate 2×10^{-8} mm^3/Nm and friction coefficient 0.03-0.05) is compared with that of a well-established MoS2 lubricant material. In the WSe_x film, the architecture and chemical composition was tailored to satisfying load bearing capacity, mechanical support and lubricity provided by the combination of soft and lubricant phases both in dry and humid atmospheres. Such solid lubricant coatings with low friction either in ambient or inert atmospheres are thus very interesting for space applications whose components are exposed to different surrounding atmospheres from their preparation until reaching the orbit.

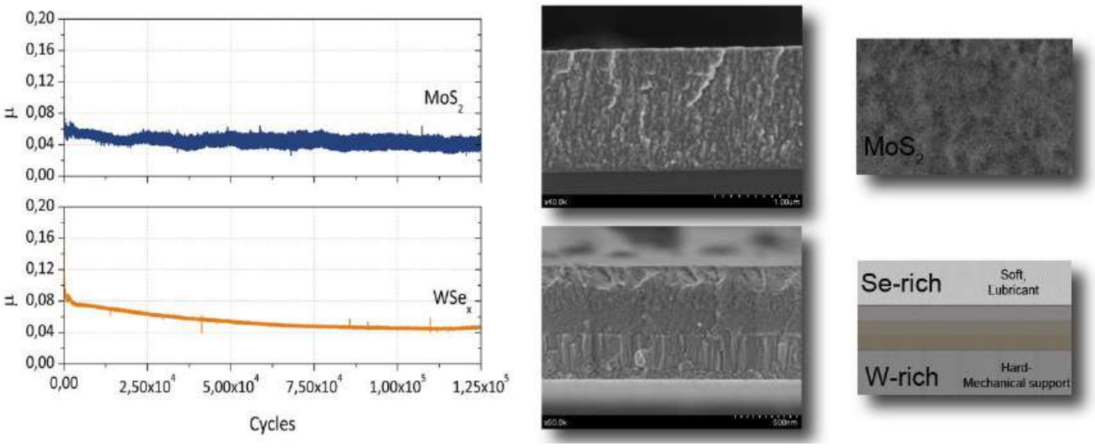

Figure 1 – Comparison of friction curves and film microstructures for MoS_2 and WSe_x films prepared by magnetron sputtering.

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Atomic transport of sputtered species in a plasma and nanostructural development of SiO_2 thin films grown by magnetron sputtering

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Session: Vacuum Science and Technology **type of contribution**: Poster

Abstract

Magnetron Sputtering is a well-known deposition technique employed to grow nanostructured thin films. Despite its wide acceptance in research centres and industry, there are numerous fundamental aspects still unclear, especially those concerning the determination and control of key fundamental processes that define the film nanostructure. In this poster we theoretically and experimentally analyse how the collisional transport of sputtered atoms in the gas/plasma affects their momentum distribution and their assembly on the film surface, giving rise to different nanostructures. From an experimental perspective, we have deposited several thin films with composition SiO_2 at different plasma pressures which, according to kinetic transport models, translate into different collisional transport of sputtered species in the plasma/gas. Given the good agreement between the nanostructures of the deposited films and those predicted by a well-tested thin film growth model [1], we have obtained the following conclusions: i) at low pressures, the atomic collisional transport is mainly ballistic, and promotes the growth of highly compact films, or with numerous well-defined tilted nanocolumnar patterns when operating at oblique angles, and ii) at high pressures, the amount of collisions in the plasma is high enough to thermalize sputtered atoms making their transport mainly diffusive. Under these conditions, films develop numerous coalescent vertical column-like porous structures.

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Propagation of the microstructure during magnetron sputtering deposition of multilayer thin films

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Session: Thin films **type of contribution**: Oral

In this work we analyze an undesired phenomenon that takes place when growing porous/compact multilayer systems by alternatively using the oblique angle and the classical configuration by magnetron sputtering. We show that compact layers develop numerous fissures rooted on the open porous structures of layer below, in a phenomenon that becomes amplified when increasing the number of stacked layers and that might cause the loss of structural control. We demonstrate that these fissures are caused by the formation and development of a discontinuous interfacial region between the porous and the compact layer. Based on these results, we propose a strategy to minimize this phenomenon by growing a thin and continuous accommodation layer on top of the porous film under the impingement of plasma ions, where the compact layer may subsequently grow homogeneously. This approach has been tested in practical situations by growing compact TiO_2/porous SiO_2 and porous SiO_x/porous SiO_2 multilayer systems intended for advanced photonic, optofluidic and near-IR mirror applications, from which preliminary results will be also presented. In these system a precise control over the microstructure and optical properties of the films has been achieved using the said accommodation layer strategy. Figure 1 shows SEM micrographs of two compact TiO_2/porous SiO_2 multilayers incorporating or not this accommodation layer. Clearly, the definition and sharpness of the interfaces, and hence the optical properties, is better with accommodation layer even though total porosity did not vary significantly from one preparation to the other.

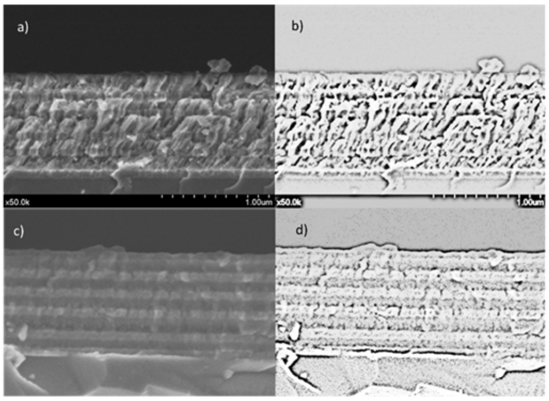

Figure 3.- a) Multilayer system made of porous SiO2/compact TiO2 layers grown under periodic deposition conditions. b) same as a) but after using a border detection and contrast enhancement software. c) Multilayer system made of porous SiO_2 + accommodation layer/compact TiO_2 layers grown under periodic deposition conditions, d) same as c) but after using a border detection and contrast enhancement software.

The STARDUST machine: an UHV station for simulating cosmic dust formation and processing

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Session: Vacuum Science and Technology **type of contribution**: Poster

Cosmic dust grains are believed to play an essential role in catalysing chemical reactions in the universe, thus promoting the formation of complex molecules in space. In addition, accretion of volatiles on dust grain surfaces leads to the formation of icy mantles, whose processing in the interstellar medium (ISM) also contributes to the large variety of molecular species found in the ISM. However, much remains unknown on cosmic dust formation in the atmosphere of Asymptotic Giant Branch stars (AGBs) and its processing during its way towards the ISM. In this sense, laboratory astrochemistry is of utmost importance so as to gain a deep knowledge on dust formation and processing, provided an accurate control of the processes is achieved, a requisite completely fulfilled by ultra-high-vacuum (UHV) technologies.

Here, we present the STARDUST machine, an UHV experimental station for simulating in the laboratory cosmic dust formation and its evolution towards the ISM. STARDUST consists of several UHV modules specially designed to mimic the conditions found in the atmosphere of AGBs. The first module is where the dust analogues are produced in a sputtering gas aggregation source, the so-called Multiple Ion Cluster Source (MICS), allowing for a precise fabrication of nanoparticles (NPs) of controlled size, stoichiometry and structure and providing a NP beam that travels through the rest of the machine. The MICS module is coupled to a diagnosis chamber in which NP beam monitoring and deposition can be performed. Afterwards, the Astrophysical Environment Simulation (AES) module imparts to the dust analogues similar physical conditions than those encountered in the atmosphere of AGBs. The AES module is comprised of a UHV chamber in which the NPs can be heated in flight by means of infrared radiation (Oven chamber) and a second UHV chamber in which the dust analogues are accelerated using electrical fields (Extraction chamber). The next module is the INFRA-ICE module in which the chemical composition of the dust analogues and/or the composition and conformational structure of the molecules produced during analogue processing can be analysed by near- and mid-infrared (NIR and MIR) spectroscopy. In addition, preparation and processing of ice analogues of astronomical interest can be performed. Finally, the ANA module serves as an analysis station in which electron spectroscopies and thermal programmed desorption (TPD) are performed both on the as prepared dust analogues and during its processing by thermal treatment, electron and ion bombardment, UV irradiation and atomic hydrogen and gas exposure. Additionally, gas mixtures can be introduced at different parts of the machine so as to promote in flight gas-dust interactions.

In summary, the STARDUST machine constitutes a unique platform for investigating cosmic dust formation and growth within the atmosphere of AGBs as well as for the study of the processes to which the dust is subjected during its fifty years journey to the ISM.

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Structure and energetic processing of interstellar hydrocarbon dust analogs formed by plasma deposition

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Session: Plasma science **type of contribution**: poster

Astronomical observations have revealed the presence of a ubiquitous absroption band at 3.4 µm in the diffuse interstellar (IS) medium. It is generally assumed that this band corresponds to some sort of amorphous hydrogenated carbon (a-C:H), whose structure has been explained by two alternative models: small aromatic islands linked by aliphatic chains [1] or large polyaromatic structures with small aliphatic substituents at the edges [2]. In addition, it has been found that the 3.4 µm absorption band related to the aliphatic component of IS carbonaceous dust disappears inside dense molecular clouds. In this environment, cosmic rays (CR) could provide a realistic destruction mechanism. In order to clarify these issues, IS carbonaceous dust analogs produced in cold hydrocarbon plasmas and processed by highly energetic electrons has been analyzed by IR absorption, and the spectral signatures have been related with chemical structures described theoretically.

Thin films and dust grains of a-C:H with a variable proportion of aliphatic and aromatic structures are produced by plasma deposition in RF discharges using mixtures of hydrocarbons and He as plasma precursors. Optical spectroscopy, mass spectrometry and Langmuir probes are used for plasma diagnostics. The a-C:H deposits are analyzed with IR absorption spectroscopy and surface analysis techniques (SEM, AFM,...). The effects of cosmic rays are investigated by irradiating the samples with 5 keV electrons. Models of a-C:H solids of variable density, based on the mentioned competing structures [1,2], are constructed using Montecarlo/Molecular Mechanics and their electronic energies and IR spectra are computed at Density Functional Theory (DFT) level.

Comparison between theoretical and experimental IR spectra [3] shows that the structure of carbonaceous dust in the diffuse IS medium is most probably intermediate between those of the two literature models but closer to that with small aromatic units [1]. Electron bombardment, which is used as a substitute for cosmic ray irradiation, induces dehydrogenation and aromatization of the carbonaceous solids but the experimental destruction rates indicate that the effects of cosmic rays are not enough to explain the disappearance of the aliphatic dust component, characterized by the 3.4 µm band, inside dense clouds [4].

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Optical and structural properties of ZnO:Ti thin films grown by reactive magnetron co-sputtering

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Session: Thin films **type of contribution**: poster

Transition metal doping and formation of mixed oxides are widely used mechanisms to improve the intrinsic properties of binary oxides. Both procedures have been decisive to explain the spectacular increase of applications based on ZnO and TiO_2 films. Proven applications of metal-doped ZnO in optoelectronic devices include photovoltaic and dye sensitized solar cells, flat panel displays, photodetectors, gas sensors, light emitting diodes and blue laser diodes. The majority of previous work on doped ZnO films is related to doping with group III elements (Al, Ga, In) but fewer studies have been performed on tetra-valent dopants as titanium, which can provide two free electrons per atom to improve the conductivity of the ZnO host [1]. In a previous work [2] we explored the structural phase and composition transitions of ZnO:Ti ultrathin films using XANES and RBS analysis. In this work, ZnO:Ti thin films with stoichiometry from very low (~0.5 at.%) to high (~25 at.%) titanium content were deposited at room temperature by DC reactive magnetron co-sputtering on (100) silicon wafers and glass substrates. The crystalline structure was studied by X-ray diffraction observing how the highly orientated grown on the (002) direction of the original ZnO is affected by the incorporation of titanium. The variation of the optical properties (transmittance and optical band gap) was also studied by UV-VIS spectrophotometry observing an improvement in the transparency at low wavelengths when titanium is incorporated in the ZnO lattice. The crystalline and optical properties were investigated as well by Raman and Photoluminescence (PL) spectroscopies. Samples with Ti concentration lower than 0.9% at. presented the most interesting optoelectrical properties from the point of view of its application as transparent conductive coatings as they provided the minimum resistivity ($4.5x10^{-2}$Ω.cm) maintaining a high transparency (≥84%).

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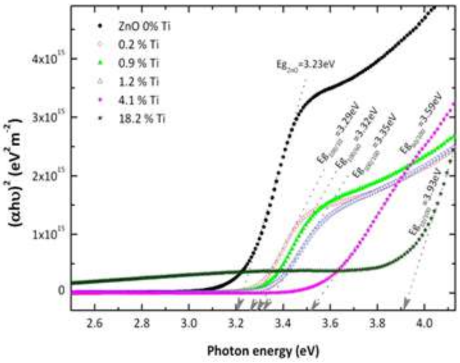

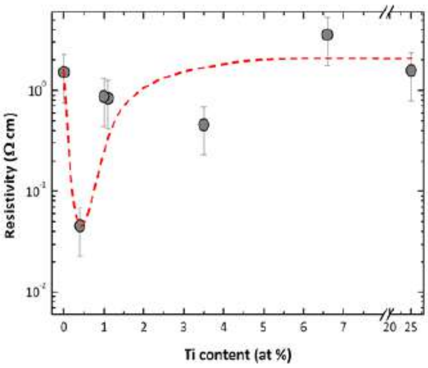

Liquids in vacuum. Coexistence and emergence

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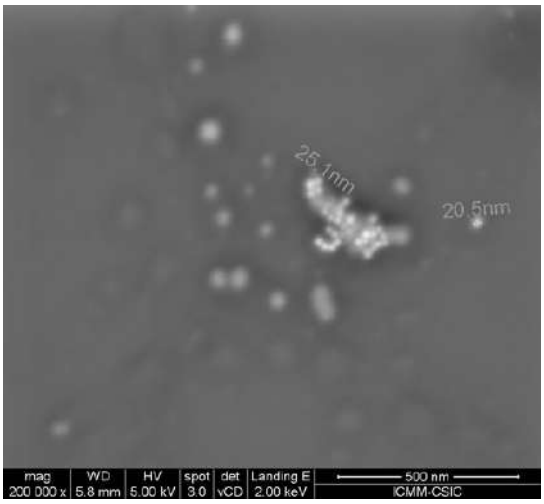
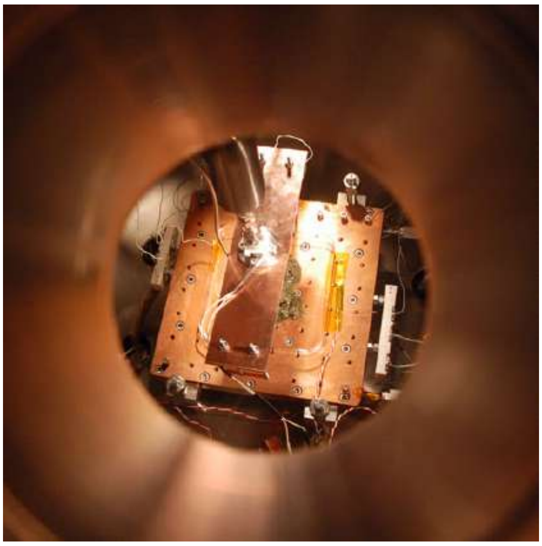
Session: Vacuum science and technology **type of contribution**: poster

Liquids and vacuum are opposite concepts. We have developed a new technique for making possible the coexistence and the emergence of liquid solutions inside a vacuum chamber. We call this technique «Atomic Layer Injection», ALI [1] and it allows to deposit sub monolayers of biomolecules, as Adenosine triphosphate (ATP), or gold nanoparticles from a liquid solution at room temperature. With this technique the molecule to be deposited or nanostructure stays in its original solution (outside of vacuum), and it is introduced inside the vacuum vessel as micro droplets.

The second application of the technique is related to space simulation [2,3]. In the Mars polar regions, cyanobacteria could survive in specific areas where ice coexists with water, or alternatively form in cycles. This process occurs at low temperature, few minibars of pressure in an environment mainly form of carbon dioxide. In a vacuum chamber it is very difficult to maintain a constant water pressure in the mbar range where the pumps are constantly working. The combination of low temperature, relatively high pressure and the correct design of pumping of the chamber with the control of water injection over a cyanobacteria registry, allow the study of the emergence of the microorganism in this extreme environments and learning about the possibility of habitability in Polar Regions of Mars.



Gold nanoparticles on a Si surface



Picture of Mars vacuum simulation chamber at CAB. Study of cyanobacteria in a Mars polar region.

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Secondary emission yield in rough dielectric surfaces.

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Session: Applied Surface Science **type of contribution**: poster

Electron Secondary Emission Yield (SEY) characterizes the number of electrons that a given material emits when an incident electron impinges on its surface. SEY depends on both the angle of incidence and the energy of the incident electrons. This is an important parameter for many vacuum-related industries where a population of electrons inside RF devices can make them malfunction and even damage them. High SEY is the main factor leading to the development of the Electron Cloud, EC, in accelerators or the multipactor effect in satellite-devices and can be tackled by just diminishing the SEY of the materials involved [1]. Materials well-fitted for this applications are typically those that exhibit SEY<1. This means that less electrons are emitted than electrons hit the surface therefore, the electron population tends to decrease in the near-vacuum of the coating.

A more complex behaviour appears when dielectric materials are exposed to this same environment. As dielectric materials have high resistivity, charge builds up in their interior and surface when irradiated by electrons. This space charge creates an electric field that tends to make the SEY=1. This means incident and outgoing charge compensate and the total charge in the material stabilizes [2, 3]. Total accumulated charge and charging rate are important parameters when dielectric materials are selected for their use in these technological applications, concretely in the space industry where replacements are not always readily available.

In this context, we study the dependence of these parameters on the surface roughness of a dielectric sample. For this, several ferrite samples with different aspect ratios where used and its charging behaviour was measured. A simulation of the trajectories of the outgoing electrons was performed to replicate such behaviour.

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Growth and vibrational properties of ultra-thin TiOPc films on Ag(111)

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Session: Surface Science **type of contribution**: Poster

The coverage dependent growth of titanyl-phthalocyanine (TiOPc) ultra-thin films on a Ag(111) surface has been studied using IR Spectroscopy, SPA-LEED, STM and TDS. In the monolayer regime three different phases were found (T_{growth}=300K), all of them with parallel orientation and in an “oxygen-up” configuration of the Ti=O: a 2D-gas phase in the low coverage regime (θ< 0.6 ML), a commensurate ($4\sqrt{3}\times7$)rect phase for 0.8-0.9 ML, and finally, a point-on-line phase when the coverage approaches saturation (1 ML). While the IR spectra of the monolayer phases vary only slightly the vibrational modes corresponding to the monolayer and bilayers of TiOPc/Ag(111) are distinctly different, so that the transition from the monolayer to the bilayer regime is clearly defined. A microscopic model for the growth of the TiOPc bilayer, which involves specific local configurations of molecules in the first and second layer is suggested based on IR and STM data (Fig.1) together with DFT calculations. Thermal desorption spectroscopy measurements reveal a high thermal stability of the TiOPc bilayer, which requires temperatures above 500K for the desorption of the second layer from the TiOPc monolayer. The unusual intrinsic stability of the TiOPc bilayer qualifies this system to be combined with other π-conjugated molecules, e.g. to design molecular heterolayer structures with a stable and well defined interface.

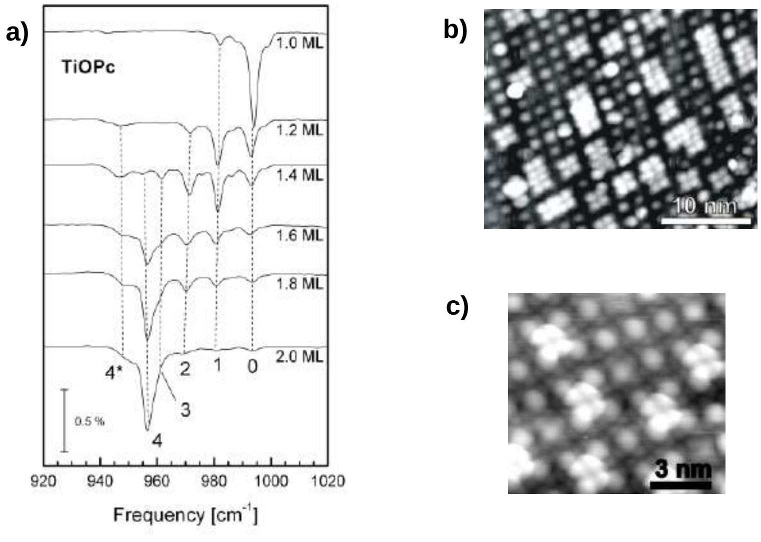

Fig. 1: (a) Evolution of IR spectra of TiOPc grown on Ag(111) with increasing film thickness. The displayed spectra focus on the frequency variation of the Ti=O stretching mode in the 1-2ML coverage regime. (b) STM measurement of 1.3 ML TiOPc/Ag(111). (c) Magnified micrograph of the sample in (c) showing the 'oxygen-up' configuration of the Ti=O group in the first layer as well as the 'oxygen-down' configuration of second layer TiOPc.

Surface reactivity of iron monosulfide (FeS) films

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Session: Surface Science **type of contribution**: Poster

Iron sulfides in their different chemical composition (pyrite, pyrrothite, trolite, greigite, etc.) are important materials in a number of different fields like electronics, prebiotic chemistry, engineering, geochemistry, catalysis, etc. Many of their technological applications are related to the thin film properties of these materials and/or to their chemical surface reactivity. Among those minerals, FeS_2 and FeS are particularly important because of the strong catalytical properties of their surfaces. Furthermore, they are in the basis of the so-called "Fe-S World" [1] a theory proposing a prebiotic route through a series of chemical reactions for the formation of simple inorganic molecules, a route ending in the synthesis of aminoacids in whose reactions the surface of the minerals plays a key role. An effort to demonstrate the experimental feasibility of the different reactions involved in that hypothesis has led to some, yet inconclusive, results [2]. Most of this experimental work in prebiotic chemistry has been done using chemical reactors: well-sealed glass containers filled with the reactants in a non reactive gas or, often, in aqueous solution, and submitted to a number of processes (varying temperature, pressure, etc.) for periods from minutes to days.

As a different strategy, we carry out ultra high vacuum (UHV) experiments using surface physicochemical techniques to study some of the basic reactions of the Fe-S world hypothesis, on the following grounds: (i) Chemical reactions on surfaces are recognized as key ingredients of the prebiotic world (ii) Surface Science techniques have access not only to the final state but, also, to intermediate reaction products. The chemical reactions that we have studied on those surfaces are

$$H_2S + FeS \rightarrow FeS_2 + H_2$$

$$N_2 + 3FeS + 3H_2S \rightarrow 3FeS_2 + 2\,NH_3$$

We have prepared stoichiometric iron monosulfides (FeS, troilite) thin films by sulfidation of Fe films in a sulfur atmosphere, and characterized these films by x-ray photoemission spectroscopy (XPS) and x-ray diffraction (XRD). Using XPS and thermal desorption spectroscopy (TDS) we study the chemical reactivity of the FeS surface under nitrogen and hydrogen sulfide exposures corresponding to the above basic reactions. Here, we present evidence of these reactions on the FeS surface, under well-defined conditions.

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Multiscale patterning of cell guides and traps through fs laser writing

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Session: Biointerfaces **type of contribution**: Poster

A better understanding of cell-biomaterial interaction in vivo passes still through the need of studying cell cultures in non conventional in vitro conditions (i.e. on substrates with 1D, 2D or 3D anisotropies). Natural biomaterials, such as bone, are characterized by a hierarchical structure with characteristic features in the micro and nanoscales [1]. In this frame, the control of the surface topography of different biomaterials has been observed to drastically influence their biocompatibility. In line with this research, pulsed laser micro/nano machining technology has been used in this work to directly write multiscale surface structures on stainless steel and titanium alloys [2]. Laser induced periodic surface structures (LIPSSs) have been obtained by fs pulsing aiming at designing cell guides and traps. The irradiated stainless steel and titanium patterns have been imaged by scanning electron microscopy and atomic force microscopy. While a microscale periodicity is induced by the spot size of the focused laser, a nanoscale topography is superposed by the appropriate selection of light polarization. The surface spectroscopic analyses by X-ray photoelectron spectroscopy further illustrate the absence of surface chemistry differences between the pristine and the irradiated samples. The culture of human mesenchymal stem cells (hMSCs) show that cells tendency to adhere and polarize on the LIPSSs depend on both the nature of the alloy and the periodicity. While cells preferentially adhere on and align through the stainless steel LIPSSs when supported by orthogonal nanoripples, the cells on TiAlV appear to be insensitive to such periodicities and adhere mostly to flat areas. In specific 1D configurations, stainless steel substrates behaved as efficient cell guides (Fig. 1.a). Meanwhile, 2D structures with isolated pristine squares (irrespective of the material) actuated as trapping networks ideal for structuring tissues (Fig. 1.b). The flexibility and reliability of the process allows envisaging an extension of the studies to alternative alloys and other non-metallic materials.

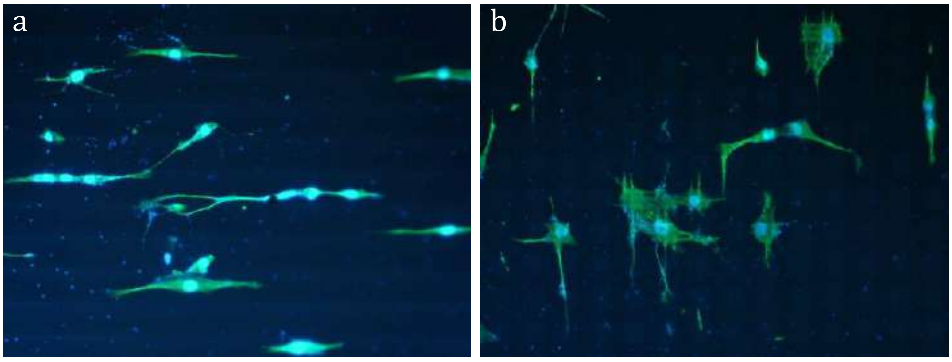

Figure 1. Fluorescence images of hMSCs on 1D and 2D LIPSSs on TiAlV (frame base 600 μm).

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Sol-gel tailoring of surface chemistry towards controlled adsorption of icosahedral P22 virus capsids

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Session: Biointerfaces **type of contribution**: Poster

The adsorption of structured virus capsids in designed stable configurations is a desirable objective towards the ulterior analysis of their mechanical properties. In this work, we have tailored surfaces with different dominant surface tension components aiming at studying the affinity of the facets of icosahedral P22 virus capsids towards one specific surface tension component. The surfaces have been prepared by the sol-gel process, using a titanium isopropoxide sol as condensing agent [2] of each one of the following organosilanes: 3-glycidyloxypropyl-trimethoxy-silane (GPTS), 3-aminopropyl-triethoxy-silane (APTS) and 1H,1H,2H,2H-perfluorodecyl-triethoxy-silane (PFDS). The optimization of the surface properties has implied the analysis of both the surface chemistry and topography of the surfaces. Fourier transformed infrared spectroscopy has allowed identifying the different functional groups of the organosilane molecules on the thin spin casted films deposited on Si (100). The surface topography, investigated by atomic force microscopy (AFM), shows that, irrespective of the organosilane used, the final root mean square roughness remains below 1 nm. Under these conditions, the surface tension of the surfaces has been estimated by measuring the contact angle with three representative liquids and using the Good- Van Oss- Chaudhury approximation. The results confirm the effective formation of a set of surface chemistries exhibiting different dominant surface tension components. The use of such surfaces to study the adsorption of P22 virus capsids has involved the analysis of the dynamics of virus immobilization by fluorescence microscopy and the interpretation of the final capsid conformation obtained by AFM. These analyses give rise to preliminary statistical distributions pointing towards a dominant 5 fold conformation in the hydrophobic surface, but 3 and 2 fold symmetries dominating on hydrophilic surfaces (Figure 1).

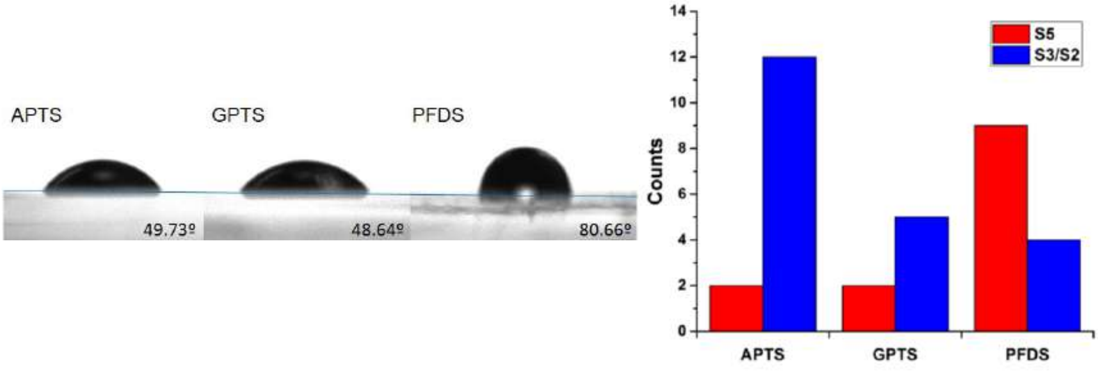

Figure 1: Water contact angle on hydrophilic APTS and GPTS and on hydrophobic PFDS. Comparison of P22 virus symmetries on each surface.

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ZnO:Al,Bi thin film electrodes for perovskite solar cells

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Session: Applied Surface Science **type of contribution**: poster

Nowadays, the need for clean renewable energies is no longer a novelty. The answer for a more sustainable future dwells on the development of new and better clean energies, as the energy demands for a close upcoming future requires. Among the several "clean" energy possibilities, photovoltaic systems have been thoroughly and systematically researched and improved, and the thermoelectric technology has been target of intense investigation. Thermoelectric materials can convert thermal differences into electric energy or the other way around, and recent research has demonstrated good results towards ZnO-based coatings for thermoelectric applications [1, 2]. In this work, ZnO:Al,Bi thin film electrodes were developed with the objective to enhance the efficiency of photovoltaic systems [3]. To play this specific role, such films must be optically transparent and possess good electric and thermoelectric properties. Thus, it is crucial to study and understand the inherent physical properties of such films: optical transmittance in the visible region; transport properties (carrier concentration, mobility) and electrical conductivity. It is also very important to establish a relation of these properties with both crystal structure and chemical composition of the films. Given so, several Al-doped ZnO thin films with several Bi concentrations and thermal post-treatment temperatures are described, along with the respective production method, magnetron sputtering.

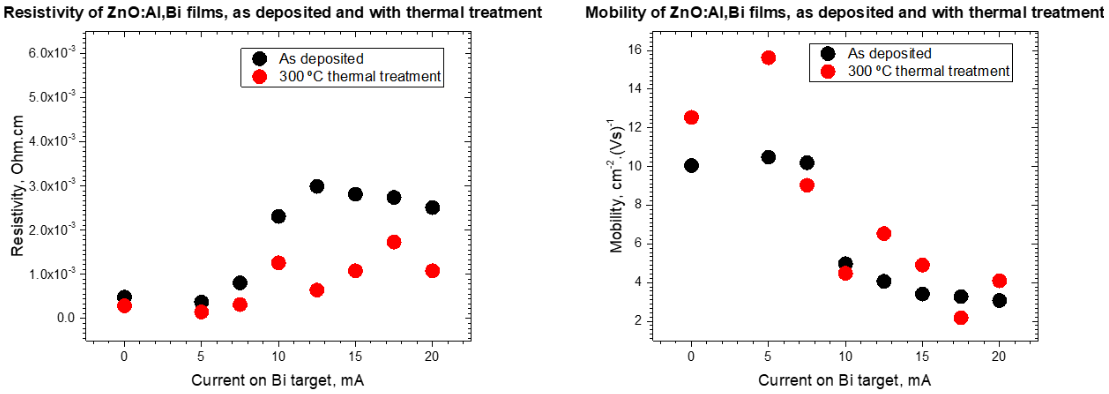

Figure 1 – Graphical representation of both resistivity (left) and mobility (right) of ZnO:Al,Bi films, as functions of the current applied to the Bi target, as deposited and with a 300 ºC thermal treatment.

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On the reactive element effect of yttrium in the oxidation behavior of multilayered CrAlYN coatings

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Session: hard coatings or surface engineering or applied surface science **Type of contribution:** Oral

Multilayered $Cr_{0.50}Al_{0.50}N$ and $Cr_{0.51}Al_{0.46}Y_{0.03}N$ coatings (c.f. Figure 1) were deposited on M2 and 316 steel substrates and heated to 1000 ºC in air for 2 h to study their oxidation mechanism and thermal stability. X-ray diffraction, glow-discharge optical emission spectroscopy and transmission electron microscopy coupled with spatially resolved microanalysis techniques are used to investigate the nanostructure, constituent phases and chemical elemental distribution of the as-prepared and oxidized samples. The incorporation of Y in low contents (< 4 at.%) in metallic nitride coatings has been demonstrated to increase the thermal stability and oxidation resistance above 900ºC but less is known about the action mechanisms. In this work, we confirm the reactive element effect of Y but displaying a different pattern from the typical observed in metallic alloys. The interdiffusion of substrate elements plays an important role in the oxidation process influencing the corrosion products. The presence of yttrium retards the iron outward diffusion by forming oxides in M2 and yttrium nitride in 316 steels. The microstructural analysis determined that yttrium migrates to the grains and interface of the oxide scale and to the nitride column boundaries.

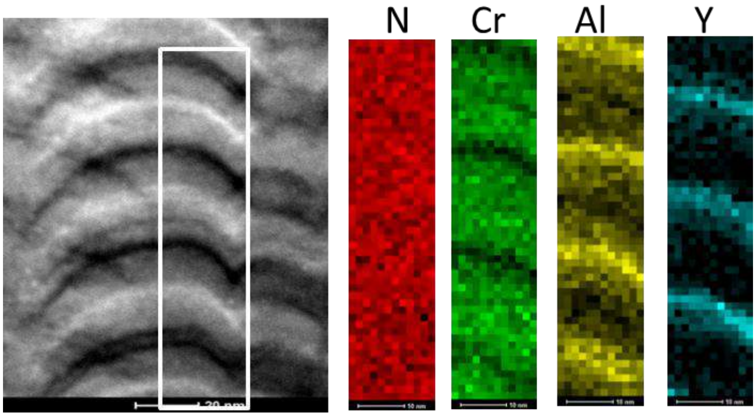

Fig. 1. HAADF-STEM image of the CrAlYN coating and X-EDS elemental maps

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Laser carbonization of porous silicon for locally tuning the surface wettability

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Session: Surface Engineering **type of contribution**: poster

Nanostructured porous silicon has been widely studied as a low cost nanomaterial for the development of biosensors, mainly due to its ease of fabrication and surface chemistry modification, and the ability to functionalize it with a variety of biomolecules. [1] In these devices, surface wettability plays a key role to control the interaction between the sensing surface and the sample being sensed, since it rules the ability of the latter to infiltrate the porous surface. Carbonization and hydrocarbonization of porous silicon by acetylene decomposition has been shown to passivate the porous surface while achieving an hydrophobic (hydrocarbonization) or hydrophillic (carbonization) surface termination. [2] In this work, hydrophobic hydrocabonized porous silicon (HCPSi) has been irradiated with a scanning focused laser in an acetylene atmosphere to locally achieve hydrophillic carbonized porous silicon (CPSi). Water contact angle and X-ray photoelectron spectroscopy measurements confirm that hydrophillic patterns have successfully been defined on the initial hydrophobic surface, while retaining the high surface area of the original porous silicon layers.

With the technique proposed, it is possible to achieve microfluidic devices with hydrophobic/hydrophillic surface contrasts at the submilimeter level to enhance the interaction between sample and sensor and thus enhance the sensitivity of porous silicon biosensors.

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The industrialization of HIPIMS: High Power Impulse Magnetron Sputtering

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Session: Hard Coatings **type of contribution**: Oral

HIPIMS (High Power Impulse Magnetron Sputtering) is a magnetron sputtering technology devoted to produce thin film coatings with enhanced properties. The technology offers advantages such as denser coatings, higher hardness values and smoother surfaces. Even though the HIPIMS technology has already been validated in both laboratory and industrial relevant environment, and despite the many advantages, the industry has not yet adopted in large scale HIPIMS for high volume manufacturing. The reason may be due to some of the intrinsic difficulties the HIPIMS technology presents, such as high complexity, lower deposition rate hence reduced throughput in production, higher costs for the power supplies with historically poor reliability.

The aim of this presentation is to explain the benefits of the HIPIMS technology, show the current state of the art of HIPIMS in industry, improved reliability and demonstrate how this technology could solve actual problems in fields such as the automotive (smooth surfaces for tribological contacts in engines) or the cutting tool industry (hard coatings on microdrills). The high added value of the coatings achieved by HIPIMS will be able to overcome the difficulty of the technology implementation.

The influence of target erosion grade in the optoelectronic properties of AZO coatings growth by magnetron sputtering

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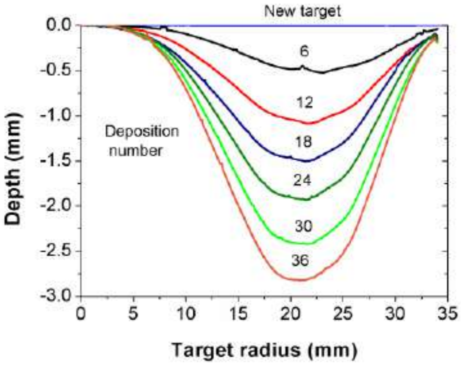
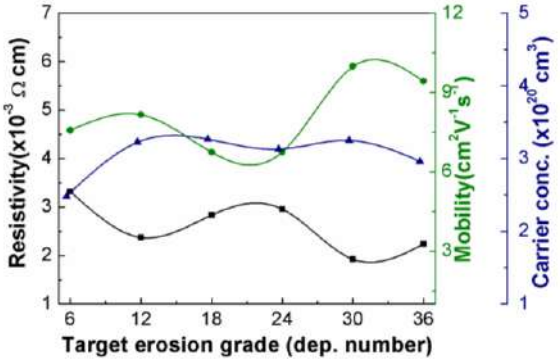
Session: thin films **type of contribution**: oral presentation

Aluminum-doped zinc oxide (AZO) transparent conductor coating has emerged as promising substitute to tin-doped indium oxide (ITO) as electrode in optolectronic applications such as photovoltaics or light emitting diodes (LEDs). Besides its high transmission in the visible spectral region and low resistivity, AZO presents a main advantage over other candidates such as graphene, carbon nanotubes or silver nanowires; it can be deposited using the technology industrially implemented to manufacture ITO layers, the Magnetron Sputtering (MS). This is a productive, reliable and green manufacturing technique. But to guarantee the robustness, reproducibility and reliability of the process there are still some issues to be addressed, such as the effect and control of the target state. In this paper a thorough study of the influence of the target erosion grade in developed coatings has been performed. AZO films have been deposited from a ceramic target by RF MS. Structure, optical transmittance and electrical properties of the produced coatings have been analyzed as function of the target erosion grade. No noticeable differences have been found neither in optoelectronic properties nor in the structure of the coatings, indicating that the RF MS is a stable and consistent process through the whole life of the target





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Pressure evolution inside cork cells

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Session: Vacuum science and Technology **type of contribution**: oral

Cork is a well-known cellular material; cells are hollowed of cytoplasm and filled with gas. Although usually referred as impermeable and commonly used to seal, many gases and vapors can be transported through cork. The cells are interconnected by very small channels (plasmodesma, plural: plasmodesmata), as commonly found in plant cells. It has been proposed that these channels play a major role in the transport of gases when cork is not compressed [1]. The aim of this work is to model pressure evolution inside a cork stopper subjected to vacuum.

Evidently, not all cork cells have the same volume and plasmodesmata connections do not have the same open diameter. Moreover, cork also has large inhomogeneities as lenticular channels and other natural defects. In this work, we assume that all cells and plasmodesmata are identical. The cell volume and plasmodesma conductance in our model equal their mean values (2×10^{-11} L and 7×10^{-11} L/s, respectively), obtained from permeation measurements [2]. There are about 7×10^{8} cells in a cork stopper. Cork defects were not considered due to their large variability.

When subjected to vacuum, the gas inside the cork will flow out through the cells towards the exterior. Pressure in inner cells will be changing slowly, due to the small conductance of plasmodesmata. The purpose of this work is, first, to calculate the total flow as a function of time coming out from a 3D array of interconnected cells, and secondly, to describe the pressure evolution at the inner volume. The dynamics of this problem is identical to that of discharging a 3D array of *n* capacitors C, interconnected by resistors R, having all resistors at the borders shunted and connected to a power supply. The flow rate and the pressure are equivalent to the electrical current and the voltage, respectively. The mathematical description of the process is in the form of a set of *n* linear differential equations, which has an analytical solution of the form:

$$U(t) = \sum_{n} a_n e^{-\frac{b_n}{RC}t}, \quad \text{Eq. 1}$$

where a_n and b_n are constants to be calculated and RC is the time constant of a single RC circuit. The, analytical solution has as many terms as the number of nodes in the array i.e. $n \approx 7\times10^{8}$ which is a challenge to find even numerically.

The advantage of using electrical equivalents to describe gas flow and pressure evolution is in the existence of many options to solve electrical circuit problems. Since the conductance is constant, as the gas flow is in the molecular regime even at atmospheric pressure [1], so will be the resistivity in the equivalent electrical circuit. Authors present different approaches in treating the pressure evolution inside the cork cells using equivalent electrical schemes.

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High-quality, one-step production of Au@TiO$_2$ nanoparticles by gas-phase synthesis

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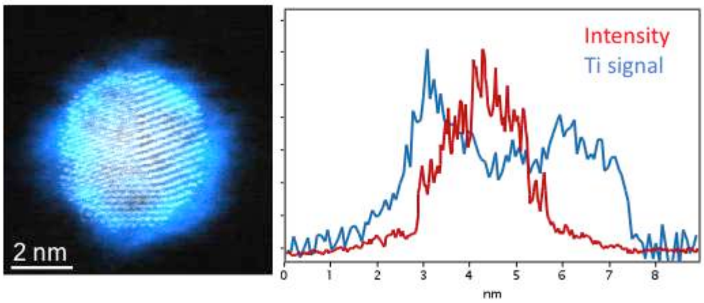
Session: Nanometer Structures **type of contribution**: oral

The gas-phase synthesis of nanoparticles is an attracting method for the production of nanoparticles, as purity and size distribution of resulting material are well-controlled [1]. The recent advent of the multi magnetron approach [2] also known as Multiple Ion Cluster Source (MICS) has added the versatility to produce nanoparticles with adjustable chemical composition and even tunable structure where core@shell nanoparticles with sharp, clean interfaces can be produced in a one-step process and avoiding the restrictions of chemical processes [3-4].

In the present communication we present the results on the growth and characterization of core@shell nanoparticles where the Au core of 4 nm diameter is surrounded by a thin (1 nm) titanium oxide shell. The production strategy will be exposed together with the characterization results including morphology (Atomic Force Microscopy, AFM), atomic structure (C_s-corrected Scanning Transmission Electron Microscopy, C_s-corrected STEM), electronic structure (X-ray Photoemission Spectroscopy, XPS) and chemical composition (XPS and STEM).



Left: High resolution C_s-corrected STEM image of a representative AuTiO$_2$ nanoparticle. Right: cross section chemical profile of the nanoparticle.

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Real-Space Atomic-Scale Imaging Circumstellar Carbon Cluster Analogues

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Carbon clusters formed after magnetron sputtering of a carbon target in an inert gas aggregation chamber represent a reliable source of chemical analogues of the inner envelopes of C-rich AGB stars. Despite their importance, a detailed characterization of the carbon products obtained in aggregation sources is complicated due to the large number of different species generated during the experiment. Here we report a methodology for studying individual carbon nanoparticles and clusters generated in the STARDUST machine, a state-of-the-art multi-technique facility specifically designed to tackle astrochemical problems from a laboratory perspective.

By profiting from ultra-high vacuum scanning tunneling microscopy (STM), we perform images in real-space with Å-resolution of the circumstellar analogues deposited on low reactive substrates. At room temperature (300K) adsorbed analogues diffuse on the surface at high speed impeding their rigorous identification. At low temperatures (4K) the adsorbed products agglomerate and rest on the surface. We find a number of sub-nanometer linear structures that can be identified as short carbon chains, C_n, $2<n<5$ (see inset in Fig. 1). The carbon chains self-organize in planar domains (see Fig. 1) maximizing the intermolecular interaction on the surface. In addition, we find a wide plethora of small cluster structures that could be ascribed to amorphous carbon species. Comparison between experimental STM images and ab-initio simulations permits us to characterize the local physical-chemical environment of the analogues with an unprecedented level of detail. Our methodology permits to address the structural identification of sub-nanometer clusters, an important step towards the full characterization of the circumstellar regions chemistry and their evolution.

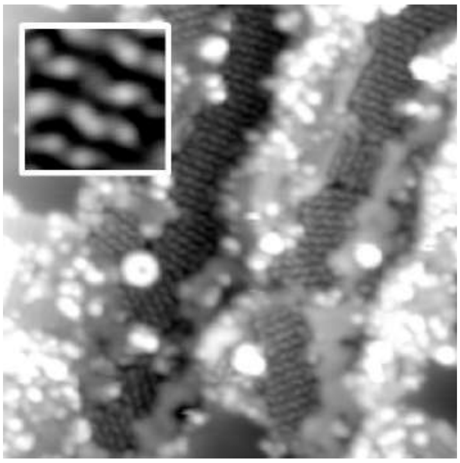

Figure 1: 25x25 nm^2 STM image obtained at low temperature (4K) of carbon cluster analogues produced in STARDUST machine and deposited on Au(111) surface. The small linear carbon chains, see upper left inset, form ordered islands on the surface. Inset,2x2 nm^2, V=1.4V, I=10pA

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Optimization of dye-sensitized TiO2 nanorod solar cells

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Session: thin films **type of contribution**: oral presentation

Keywords:
Titanium dioxide TiO2; Nanorods; Sputtering; Dye sensitized solar cells (DSSCs)

Abstract:

TiO_2 nanorods have been prepared by DC reactive magnetron sputtering technique and applied to dye-sensitized solar cells (DSSCs).

From the scanning electron microscopy images, it is known that the nanorods are formed in a configuration perpendicular to the substrate. The crystal structure of the nanorods presents an anatase phase, as verified X-ray diffraction and Raman spectroscopy. These nanorods were used as working electrodes in the DSSCs.

The influence on the conversion efficiency of several preparation parameters (the effect of a blocking layer, the effect of the annealing temperature, the variation with the nanorods length and/or diameter, the structural modifications induced by the variation of the content of oxygen). An optimized photoelectric conversion efficiency of 4.8% has been achieved.

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Chemistry Below Graphene: Decoupling Graphene From Metals By Electrochemical Oxidation

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Session: Surface science **type of contribution**: oral

While high-quality defect-free epitaxial graphene can be efficiently grown on metal substrates, strong interaction with the supporting metal quenches its outstanding properties. Thus, protocols to transfer graphene to insulating substrates are mandatory, and these often severely impair graphene properties by the introduction of structural or chemical defects. Here we describe a simple, fast and easily scalable general methodology to structurally and electronically decouple epitaxial graphene from metal surfaces. A multi-technique characterization of the different steps involved in the process, combined with ab-initio calculations, shows that after a controlled electrochemical oxidation process a single-atom thick metal-hydroxide layer intercalates below graphene decoupling it from the metal substrate. The decoupling process takes place without disrupting the morphology and electronic properties of graphene. The electrochemical protocol has been proved to work on Gr/Pt(111) and Gr/Ir(111) substrates. Epitaxial graphene was grown in UHV conditions by thermal decomposition of fullerenes [1] and the samples were characterized in-situ by STM and LEED. Subsequent ex-situ characterization with AFM, XPS and Raman before and after the electrochemical treatment demonstrates the efficiency of the decoupling process. This work suggests that suitably optimized electrochemical treatments may provide viable alternatives to transfer protocols for graphene and other 2D materials on diverse metal surfaces.

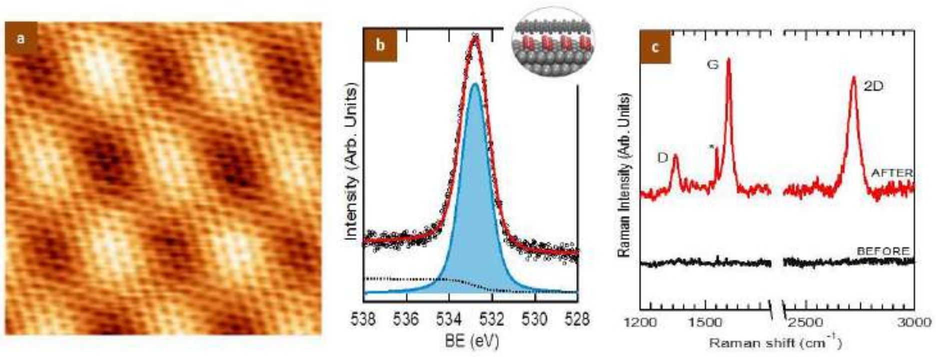

Figure 1: a) STM image of Gr/Pt(111) showing a characteristic Moiré ((4x4)nm^2, I=4nA, V=10mV). b) O1s XPS spectrum after the electrochemical treatment and a soft annealing of a Gr/Pt(111) sample. The peak can be fitted with one main component that corresponds to the hydroxide species. Inset: optimized representative Gr/Pt$_2$(OH)@Pt(111) interface with a coverage of 1/2 ML of intercalated-OH between the graphene and the Pt(111) surface. c) Raman spectra of graphene on Pt(111) before (black curve) and after (red curve) electrochemical oxidation. The decoupling of the graphene sheet from the metallic substrate is clear by the emergence of D, G and 2D bands

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On the reactive element effect of yttrium in the oxidation behavior of multilayered CrAlYN coatings

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Session: hard coatings or surface engineering or applied surface science **Type of contribution:** Oral

Multilayered $Cr_{0.50}Al_{0.50}N$ and $Cr_{0.51}Al_{0.46}Y_{0.03}N$ coatings (c.f. Figure 1) were deposited on M2 and 316 steel substrates and heated to 1000 ºC in air for 2 h to study their oxidation mechanism and thermal stability. X-ray diffraction, glow-discharge optical emission spectroscopy and transmission electron microscopy coupled with spatially resolved microanalysis techniques are used to investigate the nanostructure, constituent phases and chemical elemental distribution of the as-prepared and oxidized samples. The incorporation of Y in low contents (< 4 at.%) in metallic nitride coatings has been demonstrated to increase the thermal stability and oxidation resistance above 900ºC but less is known about the action mechanisms. In this work, we confirm the reactive element effect of Y but displaying a different pattern from the typical observed in metallic alloys. The interdiffusion of substrate elements plays an important role in the oxidation process influencing the corrosion products. The presence of yttrium retards the iron outward diffusion by forming oxides in M2 and yttrium nitride in 316 steels. The microstructural analysis determined that yttrium migrates to the grains and interface of the oxide scale and to the nitride column boundaries.

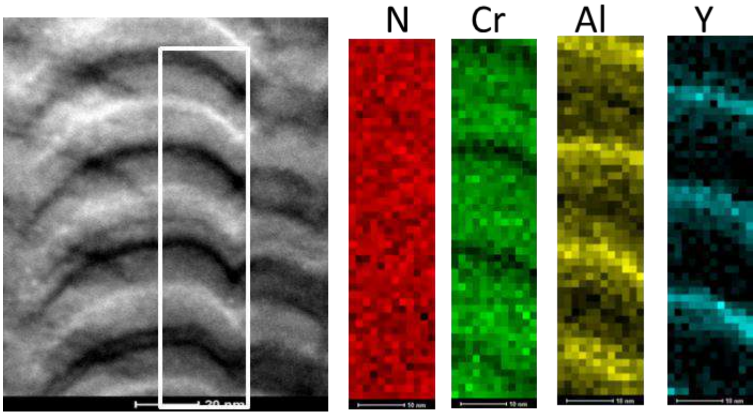

Fig. 1. HAADF-STEM image of the CrAlYN coating and X-EDS elemental maps

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Carbon evaporator for Molecular Beam Epitaxy graphene growth

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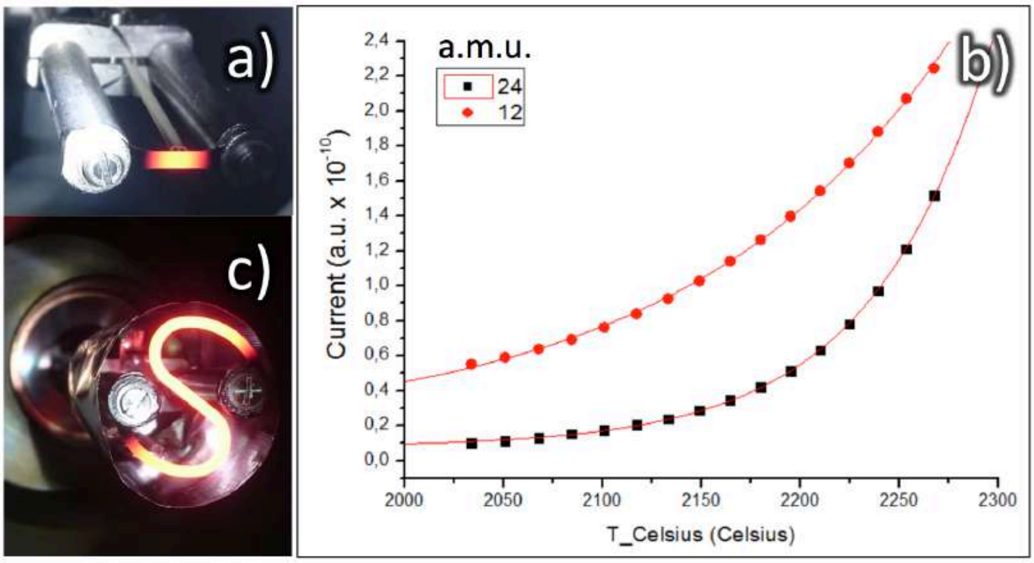
Session: vacuum science and technology **type of contribution**: oral, poster

The synthesis of graphene on insulating substrates on a large scale is still a great challenge to be achieved, in spite of all the efforts from the scientific community. It is possible to deposit carbon-containing layers using a vitreous carbon source [1] for Molecular Beam Epitaxy (MBE) growth of graphene [2, 3, 4].

The original design of the carbon evaporator (Figure 1, a) provides small evaporation rates, which are adequate for the MBE-growth of modulated, doped semiconductor structures. For the growth of graphene, it is necessary to achieve larger growth rates, keeping a low DC current operation of the cell (<= 15A). A new designed has been optimized using COMSOL simulations, constructed and tested. (Figure 1, b).

Residual mass spectrometry (Figure 1, c) shows that the ratio of chemical species C_{12}/ C_{24} depends on the temperature of operation of the cell. Recent results on the growth of graphene using this technology will be presented.

Acknowledgment: MAT2015-67021-R, MAT2014-54231



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Improving the thermal and UV stability of Kevlar through Atomic Layer Deposition

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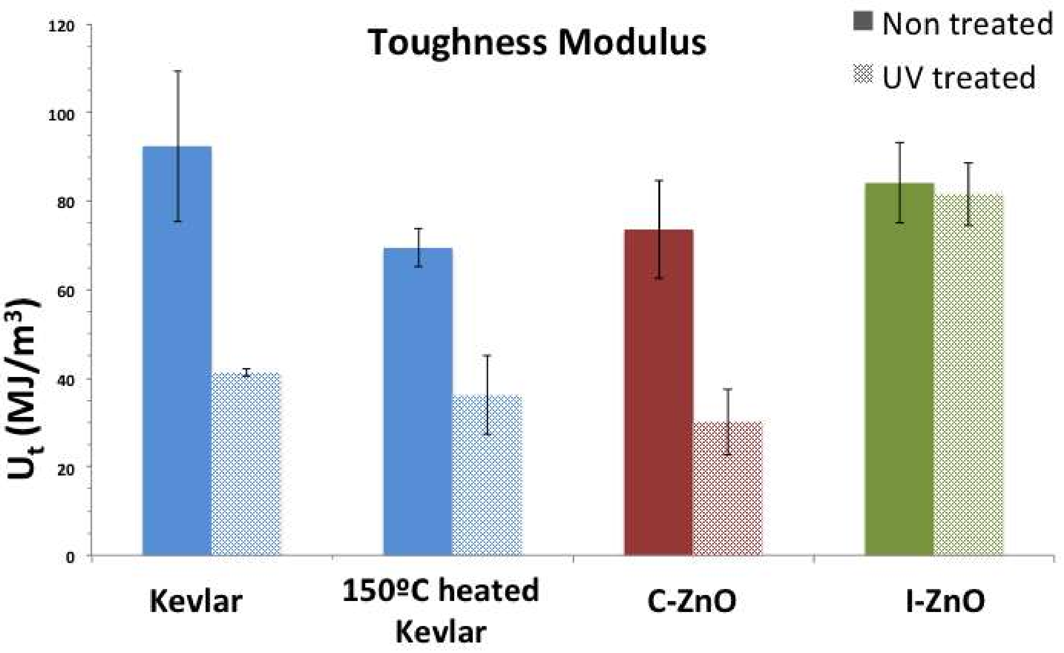
Session: thin films **type of contribution**: Oral or poster

Polyaramides, such as Kevlar®, are of great technological importance for their extraordinary mechanical performance. Kevlar fibers are used in personal safety, for reinforcement of tires and ropes, and in further material composites that require extreme mechanical stability. The origin of the mechanical robustness of Kevlar lies in the alignment on the molecular level and the intermolecular interactions of the constituting amides. The properties of the polymer are dependent on the environmental conditions. Similar to proteins, elevated temperatures and/or irradiation with UV light lower the performance of the aramide.

Nature shows an effcient way to reinforce biopolymers from the mechanical point of view. This natural way is based on incorporation of metal ions into the protein structure, which results in enhancement of the inter- or intramolecular bonding. Soft structures can thus be turned hard or vice versa by simply controlling the presence and amount of metal ions inside the biopolymer.

In our approach we apply solvent free vapor phase infiltration techniques for impregnating polyaramides with metal ions or metal oxides with the purpose of achieving extraordinary physical properties. We will show that the procedure is the method-of-choice for stabilizing the thermal sensitivity of Kevlar while at the same time introducing protection against UV-induced degradation and further properties which such polymers intrinsically do not possess.



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Low Energy Ion Scattering as a Depth Profiling Tool for Thin Layers

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Session: surface science **type of contribution**: POSTER

Low Energy Ion Scattering (LEIS) is mostly known as a method for analysis uppermost atomic layer of the surface [1]. In our work we demonstrate the ability of LEIS to be a fast and powerful tool for investigation elemental depth profile of very thin layers on the surface of compound semiconductor: Cadmium Telluride (CdTe).

Surface treatment of CdTe single crystals in Bromine- Methanol is a common method to remove damage from the crystal surface after mechanical polishing. Such treatment preferentially removes Cd and leaves approx. 4 nm thick Te-Rich layer on the surface. This thickness matches probing depth of X-ray photoemission spectrocopy.

For the analysis, we used [111] oriented single crystal of CdTe with defined Te – terminated (111)B and Cd – Terminated (111)A faces. The XPS analysis showed that the Bromine – Methanol etch has isotropic nature of etching. The ratio between Te and Cd was 1.66 for both sides of the crystal. However, Dynamic LEIS depth profile showed distinctive differences in the ratio of Te/Cd. Depth profiling with 5 keV Ne^+ ions dose of 4×10^{13} per spectrum revealed that the Te – rich area of (111)A side is twice deeper than for the (111)B orientation. Initial LEIS spectra showed Te/Cd ratio higher than 3 and converged to stoichiometric ratio of 1. For both sides, average from spectra with Te/Cd < 1 yielded the same stoichiometric value as XPS.

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Ordered arrays of Si-based nanocrystal pyramids achieved by electron-beam lithography and MBE growth on Si(001)*

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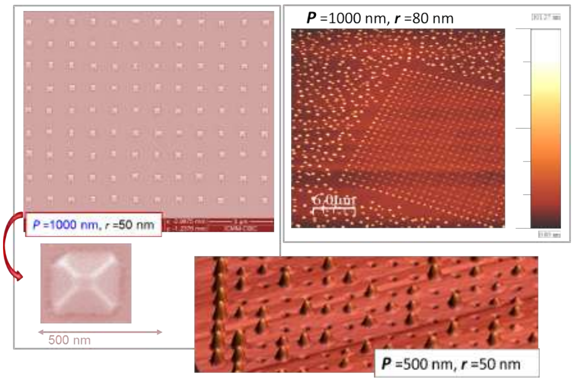
Session: Nanometer Structures **type of contribution**: Poster

The controlled development of patterns at the nanoscale attracts great scientific and technological interest since it provides appropriate routes to achieve new surface and material functionalities [1] with potential applications in a wide diversity of areas. The used methodologies often combine top-down and bottom-up strategies, in which any self-assembling phenomena of the synthesis procedure is promoted by a large scale pre-patterning of the substrate surface. By following this strategy we fabricate ordered arrays of Si-based nanocrystals with pyramidal shape, regular-size and controlled spatial arrangement. Such arrays are interesting e.g. as templates for multi-dot configurations, with illustrative examples in GeSi-derived technologies [2], to fabricate arrays of Ge quantum-dots, Ge-Si compound quantum dot molecules, etc.

Here we study the growth by Molecular Beam Epitaxy (MBE) of this type of nanostructures on patterned areas (25x25μm^2) prepared by electron beam lithography (EBL) and reactive ion etching (RIE) on Si(001) wafers. A variety of patterned fields are considered, formed by arrays of cylindrical pits with specific values of the nominal pattern periodicity (P), pit depth (d) and pit radius (r) in the ranges: 1500 nm ≤ P ≤ 370 nm; 100 ≤ r ≤ 35 nm; 80 ≤ d ≤ 27 nm. Although similar strategies combining bottom-up and top-down techniques have been successfully used in Ge/Si(001) and Ge/Si/Si(001) systems to produce highly regular arrays of Ge or GeSi islands and dots [1], for the Si/Si(001) system was a challenge, since previous works only reported changes in the shape of the pre-pattern pits.

In the present work, thin Si layers (up to an equivalent layer thickness of 5 nm) are deposited by MBE on top of both flat and pit patterned Si(001), using conditions in which the formation of nanoscale pyramid-like islands is promoted [3]. Different values of the growth parameters (substrate temperature and Si deposition rate) are considered. Our analysis focuses on two issues: i) island formation; ii) influence of the MBE growth conditions and geometry pattern parameters on the shape, size and spatial arrangement of the islands. A combination of chemical, morphological and crystal structure analysis techniques is used in the investigation: X-ray photoelectron and Auger electron spectroscopies, XPS, AES; atomic force and scanning electron microscopies, AFM, SEM; high and low energy electron diffraction, RHEED, LEED.

SEM and AFM results show that, by choosing appropriate parameter sets of MBE growth conditions and lithography pattern features, the present methodology can be used to achieve a controlled positioning of the Si-based nanostructures, allowing also control of size, shape and number density of the pyramid-like nanocrystals (see Figure).



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First of all, our **sponsors**. Our low fare for the registration has been possible thanks to them. They have also prepared an appealing technical exhibition.

We want to thank the ***Vacuum*** journal, for dedicating one number to our conference proceedings, as well as the invited editors—Jose Luis de Segovia and Irene Palacio—, for their joint effort.

We cannot forget the **scientific and organizing committees,** whose work and dedication have made possible this conference.

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