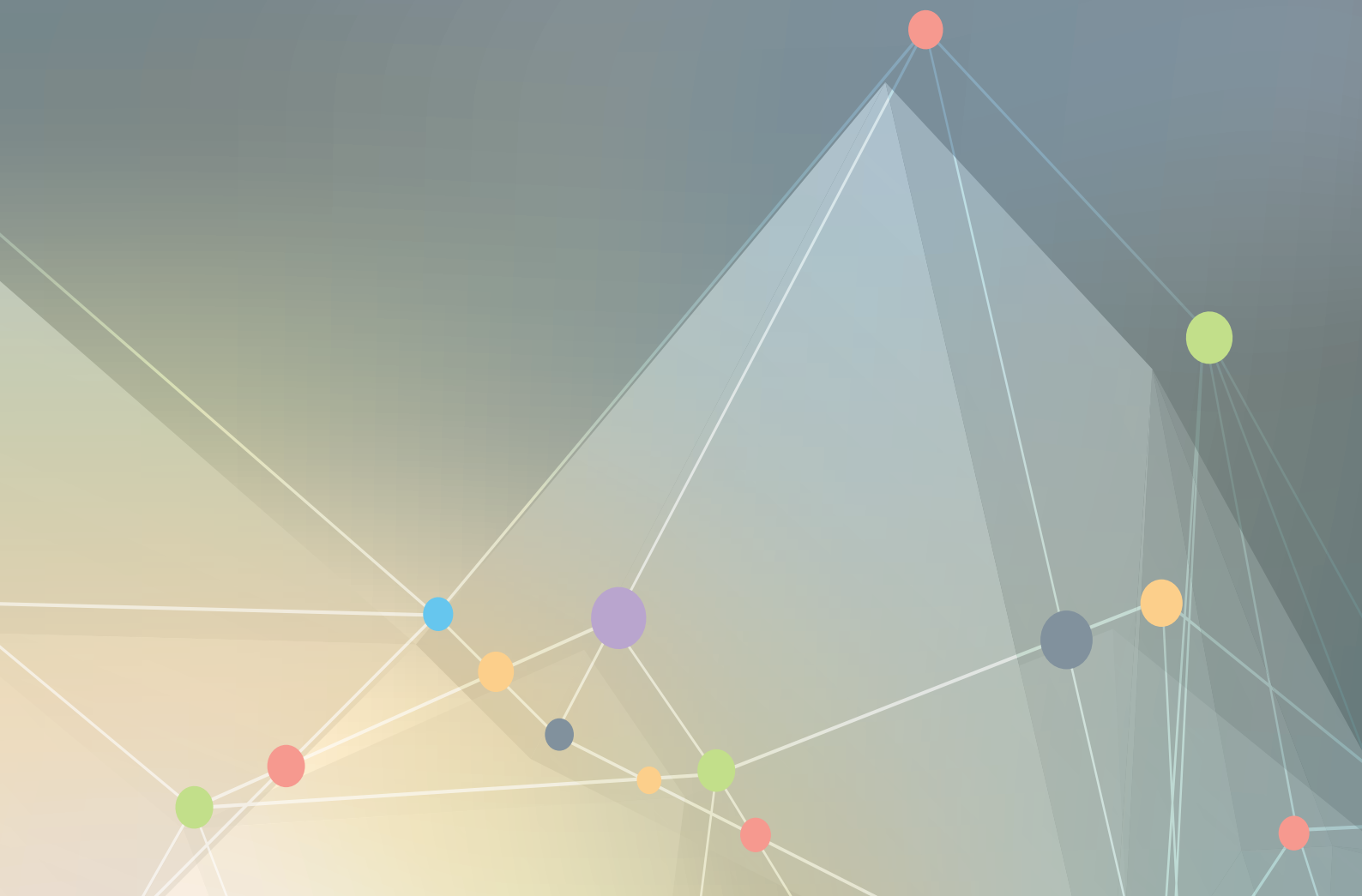


# BOOK OF ABSTRACTS

## Poster Presentations



## POSTERS AREA 3

A3

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### Thematic sessions

- Functional thin Films & Nanostructures: growth & properties
  - 2D-Materials
  - Nanoelectronics
- Nanomechanics: surface/ interface, composite nanomaterials, hybrid nanomaterials

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**Thematic Session:** Functional thin films and nanostructures: growth and properties

**Keywords:** SiC, detachment, Hydrogen implantation, thermal stress.

**Disciplinary field involved:** Physics

**Sustainable Development Goals\* eventually involved in your research:** reduction of crucial materials consumption.

## Detachment of SiC thin films by thermal stress and Hydrogen implantation

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SiC is a wide band gap semiconductor with a high potential for power electronic devices. However, issues mainly linked to the production costs of bulk SiC wafers have limited the expansion of SiC based electronics devices. Any low cost production approach is then welcome. This work deals with the production of thin films from a SiC wafer. Two techniques were used for that goal. The first method is based on stress induced spalling of bulk SiC wafers which has already been successfully applied on Si wafers [1]. Our Pioneer study on SiC using steel as stressor leads for the first time to the detachment of 62 $\mu$ m-thick SiC layer. The second method consists in ion cut of bulk SiC. For this work, SiC wafers were implanted with 2MeV hydrogen at high fluence. Implantation was followed by thermal annealing at 1300°C. We were able to detach a 32 $\mu$ m thick layer of SiC. This fits with Hydrogen range ( $R_p$ ) as simulated by SRIM. Moreover, in order to gain insight on structural changes at different stages of the detachment method, different characterization techniques such as Raman, UV-Visible spectroscopy and Photoluminescence were used and their results will be presented.

### Reference:

[1] Najoua Zayyoun *et al* 2019 *Surf. Topogr.: Metrol. Prop.* **7** 015005

**Thematic Session:** Functional thin films and nanostructures: growth and properties

**Keywords:** nanowires, sol-gel, luminescence, LED

**Disciplinary fields involved:** Chemistry, Physics

**Sustainable Development Goals\* eventually involved in your research:** Affordable and clean energy (Goal 7)

## Elaboration of multiscale nanostructured luminescent coatings by combining ZnO nanowires and $Y_3Al_5O_{12}:Ce^{3+}$ luminescent coatings

Aubry Martin<sup>1,2</sup>, Audrey Potdevin<sup>1</sup>, François Réveret<sup>1</sup>, David Riassetto<sup>2</sup>, Michel Langlet<sup>2</sup>, Geneviève Chadeyron<sup>1</sup>

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In this work, we have taken advantage of the specificities of zinc oxide (ZnO) nanowires (NWs) gratings (porosity, specific surface...) for developing efficient luminescent coatings for LED lighting. The nanowires were obtained by hydrothermal growth on a sol-gel deposited photo-sensitive seed-layer and the selective growth came from the UV photo-engraving of the seed-layer directly deposited on the sol-gel derived  $Ce^{3+}$ -doped yttrium aluminum garnet ( $Y_3Al_5O_{12}:Ce$  or YAG :Ce) coatings. NW gratings of different heights, periods and widths were developed. The addition of NWs gratings on the top of YAG:Ce coatings was expected to influence their optical properties. SEM, AFM and angle-dependent photoluminescence measurements have been carried out to study the morphological and optical properties of the obtained functional heterostructures. In particular, the optical study shows that this original design leads to a different angular distribution of light together with an increase in emission efficiency of YAG:Ce coating upon blue excitation compared to the flat coating. This enhancement is very promising since a higher efficiency is obtained without using a superior amount of rare-earth ions, which are a critical resource. Emission features have revealed to depend on the gratings parameters. Results will be discussed in reliance on multiscattering and resonance events for photons within the structure, allowing them to escape from the phosphor layer by taking optical paths different from those of the flat coating.

### **Acknowledgment:**

The authors acknowledge the French Agence Nationale de la Recherche for its financial support in the frame of the ANR SMARTLEDs project (ANR-19-CE08-0001).

**Thematic session:** Functional thin films and nanostructures: growth and properties

**Keywords:** plasmonics, conductive polymer, e-beam lithography, electrochemistry Chemistry

**Sustainable Development Goals:** Clean water and sanitation (Goal 6)

## From Noble Metal Plasmonic to Organic Plasmonic

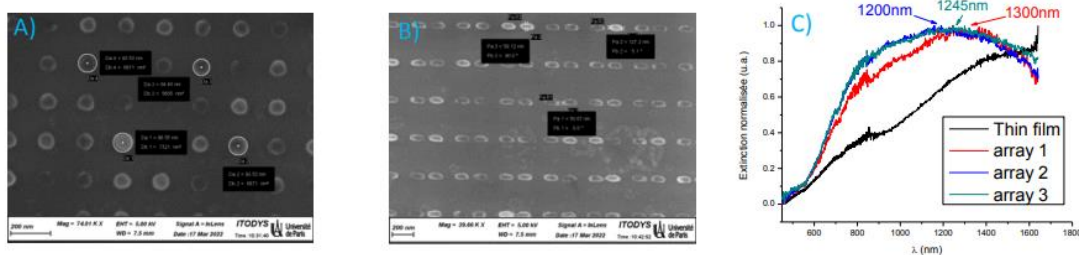
Pierre Bléteau<sup>1</sup>, Sarra Gam-Derouich<sup>1</sup>, Jean-Christophe Lacroix<sup>1</sup>

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Localized surface plasmon resonance has been extensively studied with metallic nanoparticles. The most used metals are gold, silver or platinum. However, the scarcity, the price and the pollution caused by the extraction of these metals push the scientific community to look for new materials.

Conductive polymers are an alternative that has been very little studied despite the great advantages they can bring. Conductive polymers not only avoid the use of rare and precious metals but also offer new functionalities. Thus, Magnus Jonsson's group in 2020 in *Nature*, shows that the nanostructuring of poly(3,4-ethylenedioxythiophene) (PEDOT) causes the appearance of a maximum in the infrared band around 1500-2000nm [1], [2]. With the support of theoretical calculations, the group demonstrates that the maximum of this band can be predicted by assuming that PEDOT nanoparticles are plasmonic.

We have explored by electron lithography approaches the formation of surfaces of PEDOT nanoparticles or different conducting polymers. The nanoparticle synthesis we explored allows to build any type of nanoparticles, sphere arrays, dimer arrays, nanosticks and show similar properties to Jonsson's results (**Figure 1**). We then characterized these surfaces by extinction spectroscopy, SEM, AFM and RAMAN spectroscopy in an attempt to reveal localized surface plasmon resonance.



**Figure 1:** A) Array of 90nm diameter PEDOT spheres. B) Array of nanostick dimers, 120nm\*50nm. C) Comparison of normalized extinction spectra between PEDOT nanoparticles and a PEDOT thin film.

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**Thematic Session:** Functional thin Films & Nanostructures: growth & properties

**Keywords:** Molecular beam epitaxy (MBE), Nuclear magnetic resonance (NMR), thin film, ferromagnetism, anti-ferromagnetism.

**Disciplinary field involved:** Physics

## Growth and NMR study of high quality ordered $Mn_5(Si_x Ge_{1-x})_3$ thin films on Ge(111) substrate

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This poster will present the controlled and epitaxial growth of  $Mn_5(Si_x Ge_{1-x})_3$  thin films on Ge(111) substrate by Molecular beam epitaxy methods (co-deposition), as well as characterizations of their structural and magnetic properties by X-ray diffraction (XRD), Atomic force microscopy (AFM), Transmission electron microscopy (TEM), and Nuclear magnetic resonance (NMR).

$Mn_5Ge_3$  and  $Mn_5Si_3$  are two compounds exhibiting hexagonal  $D_{8h}$  structure (space group  $P6_3/mcm$ ) and they can be grown epitaxially on Ge(111) substrates<sup>1</sup>. However, they exhibit very different magnetic behavior.  $Mn_5Ge_3$  is a metallic ferromagnet that presents a high spin polarization of the conduction electrons at the Fermi level, a Curie temperature of 296K and a strong uniaxial magnetocrystalline anisotropy along the hexagonal  $c$  axis<sup>2</sup>. On the other hand,  $Mn_5Si_3$  is an antiferromagnetic alloy exhibiting a (meta)magnetic phase transition: antiferromagnetic with a chiral spin structure below 65K and collinear above<sup>3</sup>.

In earlier time, the electrical and magnetic properties of the bulk  $Mn_5(Si_x Ge_{1-x})_3$  materials have only been studied in the bulk phase by few research groups<sup>4,5</sup>, however, no studies were carried out on the thin films. Our work, studying on high quality ordered thin films, expands the structural and magnetic knowledge on these complex materials through various and complementary characterizations. <sup>55</sup>Mn NMR spectrum reveals the changes of local magnetic properties over Si concentrations. XRD shows the correlation between Si concentration and lattice structural parameter deformation and crystallinity. Through comprehensive analysis, we bring further insights on the transition between the ferromagnetic behaviors of the  $Mn_5(Si_0 Ge_1)_3$  films and the anti-ferromagnetic  $Mn_5(Si_1 Ge_0)_3$  films.

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## Acknowledgment:

S K thanks the COST-OPERA Short-Term Scientific Mission program.

The authors thank C Coudreau for the technical assistance on the MBE cluster.



**Thematic Session:** Nanomaterials

**Keywords:** Nanowires, hexagonal Ge, nanostructures

**Disciplinary field involved:** Material Science

**Sustainable Development Goals\* eventually involved in your research:** Industry, Innovation, and Infrastructure (Goal 9)

## Hexagonal Ge on self-assisted GaAs Nanowires in MBE

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Hexagonal Ge is predicted to have novel electronic and optoelectronic properties therefore attracting great interest in the field of optoelectronics [1]. So far, hexagonal (Si)Ge with direct bandgap and wavelength tunability have been fabricated using nanowires with gold as a catalyst [2]. However, it is not compatible with the current CMOS technology [3].

In our work, hexagonal Ge has been grown on the facets of self-assisted GaAs nanowires by MBE using VLS mechanism [4]. An extended pure wurtzite segment was maintained by tuning the V/III ratio to appropriate values [5]. Following the growth of the GaAs core, a Ge shell has been grown with a long hexagonal segment. The crystal structure of the nanowires has been characterized with high-resolution scanning transmission electron microscopy (STEM) and dark field transmission electron microscope (TEM). The Ge surface chemistry was studied by X-ray photoelectron spectroscopy (XPS), and photoluminescence spectroscopy (PL) was performed to investigate the optical properties of the hexagonal Ge phase. The results have shown that the growth mechanism induce a strong As doping in hexagonal Ge, which can be controlled in a certain extent. Furthermore, the quantum confinement can be achieved in hexagonal Ge, leading to a blueshift of the emission.

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**Acknowledgment:** This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 801512.

**Thematic Session :** Functional thin Films & Nanostructures: growth & properties

**Keywords:** ZnO, nanocrystals, photolithography, photoluminescence, optical coatings

**Disciplinary fields involved :** Material chemistry, photochemistry

**Sustainable Development Goals\* eventually involved in your research:** Affordable & clean energy (Goal7) ,Industry, Innovation & Infrastructure (Goal 9)

## Laser direct writing photoluminescent patterns from ZnO nanocrystals

Quentin Kirscher<sup>1,2</sup>, Samar Hajjar-Garreau<sup>1,2</sup>, Fabien Grasset<sup>3,4</sup>, Dominique Berling<sup>1,2</sup> and Olivier Soppera<sup>1,2</sup>

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Micro- and nanopatterning of metal oxide materials is an important process to develop electronic or optoelectronic devices. ZnO is a material of choice for its semiconducting and photoluminescence properties. In the frame of the nanoarchitectonics concept, we have developed and investigated a new process that relies on direct write laser patterning in the DUV range to prepare photoluminescent microstructures of ZnO at room temperature, under air. This process is based on a synthesis of colloidal ZnO nanocrystals (NCs) with a careful choice of the ligands on the surface to obtain an optimal (i) stability of the colloids, (ii) redissolution of the non-insolated parts and (iii) cross-linking of the DUV-insolated parts. The mechanisms of photocrosslinking are studied by different spectroscopic methods. This room temperature process preserves the photoluminescence properties of the NCs and the wavelength used in DUV allows to reach a sub-micrometer resolution, which opens new perspectives for the integration of microstructures on flexible substrates for opto-electronic applications. We also show that this concept can be extended to other metal oxide nanoparticles.



Figure : Photographs of the ZnO colloidal solution (left) and patterns on Si obtained by laser direct write Deep-UV photolithography (right) under UV-light illumination

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**Thematic Session:** Functional thin films & Nanostructures: growth & properties

**Keywords:** Nanoparticle reshaping, Self-organized Nanostructure, Pump-probe Microscopy, Ultrafast Dynamics, Plasmonic Nanocomposites

**Disciplinary fields involved:** Physics

**Sustainable Development Goals eventually involved in your research:** Quality Education (Goal 4), Reduced Inequalities (Reduces Inequalities)

## Picosecond dynamics of multipulse femtosecond laser-induced transformations in Ag/TiO<sub>2</sub> nanocomposites

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2. Univ Aix Marseille, CNRS, Centrale Marseille, Institut Fresnel, Marseille, France

Exploring ultrashort laser-induced phenomena in plasmonic nanocomposites is of great relevance due to the large number of applications of such materials<sup>1,2</sup> and the numerous fundamental mechanisms that interplay on multiple timescales. The detailed literature of universal ultrafast and fast phenomena is provided by pump-probe experiments in weak excitations,<sup>3</sup> but the number of contributions conducted in strong excitation conditions triggering irreversible material response is considerably more limited. Despite some remarkable contributions investigating such phenomena,<sup>4,5</sup> several aspects on the energy relaxation above sample transformation threshold need to be explored. Our work aims to reveal additional mechanisms involved in the plasmonic nanocomposite transformation induced by ultrafast laser light. The multipulse sub-picosecond to nanosecond dynamics in Ag nanoisland ensemble encapsulated between two ultrathin TiO<sub>2</sub> layers is investigated using two-color pump-probe microscopy experiment. The sample response exhibits strong pulse number-dependent features, both on the ultrafast and hundreds of ps time-scales. The time-resolved results are supported by *ex situ* transmission electron microscopy characterizations that reveal the morphological evolution of the sample. The chronology of the laser-excited system on the ultrashort and short timescales is proposed based on the combination of experimental techniques. In addition, the dynamics in the spallation regime revealed the features of film deformation on hundreds of ps timescale. The presented results extend the literature of mechanisms triggered in ultrashort laser-excited plasmonic systems in strong excitation conditions.

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**Thematic Session** Functional thin films and nanostructures : growth and properties

**Keywords** Plasmonics, nanoalloys, electron microscopy, laser vaporization, *in situ* characterization

**Disciplinary fields involved** Physics, materials

## Plasmonic properties and structure evolution of Ag-Fe nanoparticles produced by laser vaporization under reactive atmospheres

J.Ramade<sup>1</sup>, E.Cottancin<sup>2</sup>, M-A Lebeault<sup>2</sup>, C. Langlois<sup>3</sup>, L.Piccolo<sup>4</sup>, M.Broyer<sup>2</sup>, M.Hillenkamp<sup>2</sup>, J.Lerme<sup>2</sup>, F.Calvo<sup>5</sup>, M.Pellarin<sup>2</sup> Affiliation 1 (*calibri 10, black*)

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3. MATEIS, SNMS Team, INSALYON, Lyon, France
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Multimetallic nanoparticles offer the possibility to mix elements to achieve novel systems combining their respective properties, or even generate new ones. In this context, mixing a plasmonic metal such as silver with a reactive one allows to use the optical properties, especially the localized surface plasmon resonance (LSPR) as a probe to unravel the chemical structure, as its evolution under reactive atmospheres. It is thus important to develop optical setups allowing the *in situ* monitoring of chemical processes involved in such atmospheres. Here, we show the development of an *in situ* optical spectroscopy setup (figure 1.a) used to monitor the oxidation and the reduction of Silver-Iron AgFe [1,2] nanoalloys synthesized according to the Low Cluster Beam Deposition (LECBD) Technique[3]. The optical characterization of a large assembly were combined with the investigation of single NPs by Environmental Transmission Electron Microscopy [4] and Monte Carlo simulations of the structural stability at specific temperatures. Studies were performed for two compositions (Ag<sub>80</sub>Fe<sub>20</sub> and Ag<sub>50</sub>Fe<sub>50</sub>). We show that these metals, according to their phase diagram, initially segregate with a silver-enriched surface and that iron spontaneously oxidizes when exposed to air, leading to its diffusion and the formation of iron oxide at the surface. *In situ* optical spectroscopy alternatively performed under reducing and oxidizing conditions reveals that the oxidation and reduction of iron is a reversible process, directly observable on the optical spectra (figure 1.b) and in accordance with the optical simulations. Based on these results, a scenario depicting the restructuring mechanisms under oxidation and reduction is proposed.

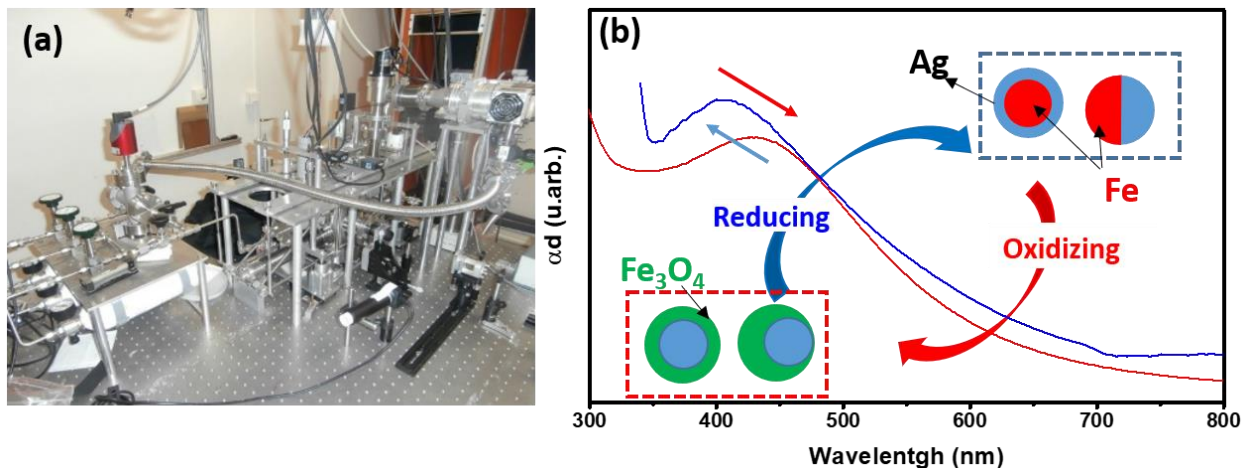


Figure 1 : (a) A picture of the environmental optical setup. (b) Optical spectra in situ acquired during after exposure of a reducing (blue) and oxidizing (red) atmosphere of Ag50Fe50 nanoparticles.

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**Thematic Session:** Functional thin Films & Nanostructures: growth & properties

**Keywords:** Plasmonics; metallic nanoparticle; growth; wetting

**Disciplinary field involved:** Physics

**Sustainable Development Goals\* eventually involved in your research:** -

## Plasmonics as a tool to reveal metal/dielectric adhesion at the nanoscale: application to buffer effect of transition metals

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The morphology and adhesion energy of nanosized metal particles supported on dielectrics escapes the rules established for large objects due the strong contribution of surface/interface in their energetics. The evolution of wetting during Volmer–Weber growth of nanoparticles is studied by *in situ* UV-vis surface differential reflectivity spectroscopy (SDRS). The integrated s-polarized SDR signal is shown to be proportional to the oscillator strength of the optically excited plasmon resonances parallel to the surface. Dielectric modelings showed that this quantity is a reliable reporter of the aspect ratio of the particles from which adhesion energy can be derived. Applied to noble (Ag, Au) or transition metals (Cr, Ni) and Zn on weakly interacting dielectric (Al<sub>2</sub>O<sub>3</sub>, SiO<sub>2</sub>, KBr) and semiconducting (TiO<sub>2</sub>, ZnO) substrates, this plasmonic approach evidences a universal “U”-shaped variation of the aspect ratio with film thickness and therefore size [1]. The first branch of the “U” is assigned to a size-dependent equilibrium shape related to surface/interface stress effects [2]. A significant decrease in adhesion energy parallels a rounding of the particles. The second branch partly stems from flattening due to incomplete coalescence. The potentialities offered by SDRS are also illustrated by the seed/adhesion effect of Cr buffer at the Zn/Al<sub>2</sub>O<sub>3</sub> interface [3].

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**Thematic Session:** Functional thin Films & Nanostructures: growth & properties

**Keywords:** Ruddlesden-Popper phases, MBE, HRSTEM, EELS, XRD

**Disciplinary fields involved:** Physics

**Sustainable Development Goals\* eventually involved in your research:** not applicable

## Structural disorder in SrTiO<sub>3</sub> based Ruddlesden-Popper phases

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(SrTiO<sub>3</sub>)<sub>n</sub>(SrO) Ruddlesden-Popper homologous series (RP phases) present outstanding physical properties such as high T<sub>c</sub> superconductivity, colossal magneto-resistance, low loss dielectricity, ferroelectricity, low thermal conductivity for heat harvesting, engineerable optical properties, all of them being tuned by the RP order  $n$  [1-3]. This flexibility of properties engineering boosts active researches.

The elaboration of these compounds is a true challenge: whereas RP phases with order  $n \leq 3$  can be synthesized by melt growth, there is no driving force for the spontaneous formation of RP phases with  $n > 3$  [4]. The latter can be elaborated by epitaxial growth, and particularly by molecular beam epitaxy (MBE) allowing layer by layer deposition. However, the RP structural quality is highly sensitive to incident elemental flux drift, which typically cause the formation of vertical SrO stacking faults [5] causing structural disorder and affecting the RP functional properties.

In this contribution, we will present a detailed High Resolution Scanning Transmission Electron Microscopy and Electron Energy Loss Spectroscopy study of the structural disorder of (SrTiO<sub>3</sub>)<sub>n</sub>(SrO) thin layers grown by molecular beam epitaxy on SrTiO<sub>3</sub> substrates. We will particularly focus on the different vertical SrO stacking fault configurations and their impact on the RP phase order. To have a multi-scaling approach, we will also compare and correlate HRTSTEM with X-ray Diffraction analysis for a better and detailed understanding of the structural disorder in SrTiO<sub>3</sub> based Ruddlesden-Popper phases.

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**Thematic Session:** Functional thin Films & Nanostructures: growth & properties

**Keywords** (max. 4-5): thin molecular layer, spin cross-over molecules, epitaxial strain

**Disciplinary field involved:** Physics

**Sustainable Development Goals\* eventually involved in your research: -**

## Structure of spin-crossover molecules ultra-thin films on Cu(110)

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Spin crossover (SCO) molecules present two spin states that can be controlled by external stimuli such as light or temperature. Their ability to switch makes them promising for incorporation in molecular spintronic devices. In this purpose, it is mandatory to understand how the properties of spin crossover molecules are modified when in direct contact with metallic substrates and how the growth of molecular films is governed by the substrate. Additionally, the bistability, i.e. the ability to reversibly switch between two stable states in the hysteretic temperature range, is an important property that needs to be controlled at the nanoscale. Grazing incidence x-ray diffraction measurements on monolayer of  $\text{Fe}[\text{HB}(3,5-(\text{CH}_3)_2\text{Pz})_3]_2$  (Pz=pyrazolyl) adsorbed on Au(111) and Cu(111) substrates enable us to evidence that an epitaxial relationship between the molecular layer and the substrates exists<sup>1</sup>. This has a direct consequence on the transition from one spin-state to the other either by using temperature<sup>2,3</sup> light<sup>4</sup> or electric field<sup>5</sup> as external stimuli. Here, we will discuss in detailed the molecular structure of  $\text{Fe}[\text{HB}(3,5-\text{Me}_2\text{Pz})_3]_2$  ultra-thin films adsorbed on Cu(110). For sub-monolayer coverage, the molecules arrange in a nearly hexagonal structure which is a reconstruction of the underlying Cu(110). For larger thicknesses, an additional molecular network appears which resemble the [100] plane of the bulk molecular crystal. By XAS measurements, we demonstrated that for a one-monolayer-high layer, the molecules are locked in the high spin state; while for a six-monolayer-high layer the molecules recovered their spin-crossover properties.

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**Thematic Session:** Functional thin film & Nanostructure: growth & properties

**Keywords:** STM, TEM, DFT, complex intermetallics, surface alloy.

**Disciplinary fields involved:** Physical chemistry /Materials science

**Sustainable Development Goals\* eventually involved in your research:** Responsible Consumption & Production (Goal 12)

## Surface and interface structures of Al-Fe thin films: from metastable to high temperature phases

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Low coefficients of friction, low adhesion or even enhanced oxidation resistance are among the surface properties that have motivated the production of several Al-based complex intermetallics as thin films. For specific deposition processes such as hot-dip aluminizing of steel or cast-iron parts, the formation of complex intermetallics can also occur fortuitously at the coating-substrate interface [1]. Here, the microstructure of the resulting coating generally consists of several layers of Al-Fe intermetallics with different interfaces which *in fine* will dictate the adhesion, the lifetime and the mechanical properties of the thin film.

To gain more insights into the formation of the Al-Fe intermetallics phases and the associated interfaces with the surrounding matrix, the adsorption of Fe on Al(100) and Al<sub>9</sub>Co<sub>2</sub>(001) surfaces has been investigated combining both experimental and theoretical methods. We will show how a structural similarity between Al(100) *fcc* planes and pure Al layers present in the metastable Al<sub>9</sub>Fe<sub>2</sub> compound stabilised this binary phase [2]. The Al<sub>9</sub>Fe<sub>2</sub>(001) surface and Al<sub>9</sub>Fe<sub>2</sub>(001)/Al(100) interface structures will be described at the atomic scale along with the epitaxial relationship. In a second part, we will demonstrate how intermetallics of various structural complexities can be selectively grown on Al<sub>9</sub>Co<sub>2</sub>(001) for different Fe coverages and dosing temperatures. The successful epitaxial growth of the high temperature Al<sub>8</sub>Fe<sub>5</sub>, B2 AlFe, and approximant Al<sub>13</sub>Fe<sub>4</sub> phases will be presented. Finally, the Al<sub>8</sub>Fe<sub>5</sub>(100)/Al<sub>9</sub>Co<sub>2</sub>(001) interface modeled by *ab initio* calculations will be discussed [3].

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**Thematic Session:** Functional thin Films & Nanostructures: growth & properties **Keywords:** Al doped ZnO, thin film, thermal treatment, AR-XPS, XAS

**Disciplinary field involved:** Physics

**Sustainable Development Goals\* eventually involved in your research: -**

## Thermal treatments effect about Al position and environment inside AZO thin films

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Al doped zinc oxide (AZO) thin films have already proved their efficiency as transparent conductive oxide (TCO) in various fields, such as solar cells or low emissivity coating, for several decades.[1] However, despite extensive literature about synthesis conditions and the optimization of conductivity features, some misunderstandings persist. The effect of thermal treatment and more precisely the possibility of formation and segregation of the second phase is still an obstacle to the control of AZO films properties.[2] In our work, AZO films were synthesized by direct current magnetron sputtering deposition. Several parameters, such as substrate deposition (ZnO or Si monocrystal), the atmosphere during sputtering (with or without oxygen), type of target (metallic or ceramic), and doping rate (1, 2, or 3 wt%) have been modified to have a large panel of samples. Afterward, each of them was submitted to high-temperature annealing (under a normal or vacuum atmosphere) to understand the influence of all these parameters. In agreement with the literature, atomic force microscopy (AFM) and X-ray diffraction (XRD) revealed an improvement in crystalline quality and an increase in grain size after annealing.[3] Angle-resolved x-ray photoelectron spectroscopy (AR-XPS) highlights aluminum surface enrichment after annealing. X-ray absorption spectroscopy (XAS) spectrums indicate  $ZnAl_2O_4$ (spinel) phase apparition after 800°C annealing under a normal atmosphere for all samples supported on silicon. All that results are a new step toward the understanding of phase formation inside AZO thin film and how to avoid it to conserve a low resistivity.

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**Thematic Session:** 2D materials

**Keywords:** Silicene, Germanene, Scanning Tunneling Microscopy, Growth

**Disciplinary field involved:** Physics

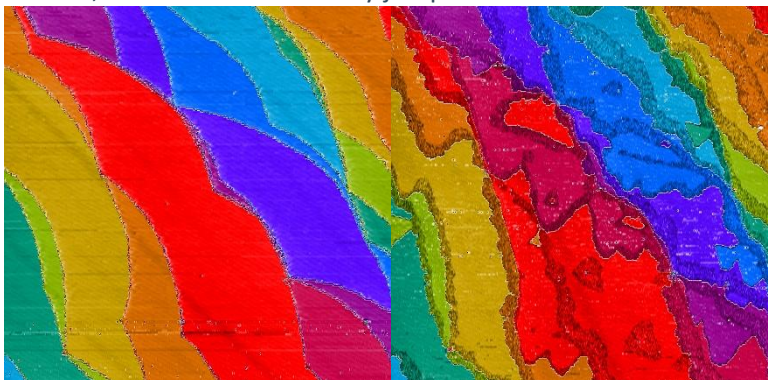
## Atomistic growth mechanisms of Xenes epitaxial layers revealed by in-situ STM

L. Florean,<sup>1</sup> K. Zhang,<sup>1</sup> A. Curcella,<sup>1</sup> R. Bernard,<sup>1</sup> Y. Borensztein,<sup>1</sup> H. Cruguel,<sup>1</sup> G. Prévot<sup>1</sup>

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2D-Xenes (where X = Si, Ge ...) are a class of two-dimensional materials from the group IVA that possess electronic properties different from those of the corresponding 3D bulk. For example, silicene (germanene), that corresponds to a buckled hexagonal plane of Si (Ge), has an electronic structure similar to the one of graphene. However, they cannot be obtained by exfoliation and must be synthesized on a substrate. The successful growth of silicene and germanene has been claimed on various metal substrate, such as Ag, Au, Pt, Al, but many of the results found are controversial since the involvement of the substrate during growth is unknown.

We have developed a series of tools to follow by Scanning Tunneling Microscopy (STM) the epitaxial growth of Xenes monolayers. For all systems studied (Si/Ag, Si/Al, Si/Au, Ge/Ag, Ge/Al), we have observed that the IVA atoms interact strongly with the substrate, in contradiction with the corresponding bulk phase diagrams showing for all cases a negligible mutual solubility in the temperature range studied [1-5]. Depending on the couple IVA /substrate, we observed either growth of Xene domains inserted in the substrate terraces, surface alloy formation or bulk alloy formation. The analysis of atomic motion and of the density of domains allows us to extract the kinetic barriers associated to the mechanisms of exchange between substrate and IVA atoms, and to the diffusion by jumps on the substrate.



**Figure.** Evolution of the Ag(111) surface before and after deposition of 0.42 ML Si at 506 K. The exact same area (600 x 600 nm<sup>2</sup>) is shown on both images.

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**Thematic Session:** 2D Materials

**Keywords:** Graphene oxide, Raman measurements, SPM measurements, Correlative approach

**Disciplinary fields involved:** Chemistry, Physics, 2D Materials

## Correlative imaging of single graphene oxide flake: sample selection and limitations

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Graphene is of major interest for a large number of applications currently under development. However, its production remains complex in large quantities. Graphene oxide (GO) is much easier to synthesize and is therefore often used as a precursor for the preparation of reduced graphene oxide (rGO), whose morphology and physicochemical properties tend more towards graphene as the reduction is more advanced. However, rGO contains a number of structural defects that influence its physicochemical properties, such as its electrical and thermal conductivity, etc. To control this reduction, it is interesting to follow the evolution of these physico-chemical properties during the GO reduction process, starting with a good characterization of the properties of the initial GO. Based on our expertise in hybrid metrology specifically developed for measuring single nano-object [1], we have chosen to characterize the GO through the correlation of various microscopy technique on single GO flake: Raman spectroscopy/microscopy, Scanning Electron Microscopy (SEM), Atomic Force Microscopy and derivate techniques (AFM, SThM, SMM, KPFM). This correlative imaging approach implies that each limitation of each technique have to be considered to select the ideal sample and substrate. Moreover, strategy must be put in place so that when correlative microscopy is performed the location of the flakes is easy and the least invasive techniques are used before the most invasive ones. We show in the poster the limitation induced by the various techniques of microscopy.

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**Thematic Session:** 2D Materials

**Keywords:** MXenes, 2D materials, Heterogeneous catalysis, Hydrogenation, CO<sub>2</sub>

**Disciplinary fields involved:** Chemistry, Material Science

**Sustainable Development Goals\* eventually involved in your research:** Climate Action (Goal 13)

## Determination of the potential of the 2D transition metal carbides (MXenes) for the heterogeneous catalysis. Application to the hydrogenation reactions in gas phase and liquid phase.

**Zheming Li<sup>1</sup>, Lola Loupias<sup>1</sup>, Gwendoline Lafaye<sup>1</sup>, Anthony Le Valent<sup>1</sup>, and Stéphane Célérier<sup>1</sup>.**

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Nowadays, the research about two-dimensional (2D) transition-metal carbides, nitrides and carbonitrides (MXenes) is growing and gaining more and more attention in many different fields, such as catalysis, electromagnetic interference shielding, energy storage, medicine and many others [1]. This is due to the high chemical richness of MXene family with more than 40 successfully synthesized configurations and more than 100 predicted stoichiometric compositions. [2] The MXenes with the general formula of  $M_{n+1}X_nT_x$ , where M is a group 3-6 early transition metal, X is carbon (C) and/or nitrogen (N),  $T_x$  are the surface termination groups (for example, -OH, -O-, -F etc.) and n, the layer number (1 to 4) are obtained by removal of the A element of their corresponding 3D precursors, the MAX phases, with  $M_{n+1}AX_n$  formula, where A is an element mainly from column 13-14 of the periodic table.

Recently, MXenes were explored in the domain of heterogeneous catalysis showing promising potential. [3] Besides their physical and chemical properties, MXenes, with a high surface/volume ratio, characteristic of 2D material, can offer the potential active sites for different heterogeneous catalytic processes. For example, Mo<sub>2</sub>CT<sub>x</sub> MXene was already successfully used as active support of copper for CO<sub>2</sub> hydrogenation. [4]

At IC2MP, molybdenum and titanium based MXenes are synthesized, characterized and studied as a catalyst and/or support for two reactions: (i) in the liquid phase for the selective hydrogenation of aldehydes (biomass valorization) and (ii) in the gas phase for the CO<sub>2</sub> hydrogenation to methanol.

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**Thematic Session:** 2D Materials

**Keywords:** MXene, 2D transition metal carbides, electrical properties, optical properties, spectroscopic ellipsometry

**Disciplinary fields involved:** Physics, Chemistry

## Optical and electrical properties of titanium and molybdenum carbide 2D layers thin films

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MXenes are a family of 2D transition metal carbides and nitrides obtained from the exfoliation of nanolaminated ceramics named MAX phases. [1] Their chemical formula is  $M_{n+1}X_nT_x$ , where M is a transition metal, X is C and/or N,  $T_x$  are surface terminations (e.g. -O, -OH, -F) inherited from the chemical exfoliation process and  $n = 1, 2$  or  $3$ . Generally speaking, MXenes are hydrophilic and have a metallic electrical behavior, making these materials promising for numerous applications, including transparent conductive thin films.[2] However, calculations based on Density Functional Theory predict some Mo-based phases to have a semiconductor like behavior [3] which would significantly increase the application range of MXenes, including e.g. thermoelectric generators.[4] In this work, we investigate experimentally the role of the Ti to Mo substitution on the electronic properties of MXene by focusing on the optical and electrical properties of  $Ti_3C_2T_x$  and  $Mo_2Ti_2C_3T_x$  spin coated thin films (figure 1). The films are a collection

of MXene flakes and their electrical transport properties comprise two contributions, namely: intra and inter flake transport. [5] Optical measurements by spectroscopic ellipsometry in infrared range allows one to probe the intra-flake transport only. By coupling optical and electrical measurements, we are thus able to better understand the electrical properties of the films and evidence the differences in terms of transport mechanisms (i.e., charge carrier densities, intra/inter flake electron mobilities) for these two compositions.

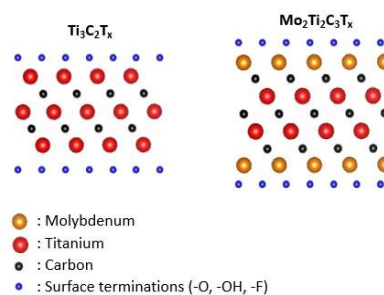


Figure 1: schematic representation of  $Ti_3C_2T_x$  and  $Mo_2Ti_2C_3T_x$  crystal

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## Acknowledgment:

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**Thematic Session:** Nanomechanics: surface/interface, composite nanomaterials, hybrid nanomaterials

**Keywords:** Twinning, Molecular Dynamics, Nanolamellar Ag/Cu, Interfaces

**Disciplinary field involved:** Physics

## Atomic Scale Simulations of Twins – Interfaces Interaction in a Nanolamellar Ag/Cu System

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1. *Prime Institute, Department of Physics and Mechanics of Materials, University of Poitiers, ISAE-ENSMA, CNRS Poitiers, France*

For a decade, modern synthesis methods, such as severe plastic deformation, were developed and applied to metallic lamellar composites in order to reduce their layer width to less than 100 nm. Nowadays, these new nanostructured materials offer outstanding mechanical properties which are partly attributed to the role increasingly played by interfaces in their plastic behavior. This role is crucial in the nanolamellar Ag/Cu composite. Indeed, silver is known to twin easily under mechanical stresses whereas copper needs more specific conditions to do so. In the Ag/Cu composite, experimental studies by transmission electron microscopy showed that the deformation twins coming from silver layers may readily cross some interfaces and spread in copper layers. In that respect, it extends the spectrum of the mechanical conditions for twinning in copper. Although these observations were then completed by atomistic simulation studies, several questions for a better understanding of elementary mechanisms remain unanswered. Atomistic simulations, and mainly molecular dynamics, fit particularly well to the nanometric scale and to the study of elementary mechanisms involved. In our study, we consider bi-metallic Cu/Ag multilayers in which different types of semi-coherent interfaces coexist, as observed experimentally. The global response of the whole system is computed, and new elementary mechanisms involved in the formation and growth of mechanical twins are identified. Special attention is given to the role of the misfit interfacial dislocations mesh in these mechanisms.

**Thematic Session:** Nanomechanics: surface/interface, composite nanomaterials, hybrid nanomaterials

**Keywords:** focused ion beam, electron microscopy, EELS, time and position sensitive detectors

**Disciplinary field involved:** Physics

**Sustainable Development Goals\* eventually involved in your research: -**

## Improved nanometric control of ions and electrons via laser ionization and coincident detection

**Clelia Bastelica, Yan Picard, Daniel Comparat**

*Université Paris-Saclay, CNRS, Laboratoire Aimé Cotton, 91405, Orsay, France*

Our projects aims at achieving breakthroughs in focused ion and electron beams, exploiting monochromaticity in the low-energy domain (eV-keV). Using ionization of a neutral atomic species and on the simultaneous production, detection and control of both the ion and the electron we propose to develop three innovative prototypes:

1. A focused ion beam using feedback control with unprecedented focused properties. This will be used to realize semiconductor circuit-editing at the (sub-)nm scale.
2. A deterministic source of (potentially) any type of ion for controlled implantation at the nm level. This will be used for on-demand doping of quantum devices.
3. A high-resolution electron-energy-loss microscope (HREELM) with precise knowledge of the electron energy and the position on the sample. It be used to realize both imaging and vibrational spectroscopy for surface analysis.

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Ion and electron ghost imaging; A. Trimeche, C. Lopez, D. Comparat, and Y. J. Picard; Phys. Rev. Research 2, 043295 (2020); <https://doi.org/10.1103/PhysRevResearch.2.043295>

Real-time trajectory control of deterministically produced ions; C. Lopez, A. Trimeche, D. Comparat, Y.J. Picard; Phys. Rev. Applied 11 064049 (2019); <https://doi.org/10.1103/PhysRevApplied.11.064049>

Design for a high-resolution electron energy loss microscope; M. Mankos, K. Shadman, R. Hahn, Y. J. Picard, D. Comparat, O. Fedchenko, G. Schönhense, L. Amiaud, A. Lafosse, N. Barrett; Ultramicroscopy, 207 112848 (2019); <https://doi.org/10.1016/j.ultramic.2019.112848>

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### **Acknowledgment:**

This project has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (Grant agreement No. 101055250). This work was also supported by the ANR FIBback (ANR-21-CE42-0010).

Funded by the European Union. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the European Research Council. Neither the European Union nor ERC can be held responsible for them.

**Thematic Session:** Nanomechanics: surface/interface, composite nanomaterials, hybrid nanomaterials

**Keywords:** Nanomechanics, molecular dynamics, load vs displacement-control, nanoparticles

**Disciplinary fields involved :** Physics, Computer science

## Load versus displacement controlled nanomechanics : insights from atomistic simulations

**Hugo Iteney<sup>1\*</sup>, Olivier Thomas<sup>1</sup>, Thomas W. Cornelius<sup>1</sup>, Jonathan Amodeo<sup>1</sup>**

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The characterization of nano-objects takes a particular interest due to their enhanced mechanical properties when compared to bulk materials. In nanomechanical experiments, two ways of controlling the load are currently available depending on the brand device used *i.e.*, namely the load and the displacement-controlled modes. Most of SEM compression setups used for compression tests on pillars or nanoparticles are load-controlled or benefit of a software-based feedback loop on displacements that is less accurate than the scarcer intrinsic displacement-control setups. On the other hand, displacement-control molecular dynamics (MD) simulations are generally designed for the sake of simplicity.

Thus, the comparison between simulations and experiments is not always straightforward. On one hand, simulations where the displacement of the indenter is monitored show a huge stress drop when the first dislocations nucleate while huge strain bursts are observed in load-controlled experiments.

In this study we present an original load-control MD setup to discuss load vs displacement control experiments and simulations. Here we apply our approach to the cases of Wulff-shaped Au and Ag nanoparticles (NPs) recently investigated using experimental nanocompression tests [1, 2]. First, the mechanical response of Au NPs obtained using the load-control model is investigated. In contrast with the displacement-controlled simulations, the strain bursts are captured and the magic “pancake” shape of metal NPs often observed at the end of nanocompression experiments is now explained. A specific attention is paid to the evolution of the dislocation microstructure during the test in comparison to the displacement-controlled simulations. A similar approach is then applied to Ag NPs for which the load-control analytical model proposed in ref. [1, 2] is directly faced to the simulation’s outcomes. In the both cases, implications for nanomechanics experiments are discussed.

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THE NANOSCIENCE MEETING

# Poitiers

March, 15, 16 and 17

# 2023



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**Thematic Session:** Nanomechanics: surface/interface, composite nanomaterials, hybrid nanomaterials

**Keywords:** cracking, plasticity, nickel, thin film, X-ray diffraction

**Disciplinary field involved:** Physics

**Sustainable Development Goals\* eventually involved in your research:** none

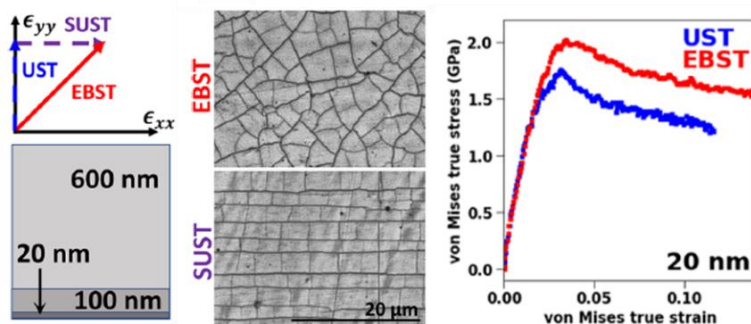
## Strain ratio and thickness effects on plasticity and cracking of nickel thin films

Pierre Godard<sup>1</sup>, Fatih Zighem<sup>2</sup>, Dominique Thiaudière<sup>3</sup>, Damien Faurie<sup>2</sup>, Pierre-Olivier Renault<sup>1</sup>

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2. Université Sorbonne Paris Cité, LSPM - CNRS, Villetaneuse, France
3. Synchrotron SOLEIL, Gif sur Yvette, France

We are interested in the cracking of nickel thin films deposited on flexible substrates. We have in particular illustrated that an equibiaxial loading leads to an isotropic ("dried mud") pattern, whereas if one loads first in one direction, then in the perpendicular direction, the cracks form a rectangular network. We can therefore apply the same ( $\epsilon_{11}, \epsilon_{22}$ ) strain but having different crack patterns [1]. This study is completed by a thickness effect, with films of 20, 100 or 600 nm [2].

We combine digital optical image correlation to characterize the applied strain with X-ray diffraction to measure the stresses in the film. First, well-known effects are found: for example, the thinner a film, the greater its mechanical resistance, or the fact that the nucleation of cracks appears at increasingly large strains as the film thickness decreases.



We have also shown that the mechanical resistance, the elastic limit and the cracking limit depend on the loading path. However, the average spacing between two cracks, on these three tests, is very well approximated by  $125h$ , where  $h$  is the thickness of the film.

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### Acknowledgment:

This work was funded by the French National Research Agency, grant reference ANR-19-CE08-0007. This work also pertains to the French government program "Investissements d'Avenir" (LABEX INTERACTIFS, reference ANR-11-LABX-0017-01 and EUR INTREE, reference ANR-18-EURE-0010).



**Thematic Session:** Nanomechanics: surface/interface, composite nanomaterials, hybrid nanomaterials

**Keywords :** Iron oxide nanoparticles – Thermal decomposition – Nucleation and growth control – Nanocomposite – Mechanical properties.

**Disciplinary fields involved :** Chemistry, Mechanics

**Sustainable Development Goals\* eventually involved in your research:** Positively impact the thermal and mechanical characteristics of the packaging material.

## Study of the mechanical properties of polymers reinforced with nanoparticles of adjustable size, shape and surface chemistry

**Sakina MEFTAH<sup>1,2</sup>, Fahmu BEDOUI<sup>1</sup>, Djimédo KONDO<sup>3</sup>, Anh-tu NGO<sup>2</sup>, Isabelle LISIECKI<sup>2</sup>**

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3. Institut Jean-Le-Rond-d'Alembert for mechanics, Sorbonne université, 4 Place de Jussieu, 75005 Paris, France

Researchers are mainly interested in finding solutions to improve the properties of polymers by incorporating nanoparticles (NPs). The central point of the development of such materials lies in the understanding of the polymer/NP interface which plays the key role in the improvement of its properties. For this purpose, we plan to study the evolution of the mechanical properties of these materials as a function of the structural and chemical characteristics of the incorporated nanoparticles (size, shape, surface chemistry). To achieve this, we prepare our model samples of iron oxide nanoparticles by thermal decomposition of an organometallic precursor [1] through the expertise of MONARIS laboratory in colloidal chemistry [2][3]. The size of the nanoparticles (3, 6 and 12 nm) is controlled by adjusting several parameters: nature of the solvent, reaction temperature, reaction time, moisture and purity of the reagents. For each NP size, we use three different coating ligands (acids) characterized by different hydrocarbon chain lengths (C8, C12 and C18). The surface chemistry of the NPs is studied by infrared spectroscopy. We will also study other forms of nanoparticles (cubic and triangular) obtained by adding 'impurities' in the precursor. The flexibility of this system will allow a comprehensive study of the performances of these materials at the Roberval laboratory [4][5]. A final step of modelization by scale shifting is required to interpret and optimize the development factors of the material. This approach already developed at the institut Jean Le Rond D'Alembert, will be adapted to the materials studied in this thesis.

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THE NANOSCIENCE MEETING

# Positiers

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**Thematic Session:** Nanomechanics: surface/ interface, composite nanomaterials, hybrid nanomaterials

**Keywords:** Gold nanoparticles, Molecularly Imprinted Polymers, nanosensors

**Disciplinary fields involved:** Physical chemistry

**Sustainable Development Goals\* eventually involved in your research:** simple approach for synthesis of hybrid nanoparticles

## Synthesis of molecularly imprinted polymer-based hybrid nanosensors by optical near-field photopolymerization

**Amine Khitous<sup>1,2</sup>, Céline Molinaro<sup>1,2</sup>, Simon Gree<sup>1,2</sup>, Karsten Haupt<sup>3</sup>, Olivier Soppera<sup>1,2\*</sup>**

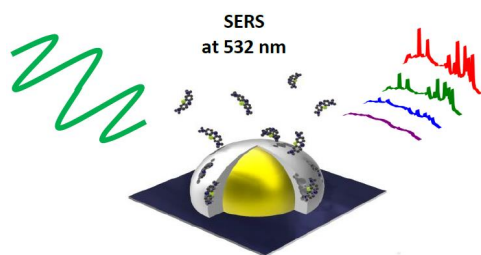
*1 Université de Haute-Alsace, CNRS, IS2M UMR 7361, F-68100 Mulhouse, France*

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A new simple, fast and versatile method for the functionalization of gold nanoparticles (AuNPs) by a nanoscale layer of molecularly imprinted polymers (MIPs) was developed. The key step is based on near-field radical photopolymerization of a MIP pre-polymerization mixture. This allows the preparation of hybrid AuNPs@MIPs nanoparticles which are used as substrates for LSPR and surface enhanced Raman spectrometry (SERS) analyses with excellent sensitivity and specificity. To demonstrate the performance of AuNPs@MIPs, MIPs specific to methylene blue (MB) were prepared. The sensitivity of spectroscopic detection is in the range of 10 nM. Specificity is demonstrated by comparing the response with a control non-imprinted polymer (NIP) and by interference tests with two analogues (Rhodamine 6G and Rhodamine 110). This fabrication method allowed us to obtain robust and recyclable sensing surfaces with high sensitivity and selectivity. The nanometric thickness of MIP allows a short analysis time (10 min), which improves the performance of MIP-based sensors and opens new perspectives to detect molecules at very low concentrations.



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**Thematic Session:** Nanomechanics & Nano-electronics

**Keywords:** Phononic resonator, Simulations, Piezoelectricity , Mechanical qubit

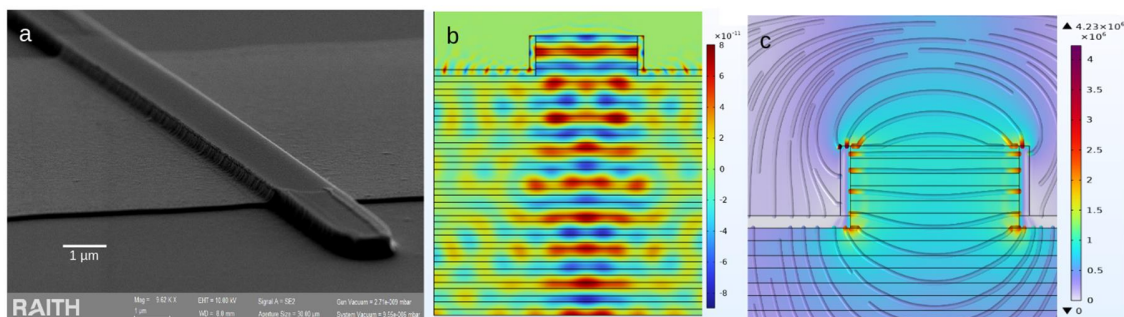
**Disciplinary fields involved :** Physics

## Towards an electrically driven high Q, GHz mechanical resonator for quantum information applications

Marie Joly<sup>1</sup>, Paola Atkinson<sup>1</sup>, Daniel Garcia-Sanchez<sup>1</sup>

<sup>1</sup> Sorbonne Universités, UPMC Univ. Paris 06, CNRS-UMR 7588, Institut des NanoSciences de Paris, F-75005 Paris, France

In recent years, efforts have been put towards realizing a mechanical qubit by coupling a macroscopic mechanical resonator with a transmon qubit<sup>[1, 2]</sup>. One of the challenges here is to create a mechanical resonator that has both a high quality factor and which can be strongly coupled to the transmon. Here, we discuss different strategies to achieve a high frequency, high Q, electrically driven mechanical resonator based on a GaAs/AlAs superlattice<sup>[3]</sup>. This consists of a succession of different layers forming acoustic mirrors with a central cavity which confines phonons with specific wavelengths. We will describe in detail the fabrication of a micropillar where a lateral electrical field is applied to generate a mechanical mode, and present models of the displacement field and electrical impedance of the different designs.



(a): SEM image of a GaAs micropillar with side Au electrodes, (b-c): Displacement field along Y (out of plane) and electric field across a GaAs/AlAs superlattice with lateral gold electrodes, Comsol simulations.

References: [1]: F. Pistoiesi and al., Proposal for a Nanomechanical Qubit, 0.1103/PhysRevX.11.031027, [2]: K. J. Satzinger and al., Quantum control of surface acoustic wave, [3] D.Garcia-Sanchez and al., Acoustic confinement in superlattice cavities, 10.1103/PhysRevA.94.033813 phonons

## Map of Stands & Posters Exhibition

