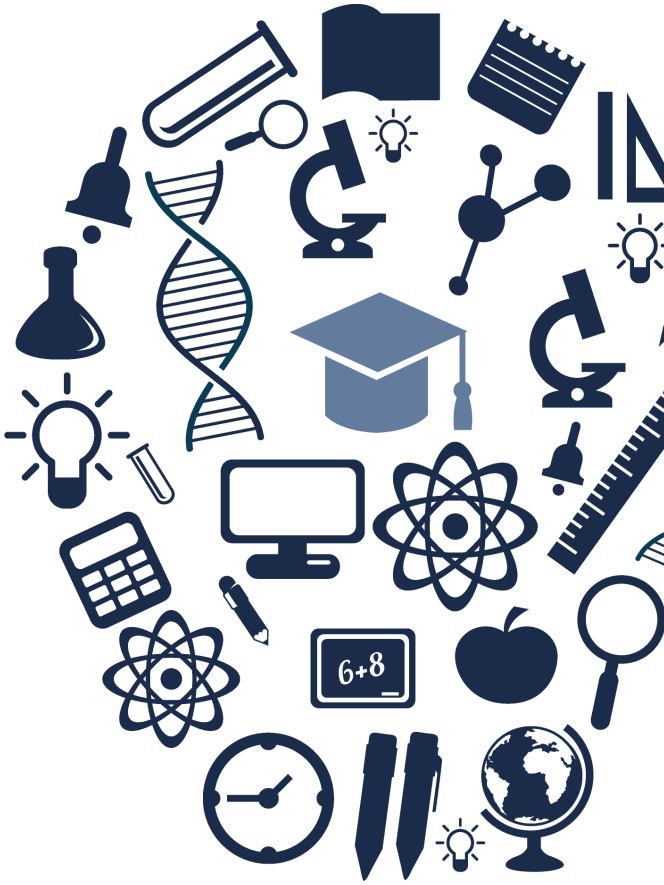
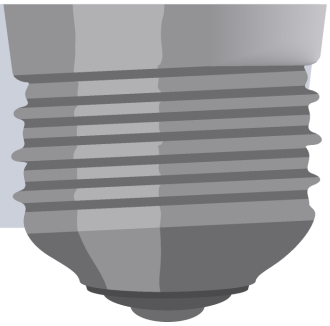
ALBA



5 October 2018
09:30 - 12:15 h

ALBA Synchrotron
Maxwell Auditorium

2nd EARLY-STAGE RESEARCHER DAY



Students doing their PhD at the ALBA Synchrotron **will present the status of their projects** in areas such as the application of synchrotron light as well as accelerators development.

Closing remarks by Caterina Biscari, director of the ALBA Synchrotron.

Open to ALBA staff

Further information and presentations
https://indico.cells.es/indico/event/176/

www.albasynchrotron.es

Programme

09:30	Welcome	Miguel Ángel García Aranda, head of Experiments division, & Francis Pérez, head of Accelerators division
09:45	Development of a 1.5 GHz Solid State Amplifier for the 3rd Harmonic Cavity for ALBA Synchrotron Light Source	Zahra Hazami, Accelerators division
10:00	Evaluation of the Surface Impedance of High-Temperature Superconducting Coated Conductors (HTS-CC) and Requirements for Their Use as Beam Screen Materials for the FCC-hh	Patrick Krkotic, Accelerators division
10:15	Conventional Pd/CeO_2 vs CeO_2/Pd inverse catalysts for CO oxidation: Identification of the electronic nature of the nanoparticles and their interaction with the support	Xènia Garcia, Experiments division
10:30	Coffee Break	
11:00	Electrically conductive nanocomposites for additive manufacturing (3D printing)	Imran Khan, Experiments division
11:15	Ultrathin antiferromagnetic oxides with tunable properties	Anna Mandziak, Experiments division
11:30	Prevention of the spread of antibiotic resistance by conjugation, via the study of crucial proteins of the PLS20 conjugative plasmid at a structural and functional level	Nerea Bernardo, Experiments division
11:45	Molecular and structural biology of Auxin Response Factors	Isidro Crespo, Experiments division
12:00	Closing remarks	Caterina Biscari, ALBA Synchrotron director
12:15	End of the event	

Abstracts

Development of a 1.5 GHz Solid State Amplifier for the 3rd Harmonic Cavity for ALBA Synchrotron Light Source

Zahra Hazami
Thesis director: Francis Perez[1] & Yuri Koubychine[2]
1. ALBA Synchrotron, 2. Universitat Politècnica de Catalunya

Accelerators division

The 3rd harmonic system of ALBA storage ring, which is in the development phase, has been designed to achieve brighter beam with lower emittance and more current. For this system, 20kW RF power for each of the four scaled dampy cavities is needed. These cavities could provide 1MV of voltage to the beam at 1.5GHz.

To achieve this power, the solid state technology have been chosen, with an architecture of the transmitter system containing a tree diagram of 250W power amplifier modules based of transistors which sit in parallel by a combination technique.

There are many choices to set this array and the one which has been selected is to divide the 20kW overall power per cavity in 1kW modules.

This PhD project concentrates on the design, construction and tests of a 1kW module solid state power amplifier with all the belongings.

Abstracts

Evaluation of the Surface Impedance of High-Temperature Superconducting Coated Conductors (HTS-CC) and Requirements for Their Use as Beam Screen Materials for the FCC-hh

Patrick Krkotic
Thesis director: Montse Pont[1] & Joan O'Callaghan[2]
1. ALBA Synchrotron, 2. Universitat Politècnica de Catalunya

Accelerators division

The International Future Circular Collider (FCC) study is working on a conceptual design for a post Large Hadron Collider (LHC) particle accelerator using 16 T Nb_3Sn superconducting dipoles for achieving p-p centre-of-mass collision energies up to 100 TeV on a 100 km circumference machine. The baseline design of the FCC-hh beam screen is based on an octagonal shaped stainless-steel tube coated in its interior with copper. However, the low revolution frequency of the protons combined with a relatively high operating temperature of 40 K to 60 K provides a beam coupling impedance too close to the acceptable limit for a stable beam. The arising limitations might be overcome by looking for materials others than Cu. In this work we concentrate on the possible use of high-temperature superconductor coated conductor (HTS-CC) tapes. The HTS-CC envisages a lower surface resistance than copper under the required operating conditions (< 4 GHz, 16 T, 40-60 K). This motivates the exploration of the RF-performance of HTS-CCs based on $ReBa_2Cu_3O_7$ (Re=Y,Gd) as a function of temperature and magnetic fields, using a microwave non-contact dielectric loaded resonator technique and further, by developing a surface resistance measurement facility close to FCC operating conditions.

Abstracts

Conventional Pd/CeO_2 vs CeO_2/Pd inverse catalysts for CO oxidation: Identification of the electronic nature of the nanoparticles and their interaction with the support

Xènia Garcia
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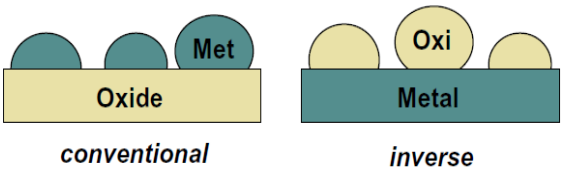
1. ALBA Synchrotron, 2. Universitat Politècnica de Catalunya

Experiments division

Cerium dioxide exhibits very interesting redox properties, given by its electronic configuration ([Xe]$6s^2 5d^1 4f^1$). The ability to easily change between its Ce^{3+} and Ce^{4+} oxidation states and the capacity to accommodate oxygen vacancies on its structure is known as oxygen storage capacity (OSC)[1], and makes ceria an ubiquitous constituent in catalytic systems for different applications, for instance as a component of automotive three-way catalysts (TWCs)[2,3].

The design of a catalyst usually includes a support with good redox properties loaded with a metallic active phase. Conventional Pd(NPs)/ceria (NPs: nanoparticles) and inverse ceria(NPs)/Pd catalysts (Scheme 1) have been shown to be excellent systems for fundamental studies[4]. The metal/oxide configuration is by far the most common in industrial applications while the inverse oxide/metal configuration is less common in technical applications but quite useful for fundamental studies in catalysis since it can lead to special structural and catalytic properties due to strong metal-oxide interactions, difficult to attain when depositing a metal on a regular oxide support. Thus, this inverse catalytic system can be used to study the interface between the ceria and the supporting metal, as well as the role of the oxide in a catalytic process and how the stability of different reaction intermediates depends on the nature of the oxide. Indeed, it has been shown that inverse model ceria catalysts are very convenient to clarify the reaction mechanism of important industrial reactions such as CO oxidation and CH_4 combustion[5]. Scanning electron microscopy (SEM) analysis allowed the characterization of the size of the synthesized CeO_2 polycrystals, which measured between 5 and 20 nm, with 10 nm as an average size.

Abstracts



Scheme 1. Different metal-oxide configurations of ceria-based catalysts[6]

On the other hand, X-Ray Diffraction (XRD) technique was performed to determine the size of Pd nanoparticles generated in the conventional Pd/CeO_2 catalyst, which measured about 8 nm, and also to confirm that the Pd weight loaded over ceria nanoparticles was of 4 wt%. Interferometric microscopy analysis provided information about the surface roughness of the inverse and direct catalyst configuration, with 100 and 2100 cycles of ALD reaction, respectively. The dispersion of Pd nanoparticles over the 2100 cycles ceria film produced an increase of the Ra value, directly related to its surface roughness, but it was still smoother than the inverse catalyst surface.

Lastly, Ambient Pressure X-Ray Photoelectron Spectroscopy experiments (NAP-XPS) were performed to characterize the near surface region of the samples during CO oxidation under operando conditions. The results demonstrated differences on the capacity of the catalysts to oxidize CO owing to palladium and ceria oxidation states of each sample. CeO_2 and palladium of the conventional Pd/CeO_2 catalyst appeared more oxidized than the other samples and, consequently, with higher ability to transfer oxygen atoms and thus to oxidize the CO.

1. Aneggi, E., Boaro, M., Leitenburg, C. De, Dolcetti, G. & Trovarelli, A. Insights into the redox properties of ceria-based oxides and their implications in catalysis. J. Alloys Compd. 412, 1096–1102 (2006).

2. Kim, G. & Grace, W. R. Ceria-Promoted Three-Way Catalysts for Auto Exhaust Emission Control. Ind. Eng. Chem. Prod. Res. Dev. 21, 267–274 (1982).

3. Trovarelli, A., Leitenburg, C. De, Boaro, M. & Dolcetti, G. The utilization of ceria in industrial catalysis. 50, (1999).

4. Rodriguez, J. A., Grinter, D. C., Liu, Z., Palomino, R. M. & Senananayake, S. D. Ceria-based model catalysts: fundamental studies on the importance of the metal – ceria interface in CO oxidation, the water-gas shift, CO2 hydrogenation, and methane and alcohol reforming. Chem. Soc. Rev. 46, 1824–1841 (2017).

5. Graciani, J., Vidal, A. B., Rodriguez, J. A. & Sanz, J. F. Unraveling the Nature of the Oxide – Metal Interaction in Ceria-Based Noble Metal Inverse Catalysts. J. Phys. Chem. C 118, 26931–26938 (2014).

6. Senanayake, S. D. et al. Probing the reaction intermediates for the water-gas shift over inverse CeOx /Au(111) catalysts. J. Catal. 271, 392–400 (2010).

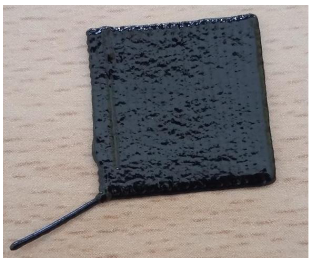
Electrically conductive nanocomposites for additive manufacturing (3D printing)

Imran Khan
Thesis director: Christina Kamma-Lorger[1] & Geoffrey Robert Mitchell[2]
1. ALBA Synchrotron, 2. Institute Politechnic Leiria

Experiments division

Additive manufacturing is a digital layer-by-layer printing process in which a computed aided design file provided to a machine with 3D dimensional control to print material additively. The project has number of phases including preparation of electrically conductive nanocomposites employing carbonaceous and metallic nanostructures and development of printing system for thermoset polymers. Thermoplastic polymers are reprocess able and upon application of the heat (extrusion) In this project, two different classes of polymers namely thermoplastic and thermosets will be used to prepare electrically conductive nanocomposites for additive manufacturing applications. Electrically conductive nanocomposites of biodegradable thermoplastic polymer (polycaprolactone) were printed in a layer-by-layer fashion using a bio extruder while a custom designed printer used to print epoxy resin based nanocomposites. 3D printed strands of polycaprolactone-based nanocomposites contained multiwall carbon nanotubes were prepared and subjected to uniaxial deformation. Electrical conductivity was measured under the effect of uniaxial deformation and the changes in the microstructure was studied using small angle x-ray scattering. A custom designed printer (Figure 1) was prepared to overcome limitations in material choice for additive manufacturing and offer functionality to 3D printed structures. The nanostructure materials used in this study are multiwall carbon nanotubes. The epoxy resin selected for this work is a colourless solid that melts slightly above room temperature and commonly known as bisphenol A diglycidyl ether. Triethylenetetramine is an amine based organic compound used to crosslink the epoxy resin. The print process is based on extrusion mechanism with/without the aid of a curing system (radiation or other form of energy) to cure the nanocomposites.

(a)



(b)

Figure 1: (a) The Custom designed printer to print electrically conductive epoxy-based nanocomposite. (b) 3D printed electrically conductive nanocomposite using the printer shown in (a).

The success of additive manufacturing in such kind of nanocomposites depends on extent of crosslinking or cure of epoxy nanocomposites to achieve optimum layer formation without collapsing. Moreover, layer adhesion is also important to acquire a 3D structure. In this context, the rheology of epoxy resin/carbon nanotubes nanocomposites will be achieved with the help of a thermoplastic polymer (polycaprolactone) to achieve an optimum print quality besides the processing parameters. The processing parameters include extrusion and flow rate of the material. The nanocomposites strands were printed and additively pilled to acquire a desired structure (Figure 1b) using a Computer-aided design file. The print quality and functionality (electrical conductivity) of the printed nanocomposites samples will be studied through morphological and electrical characterization of the printed samples using different characterization techniques including four probe method, small angle x-ray scattering (Figure 2), and high- resolution electron microscopy techniques (Figure 2c). The extent of epoxy reactions will be studied with Fourier transform infrared spectroscopy. The dynamic scanning calorimetry will be used to study Cure kinetics and hence to quantify the extent of chemical reaction or degree of cure in the printed nanocomposite samples. Electrical conductivity will also be measured during 3D printing of nanocomposite samples. Effect of relatively relevant print parameters will be concerned subject throughout this project. The project will give a new insight to additive manufacturing with nanocomposites for variety of other applications as well. Some of the recent results from epoxy based electrically conducting 3D printed nanocomposites are shown in Figure 2.

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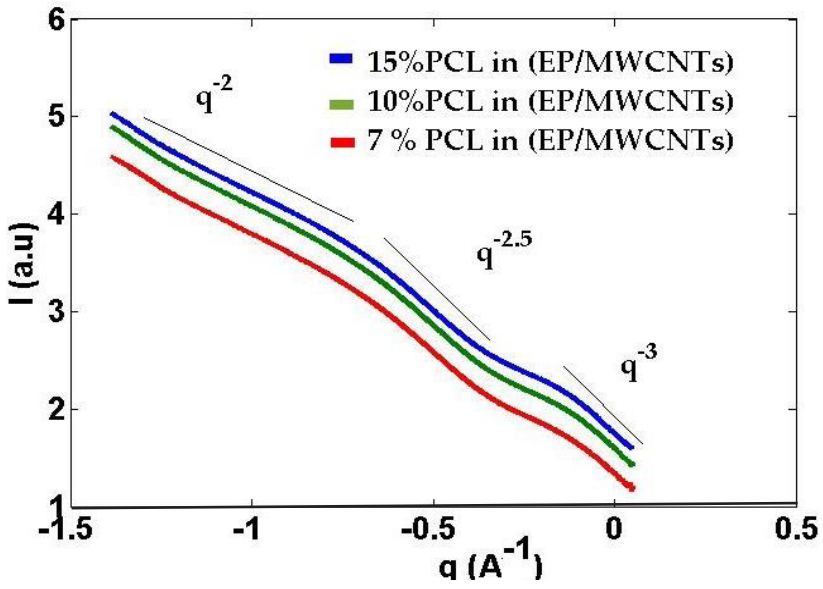
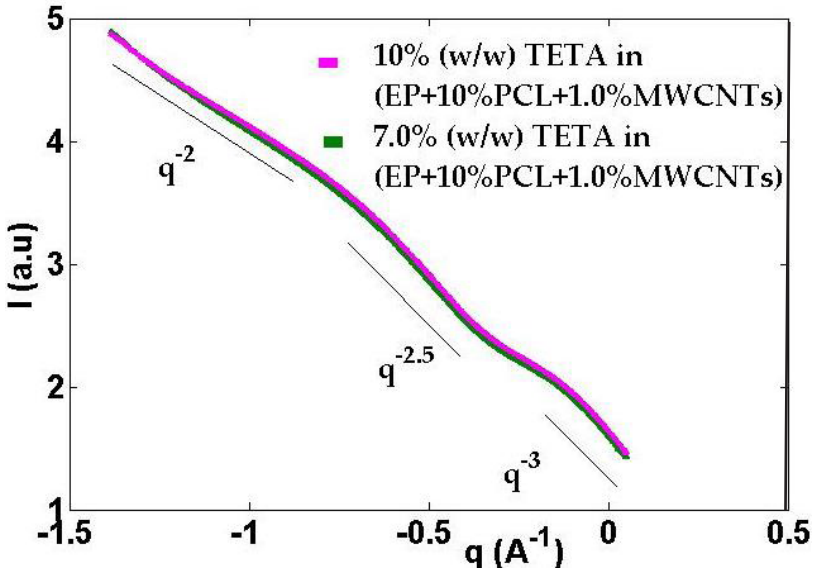
The potential applications for this study include electrical circuits, electrocardiogram and electroencephalogram electrodes and 3D printed energy storage devices. The results from this study will be used to compile the doctoral thesis.



(a)



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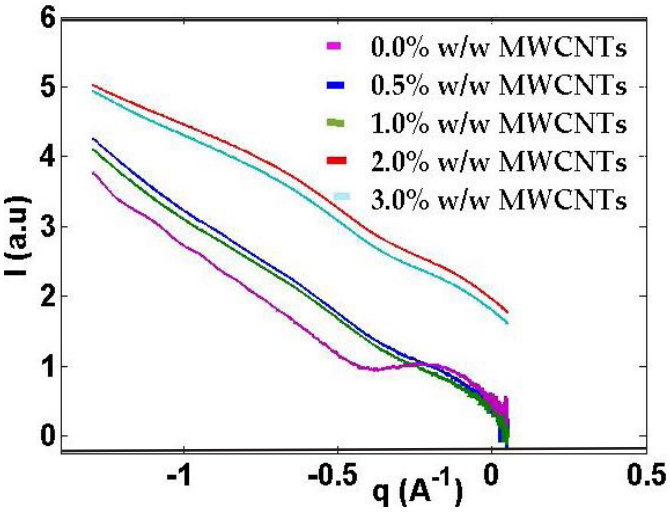

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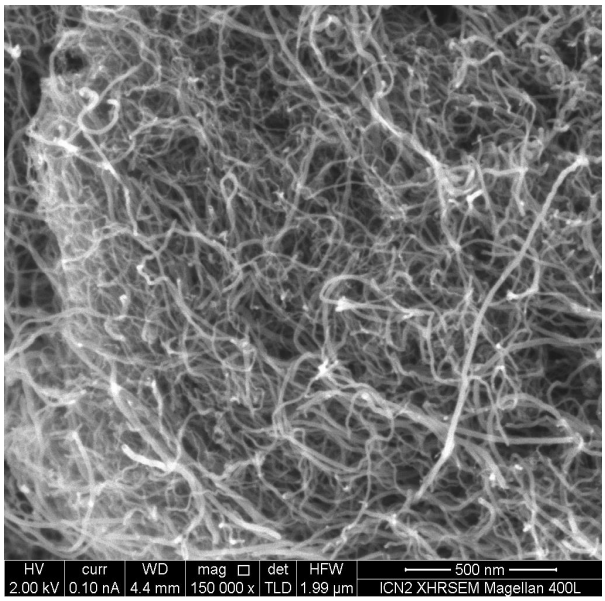
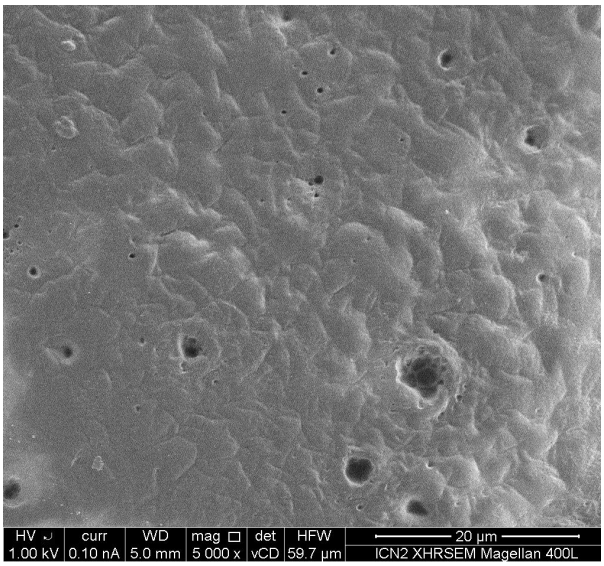


(d)



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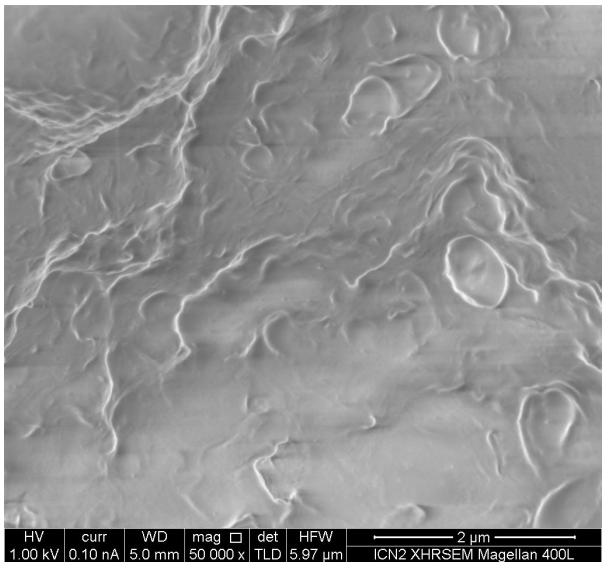

(f)

Figure 2: Fractal morphology evidenced from log-log plots obtained after integration of 2D patterns recorded in the SAXS experiments with variation in (a) PCL (b) TETA and (c) MWCNTs. Electron microscope images obtained from (d) pristine MWCNTs, (e) pure epoxy and (f)nanocomposites.

Abstracts

Ultrathin antiferromagnetic oxides with tunable properties

Anna Mandziak
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1. ALBA Synchrotron, 2. Instituto Física Química Rocasolano

Experiments division

Antiferromagnetic (AFM) oxides are attracting attention in spintronic applications due to a combination of interesting features: they are robust against perturbation due to external magnetic fields, they have no stray fields, and present ultrafast dynamics and large magneto-transport effects. We demonstrate the growth of ultrathin micrometric islands of antiferromagnetic metal monoxides with different compositions and heights in the range of nanometers. By combining high-temperature oxygen-assisted molecular beam epitaxy and low-energy electron microscopy we are able to optimize the external parameters so micrometric islands grow each from a single nucleus, resulting in an extremely low density of pinning centers and large antiferromagnetic domains, providing an ideal playground to understand fundamental properties of ultrathin microstructures.

In particular we study mixed Co-Ni monoxides, which share the same rocksalt structure. The chemical and magnetic characterization is performed by x-ray absorption spectroscopy and x-ray magnetic linear dichroism spectromicroscopy, as presented in Figure 1. Both end members are Mott insulators with antiferromagnetic order, and Neel temperatures that range from 291 K (CoO) to 525 K (NiO). We find that while NiO does not grow on Ru in a 3D form, precluding the formation of highly perfect micrometric islands, the addition of Co modifies the growth mode decreasing greatly the number of nucleation points. By varying the Co:Ni composition both the size and Neel temperature of laterally micrometric ultrathin islands can be adjusted at will.

Abstracts

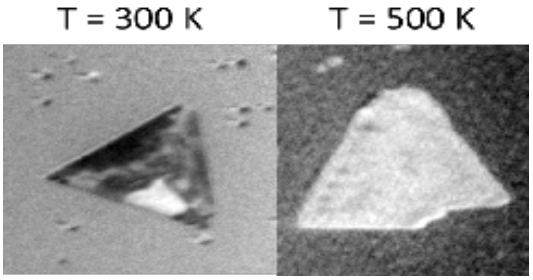

Figure 1. XMLD-PEEM images obtained at the Co L3 below (300 K) and above (500 K) the Neel temperature of the mon-oxide islands. Field-of-view for the 4 images is 2 μm.

[1] Z. Qiu, D. Ho, J. Barker, K. Yamamoto, O. Gomonay and E. Saitoh, Nature Materials, 2018.

Abstracts

Prevention of the spread of antibiotic resistance by conjugation, via the study of crucial proteins of the PLS20 conjugative plasmid at a structural and functional level

Nerea Bernardo
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1. ALBA Synchrotron

Experiments division

Antibiotics have always been considered one of the most important discoveries of the 20th century. This is indeed true, but nowadays we are facing a real issue, and that is the rise of antibiotic resistance. Genetic capacity of bacteria has improved due to mankind's overuse of antibiotics and, therefore, they have developed antibiotic resistance genes (ARG) during these last decades. Antibiotic resistance genes can be spread among bacterial populations via horizontal gene transfer (HGT). Conjugation is the HGT route that is predominantly responsible for the spread of ARG. Conjugative elements can be placed in the bacterial chromosome or they can also be integrated into plasmids, which are extrachromosomal, autonomously replicating units. Although several aspects of conjugation have been studied deeply over the last years, most of these studies concern Gram-negative (G-) bacteria. The gut microbiome of humans and animals, which has been proved to function as a ARG pool, contains both G- and Gram-positive bacteria (G+). The studies that will be performed will be focused on the native conjugative plasmid pLS20 of the G+ bacterium Bacillus subtilis.

Understanding the process by which ARG are transferred within the bacterial population, we realize about the relevance of studying relaxases and conjugation elements in a functional, biochemical and structural level. Hence, we will be able to gain insight into the mentioned process and devise rational approaches to reduce the development and spread of antibiotic resistance and, thus, avoid a critical situation in therapy, a return to a pre-antibiotic era.

Abstracts

Molecular and structural biology of Auxin Response Factors

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Thesis director: Roeland Boer[1] & Dolf Weijers[2]
1. ALBA Synchrotron, 2. Wageningen University and Research

Experiments division

Auxin regulates numerous growth and developmental processes in plants by controlling gene expression via a family of functionally distinct DNA-binding auxin response factors (ARFs). ARFs act as transcription factors bound to auxin response DNA elements (AuxRE) in the promoters of auxin-regulated genes and confer specificity to auxin response through selection of target genes. Sequence alignments reveal that the degree of conservation in DNA-interacting residues is very high, so how the specificity to the auxin response is mediated by ARFs is still unknown. On the one hand, a possible explanation for specificity to gene expression can be the fact that ARFs recognize two AuxRE forming a dimer. The spacing between the AuxREs can highly affect the protein dimerization due to the displacement and rotation of the major groove of DNA. Changing the spacing will force the ARF dimer to open and tilt, leading to an overall conformational change that could select the binding ARF. On the other hand, ARF-interacting partners can be conferring specificity. ARFs consist on three differentiated domains, DBD which binds to DNA, PB1 (III/IV) which is involved in protein-protein interactions and the middle region (MR), an unstructured domain. MR has been proposed to bind Brahma (BRM), a SWI/SNF ATPase that 'unlock' the chromatin for transcriptional activation. The exact sequence of MR and BRM that interact is still unknown. We are performing protein-protein interaction assays to find these sequences, which could reveal the interacting mechanics and gene specificity.