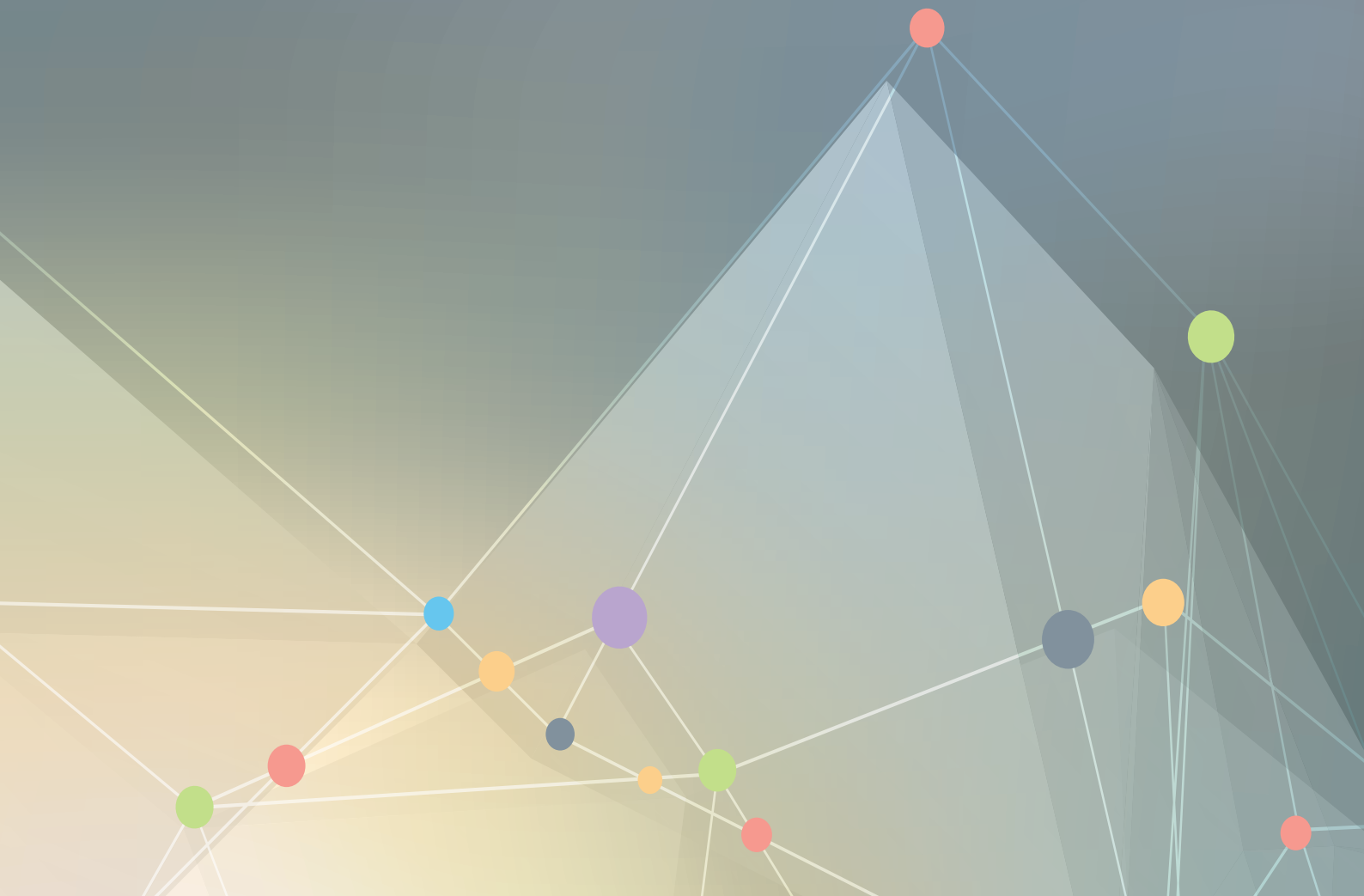


# BOOK OF ABSTRACTS

## Oral Presentations



# 2023



## Nanomechanics:

### surface/interface, composite nanomaterials, hybrid nanomaterials

(Last update: November 4<sup>th</sup>, 2022)

#### description

This « Nanomechanics » session aims at bring together researchers working on the mechanical properties of nanometric-sized objects, whose deformation mechanisms are specific due to their significant surface/volume ratio. The investigations from the micron-scale down to individual atoms require the development of new experimental and simulation tools and techniques. At such a scale, the physical and/or chemical phenomena may be strongly modified/affected, revealing new material laws that can be tuned to exploit these original properties.

The issues are double 1- fundamental on mechanisms (elasticity, plasticity, fracture) and 2- applicative since the strain fields are often coupled to functionalities (electrical, magnetic, optical, ...). The targeted field of study concerns nanoparticles/nanostructures and nanometric thin films as well as the development of their mechanical characterization and/or the simulation of their mechanical properties.

The main points addressed in this session are the following:

- Nanoparticles, vibration, elasticity
- Nano/micro-pillars, plasticity, and fracture
- Nanostructured/nanocomposite thin films, hybrid materials
- Couplings between deformation mechanisms and functional properties
- Atomistic and multi-scale simulations
- Experimental developments: electron microscopy, synchrotron, near field microscopy, vibrational spectroscopy.

#### Keywords

Nano-objects, thin films, small-scale mechanics, experimental techniques, simulations

#### organizing committee

**Aurélien CRUT** (Univ. Lyon – ILM, Lyon)

**Stéphanie ESCOUBAS** (AMU – IM2NP, Marseille)

**Damien FAURIE\*** (Univ. Poitiers – Univ. Sorbonne Paris Nord – LSPM, Villetaneuse)

**Julien GODET\*** (Univ. Poitiers – Pprime, Poitiers)

**Barbara PUTZ** (Montanuniversität Leoben – Structural and Functional Ceramics, Leoben)

\* session Coordinator

**2023**

**Wednesday March 15<sup>th</sup>**

**3.30 pm – 6.00pm**

**Amphi 150**

**Program of the session**

**Chairs: Julien GODET & Barbara PUTZ**

**NANOMECHANICS**

<b>15:30</b>	<b>Nanomechanics: Playing the nanoguitar to explore the dynamics of harmonic oscillators and two-level systems</b>	<b>Eva Maria WEIG</b> • <i>Technical University of Munich – Chair of Nano &amp; Quantum Sensors, Munich – Germany</i>
<b>16:00</b>	Multifrequency-AFM platform for chemical and local property analysis	<b>Eric LESNIEWSKA</b> • <i>Univ. Bourgogne - ICB, France</i>
<b>16:15</b>	Elastic study of self-suspended nanowires by pump-probe spectroscopy	<b>Laurent BELLARD</b> • <i>Sorbonne Univ. - INSP, France</i>
<b>16:30</b>	Plasmo-electronic effects in self-organised gold nanoparticles strain gauges	<b>Jérémie GRISOLIA</b> • <i>INSA Toulouse - LPCNO, France</i>
<b>16:45</b>	<b>Coffee &amp; tea break</b>	
<b>17:15</b>	Nanomechanical characterization by AFM of a composite material: method and analysis	<b>Rosine COQ GERMANICUS</b> • <i>Univ. Caen Normandie CRISMAT, France</i>
<b>17:30</b>	Small-scale experimental techniques to study thin film delamination	<b>Alice LASSNIG</b> • <i>Austrian Academy of Sciences. - ESI, Austrian</i>

# Keynote Speakers

## NANOMECHANICS



### Eva WEIG

**Technical University of Munich | Professor**

*Chair of Nano & Quantum Sensors*

<https://www.ee.cit.tum.de/nan/home/>

### BIOGRAPHY

Eva WEIG is a Full Professor at the School of Computation, Information and Technology of the Technical University of Munich (TUM) in Germany. She holds the Chair of Nano and Quantum Sensors and is a Director of the TUM Center for QuantumEngineering. Before joining TUM in 2020, she spent eight years as a Full Professor at the Department of Physics of the University of Konstanz in Germany. Eva got a PhD in Physics from Ludwig-Maximilians-University (LMU) in Munich, Germany, in 2004, where she also worked as a Junior Research Group Leader following her postdoc at the California NanoSystems Institute at the University of California at Santa Barbara (UCSB).

Research at the Chair of Nano & Quantum Sensors is dedicated to nanomechanical systems. Among others, the group has pioneered the integrated dielectric control of high Q nanomechanical resonators. Research interests include the nonlinear dynamics and the coherent control of nanomechanical systems, the study of coupled nanoresonators and nanomechanical arrays, as well as cavity opto- and electromechanical systems.

### NANOMECHANICS: PLAYING THE NANOGUITAR TO EXPLORE THE DYNAMICS OF HARMONIC OSCILLATORS AND TWO-LEVEL SYSTEMS

Nanomechanical resonators are freely suspended, vibrating structures with nanoscale dimensions. They show great promise as versatile linking elements in hybrid nanosystems, as sensors or signal transducers both in the classical and in the quantum realm, generating an increasing amount of attention both for fundamental explorations and for practical applications. Here I will focus on doubly-clamped pre-stressed nanostring resonators. These seemingly simple devices exhibit remarkably large room temperature quality factors and enable electrostatic control [1]. Nanostrings are thus an ideal testbed to explore a variety of dynamical phenomena. Recent progress in controlling the coherent as well as the nonlinear dynamics of high Q nanostring resonators will be reviewed. In particular, I will discuss the interplay between the two orthogonal fundamental flexural modes of the string vibrating in- and out-of-plane with respect to the sample surface. These two modes are strongly coupled and reveal a pronounced avoided crossing [2], which can be described as a classical two-mode system mimicking the coherent dynamics of a quantum two-level system [3,4]. Further, the nonlinear dynamics of the resonantly driven nanostring will be highlighted, which gives rise to thermomechanical squeezing [5], and has recently been shown to lead to the generation of a novel type of frequency comb [6].

### KEYWORDS:

Nanomechanics; high quality factor; nonlinear dynamics; coherent control; nanoelectromechanical systems

### REFERENCES

- [1] Q. P. Unterreithmeier et al., Nature 458, 1001 (2009)
- [2] T. Faust et al., Phys. Rev. Lett. 109, 037205 (2012)
- [3] T. Faust et al., Nature Physics 9, 485 (2013)
- [4] A. Chowdhury et al., arXiv: 2204.04736
- [5] J. S. Huber et al., Phys. Rev. X 10, 021066 (2020)
- [6] J. S. Ochs et al., Phys. Rev. X 12, 041019 (2022)



**Keywords:** Ultrasound, IR, and microwave spectroscopy, chemical identification, strain analysis  
**Disciplinary fields involved:** Physics, Material Science, Biophysics

## Multifrequency-AFM platform for chemical and local property analysis

Lesniewska E.<sup>1</sup>, Custovic I.<sup>1</sup>, Piétrement O.<sup>1</sup>, Pocholle N.<sup>1</sup>, Bourillot E.<sup>1</sup>

1. Laboratory ICB UMR CNRS 6303, University of Bourgogne, Dijon, France

A new AFM-based platform combining IR spectroscopy ( $700\text{--}1900\text{ cm}^{-1}$ ), tomography using the frequency range  $1\text{ MHz--}20\text{ GHz}$  has been developed to detect specific bodies inside organic or inorganic elements, and/or structural modifications.

Combining AFM and IR, we can assist in the design of nano-hybrids illustrated by an example on DNA and inorganic nanoparticles. Combining AFM and microwave ( $0.3\text{--}20\text{ GHz}$ ), we can detect light chemical elements in materials and local sub-surface mechanical stresses. Combining AFM and ultrasonic wave ( $1\text{--}10\text{ MHz}$ ), we can access the variations of density and intrinsic porosity of the material. Examples will be developed demonstrating the potential of this new multi-frequency platform for the characterization of nanostructured interfaces and nano-objects. We have achieved a comparative study of AFM-IR and multi-frequency analysis on single stranded DNA, DNA networks, protein-DNA assemblies, reconstituted membranes, and cells transfected by viruses or functionalized nanoparticles (Fig.1). Our results indicate that the coupling of these techniques constitutes a great advantage to fully characterize chemical, topographical and volumetric parameters of biological sample or inorganic sample at the surface and sub-surface with nanometric resolution.

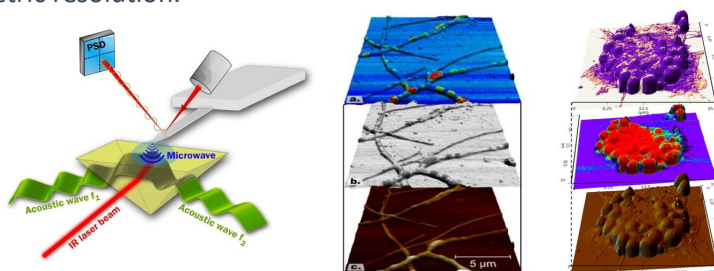


Fig. 1 – a/ Multifrequency-IR platform. b/ Detection of lipids in bacteria. c/ Detection of yeasts in macrophage

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- I. Custovic et al., *Scientific Reports in press*, available at arXiv:2201.12092 [physics.bio-ph]

### Acknowledgment:

This work has been supported by the French National Research Agency: ANR-20-CE20-MACARON, ANR-19-CE42\_OMICRON, ANR-17-EURE-EIPHI, ANR-15-IDEX-03 PIA2/iSite-BFC, Feder and BFC Region Funds.

**Keywords:** nanowire, vibrational mode

**Disciplinary field involved:** Physics

## Elastic study of self-suspended nanowires by pump-probe spectroscopy

L. Belliard<sup>1</sup>, R. Delalande<sup>1</sup>, B. Perrin<sup>1</sup>, L. Burr<sup>2</sup>, M. E. Toimil-Molares<sup>2</sup>.

1. Institut des Nanosciences de Paris, Sorbonne Université, CNRS UMR7588, 4 place Jussieu, 75005 Paris, France
2. GSI Helmholtz Centre for Heavy Ion Research, D-64291 Darmstadt, Germany

The study of elasticity at the nanoscale has experienced a great expansion in the last decades. This emulation is partly related to progress on the synthesis of nanoparticles of various geometries and sizes, but also to the development of different approaches of vibrational spectroscopy. We will present here a comprehensive study of the elasticity in copper and gold nanowires using a self-suspended geometry, Fig1.

The generation and detection within these systems is provided by a time-resolved pump-probe approach so-called picosecond acoustics. By coupling the detection of localized vibrational modes to that of guided propagative modes, we will show how it is possible to traces imultaneously the longitudinal and transverse velocities of individual nanowires 1-3.

The interest of the self-suspended geometry lies in an increase of the acoustic confinement allowing the observation of a complex vibrational landscape.

Finally, we will discuss how to create new nanoscale acoustic sources through the relaxation of breathing modes in the substrate.

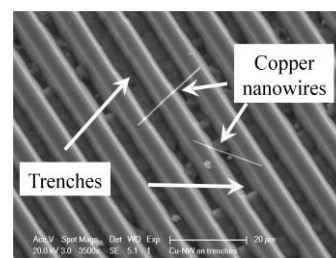


Figure1: SEM image of the nanowire crossing the trenches prepared on a silicon wafer.

### References:

- 1) S. Fernandez, C. Jean, E. Charron, P. Gentile, M.I. Richard, O. Thomas, B. Perrin, L. Belliard, Jour. Appl. Phys. **126**, 204304 (2019)
- 2) R. Delalande, L. Burr, E. Charron, M. Jouini, M. E. Toimil-Molares, L. Belliard, Appl. Phys. Lett. **115** 083103 (2019)
- 3) P.A. Mante, L. Belliard, B. Perrin, Nanophotonics **7** (11) 1759–1780 (2018)

**Keywords:** gold nanoparticles, strain gauge, photo-induced charge transport; surface plasmons

**Disciplinary fields involved:** Physics and Chemistry

## Plasmo-electronic effects in self-organised gold nanoparticles strain gauges

Louis Merle<sup>1</sup>, Adnen Mlayah<sup>2</sup>, Jérémie Grisolia<sup>1</sup>

1. LPCNO, Université de Toulouse, INSA, CNRS, UPS, 135 avenue de Rangueil, Toulouse 31077, France
2. LAAS, Université de Toulouse, CNRS, UPS, 7 avenue du Colonel Roche, Toulouse 31031, France

The coupling between charge transport and surface plasmons in metal nanostructures is the driving force of the emerging field of “plasmo-electronics”. Using this synergy in strain gauge based nanoparticles requires the understanding of quite complex phenomena involving several fundamental interaction mechanisms between elementary excitations (plasmons, electron-hole pairs, phonons), which are responsible for the conversion of light into charge carriers. In this study, we report on the plasmo-electronic properties of self-assembled monolayers of colloidal gold nanoparticles (NPs) strain gauges formed on a flexible polyamide substrate. Impedance spectroscopy measurements performed under optical excitation and applied uniaxial stress are used to investigate the plasmo-electronic properties of the NP strain gauges. The impedance spectroscopy data are interpreted using a multi-scale approach in which a local nano-junction model, composed of parallel inter-particle resistance  $R_{ij}$ , capacitor  $C_{ij}$  and photo-resistance  $g_{ij}^{-1}$ , are introduced and serves as a building block of a meso-scale nano-junctions network. The surface plasmon properties are modeled in the  $g_{ij}^{-1}$  term using electro-dynamic calculations based on the discrete dipole approximation (DDA). The electric characteristics of the mesoscopic nanoparticle network are obtained by solving the current-bias voltage equations according to Kirchhoff's laws. The combined DDA-Kirchhoff numerical simulations give the electrical properties of the strain gauges (relative resistance and capacitance, and sensitivity), as a function of the laser intensity, wavelength and also electrical frequency. These results are quantitatively compared to the experimental data. In particular, the strain gauge sensitivity is found to be enhanced under resonant plasmonic excitation and frequency dependent. This method enables strain gauge engineering and paves the way for novel applications in this emerging field.

### References:

- Plasmonic photo-current in freestanding monolayered gold nanoparticle membranes. M. Gauvin, T. Alnasser, E. Terver, I. Abid, A. Mlayah, S. Xie, J. Brugger, B. Viallet, L. Ressler and J. Grisolia\*

**Keywords:** AFM, PFQNM, composite nanomaterials, Young's modulus, adhesion

**Disciplinary field involved:** Physics

**Sustainable Development Goals\* eventually involved in your research:** materials for environment

## Nanomechanical characterization by AFM of a composite material: method and analysis

**R. Coq Germanicus<sup>1</sup>, D. Mercier<sup>2</sup>, M. Fèbre<sup>3</sup>, D. Mariolle<sup>4</sup> and Ph. Leclère<sup>5</sup>**

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Nowadays in high integrated microelectronic devices, heterogeneous materials are used to design the device packaging. Encapsulation of epoxy matrix also called Epoxy Molding Compound (EMC), a composite material, is widely used as plastic packages for automotive, aerospace coatings and integrated microelectronic devices. Composite plastic packaging ensures electrical insulation and protects the electronic devices from external environment<sup>1</sup>. Nanomechanic features are of particular interest due to their influence on macroscopic material properties and behavior. Therefore, reliability and failure analysis investigations of the different materials require a characterization, a detection and a quantification of 2D-local properties with high spatial resolution. Scanning Probe Microscopies (SPM) are powerful tools developed to probe local properties such as mechanical properties. Based on an Atomic Force Microscope (AFM), 2D-local materials properties are presented and analyzed. Firstly, topography and local mechanical properties of Epoxy Molding Compound (EMC) are investigated by the Peak Force Quantitative Nanomechanical Mapping (PF-QNM)<sup>2,3</sup>. Secondly, the method to quantify the mechanical properties (the deformation, indentation, dissipation, adhesion and Young's modulus) is presented. Results obtained from PF-QNM are compared with classical instrumented nanoindentation mapping tests. Impact of scan parameters, probe properties, reproducibility and scan resolutions are also discussed within a metrological approach.



## References:

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- Towards wireless highly sensitive capacitive strain sensors based on gold colloidal nanoparticles. H. Nesser, J. Grisolia†, T. Alnasser, B. Viallet and L. Ressler. Nanoscale, 2018, 10, 10479 – 10487
  - Plasmonic photo-capacitance of self-assembled gold colloidal nanoparticle monolayers. H. Nesser, J. Grisolia,†, A. Mlayah, T. Alnasser, D. Lagarde, B. Viallet and L. Ressler. Materials Today Nano 4 (2018) 38-45
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## acknowledgment:

This study has been supported by the EUR grant NanoX No. ANR-17-EURE-0009 in the framework of the Programme des Investissements d'Avenir. This work was performed using HPC resources from CALMIP (Grant 2020-P0996)."



**Keywords:** *in situ* delamination, thin film delamination, plasticity and stress quantification at small scale

**Disciplinary fields involved** Physics, Materials Science

**Sustainable Development Goals\*:** improve interface adhesion as a strategy to improve overall device quality

## Small-scale experimental techniques to study thin film delamination

A. Lassnig<sup>1</sup>, M. Tkadletz<sup>2</sup>, M. Meindlhumer<sup>2</sup>, J. Todt<sup>2</sup>, C. Mitterer<sup>2</sup>, S. Zak<sup>1</sup>, C. Gammer<sup>1</sup>, J. Keckes<sup>2</sup>, M. J. Cordill<sup>1</sup>

1. Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Leoben, Austria

2. Materials Science Department, Montanuniversität, Leoben, Austria

Understanding the factors accompanying thin film delamination to quantify adhesion to their substrates is important to ensure reliable multi-material components which are widely encountered in several technological applications at different length scales.

When looking at ductile thin film delamination, toughening mechanisms attributed to the intrinsic film and substrate properties are important to improve interface adhesion and ensure reliable multi material components at small scale (below micrometer film thickness). Therefore, the delamination behavior of ductile thin films was investigated using spontaneous buckling – which is rooted in Euler beam theory which does not account for plastic deformation of the delaminating structures. While it has been shown that plasticity is an important energy dissipation mechanism increasing the interface stability, the Hutchinson and Suo model which is routinely used for adhesion quantification, does not account for permanent deformations of the film and/or substrate. In a recent study we introduced a FIB based technique which decouples the elastic and plastic contributions of the delaminated thin films, proving that the films that deformed more plastically improved the interface stability as interface delamination could be delayed [1].

Using small scale experimental techniques such as cross sectional nano-beam X-ray diffraction and in-situ TEM interface fracture experiments the mechanisms occurring during thin film delamination are explored using in-situ and post mortem characterization techniques. At all length scales of the experiments we could demonstrate that significant strains occurred within the delaminating films, proving that the capacity of thin films to plastically deform prior delamination improves interface properties.

## **References:**

[1] A. Lassnig, V.L. Terziyska, J. Zálešák, T. Jörg, D.M. Töbrens, T. Griesser, C. Mitterer, R. Pippan, M.J.Cordill, E. Al., Microstructural Effects on the Interfacial Adhesion of Nanometer-Thick Cu Films on Glass Substrates: Implications for Microelectronic Devices, ACS Appl. Nano Mater. 4 (1) (2021) 61–70. <https://doi.org/10.1021/acsanm.0c02182>.

**Acknowledgment:** A. L. acknowledges funding of the Austrian Science Fund (FWF) under grant numbers T891-N36 and Y1236-N37.

**2023**

**Thursday March 16<sup>th</sup>**

**10.30 am – 12.30 pm**

**Amphi 150**

**Program of the session**

**Chairs: Julien GODET & Damien FAURIE**

NANOMECHANICS		
10:30	Single and multilayer electro-mechanical behavior studied with in-situ methods	Megan CORDILL • ESI – OAW, Leoben – Autriche
11:00	Mechanical properties of a thickness controlled multi-layered copper thin film	Silvia KALACSKA • CNRS - LGF, France
11:15	Nanoengineering the glassy state: toward novel thin film metallic glasses with outstanding combination of mechanical properties	Matteo GHIDELLI • CNRS - LSPM, France
11:30	Influence of ALD interlayers on mechanical and interfacial properties of Al thin films on polyimide	Johanna BYLOFF • ETH Zurich - EMPA, Suisse
11:45	Link between cracking mechanisms of trilayer films on flexible substrates and electro-mechanical reliability under biaxial loading	Shuhel ALTAF HUSAIN • CNRS - LSPM, France
12:00	Mechanical properties of realistic nanoporous gold ultra-thin film for flexible electronics, investigated by Molecular dynamics simulations	Gwénaél MASSE • Univ.Poitiers - Inst. Pprime, France
12:15	Nanoparticle morphology and stress evolution in metallic nanocomposite thin films produced by combined gas phase aggregation and magnetron sputtering	Barbara PUTZ • ETH Zurich - EMPA, Suisse

# Keynote Speakers

NANOMECHANICS



## Megan CORDILL

**Austrian academy of sciences | Researcher**

*Erich Schmid Institute of Materials Science*

<https://www.oeaw.ac.at/esi/institute/staff/megan-cordill>

### BIOGRAPHY

Dr. Megan J. CORDILL (she/her/hers) is the deputy director and group leader at the Erich Schmid Institute of Materials Science of the Austrian Academy of Sciences. Dr. Cordill studied materials science and engineering at the University of Minnesota and earned her PhD in 2007. Her research interests include thin film adhesion, nanoindentation, structure-properties relationships of thin films, as well as probing electrical, thermal, and mechanical properties using advanced in-situ techniques. Dr. Cordill has published more than 150 SCI papers, edited 4 special issues on materials science and diversity topics, and has an h-index of 25 (Scopus). She is an active member of TMS, MRS, and AVS. In 2008, Cordill recipient of the Lise Meitner Fellowship for post-doctoral research in Austria, and in 2020 placed 2nd for the prestigious Houska Prize, Austria's largest private prize for applied research.

### SINGLE AND MULTILAYER ELECTRO-MECHANICAL BEHAVIOR STUDIED WITH IN-SITU METHODS

Electrical and mechanical properties of thin metal films on compliant polymer substrates are important to understand in order to design reliable flexible electronic devices. Single and multilayer films of Cu and Al on polyimide (PI) substrates were examined for their use as interconnects in flexible electronic devices with and without the use of Mo, Cr, or Nb interlayers. Using in-situ tensile straining with X-ray diffraction (XRD) and confocal laser scanning microscopy (CLSM) mechanical behavior can be examined. CLSM can provide information about crack spacing and film delamination, while XRD experiments are utilized to determine the lattice strains and stresses present in the films. If these in-situ techniques are combined with in-situ 4-point-probe (4PP) resistance measurements, the influence of the mechanical damage on the electrical properties can be correlated. This combination of multiple in-situ investigations are particularly useful when studying the electro-mechanical behavior under uniaxial and biaxial loading conditions to better understand where complete electrical failure occurs. Mechanisms behind these phenomena as well as the role of film thickness, residual stresses, and film architecture will be discussed.

### KEYWORDS:

thin films; electrical behavior; mechanical behavior; in-situ; x-ray diffraction

### REFERENCES

[1] Cordill, M.J.; Kreiml, P.; Mitterer, C. Materials Engineering for Flexible Metallic Thin Film Applications. *Materials*. 2022, 15, 926, doi:10.5594/J12186.

**Keywords:** plastic deformation, micropillars, HR-EBSD, strain rate sensitivity

**Disciplinary fields involved:** Physics, Engineering

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

## Mechanical properties of a thickness controlled multi-layered copper thin film

Szilvia Kalácska<sup>1</sup>, László Pethő<sup>2</sup>, Guillaume Kermouche<sup>1</sup>, Johann Michler<sup>2</sup>, Péter D. Ispánovity<sup>3</sup>

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2. Empa Swiss Federal Labs for Materials Science, Feuerwerkerstrasse 39, 3602 Thun, Switzerland
3. Eötvös Loránd University, Dept. of Materials Physics, Pázmány P. stny. 1/a, 1117 Budapest, Hungary

Creating multi-layered thin films with alternating dissimilar sublayers is proposing unusual (electric, thermal, optical, etc.) properties to be experimentally investigated. In such a system where grain size and texture can be controlled by the deposition/annealing process represents a unique opportunity to focus on some aspects of the deformation processes driven by the collective behaviour of dislocation. Our aim was to create a system with large enough grains (500-800 nm in diameter) and engineer flat grain boundaries to study plastic deformation modified by the presence of barriers.

A hybrid thin film deposition system was used (Swiss Cluster) to create the samples by combining atomic layer deposition (ALD) and physical vapour deposition (PVD) [1]. Sequential deposition of ~1 µm thick Cu multilayers were separated by 10 nm thick Al<sub>2</sub>O<sub>3</sub> interlayers. The initial 100-250 nm grain size was increased by extensive heat treatment (@800°C for 4h under Ar atmosphere, Figure 1.). Such final specimen was quite challenging to create without porosities or major delamination from the substrate after heat treatment.

Afterwards, micropillars were fabricated using focused ion beam (FIB) milling close to the edge of the bulk sample. These micropillars were then compressed at various strain rates using a nanodeformation setup (Alemnis AG). High (angular) resolution electron backscatter diffraction (HR-EBSD) was applied to study the geometrically necessary dislocation (GND) density distribution after quasi-static (QS) and high strain rate (HSR) deformations. Sequential FIB-slicing [2] was applied to create 3D reconstructions of the deformed volumes.



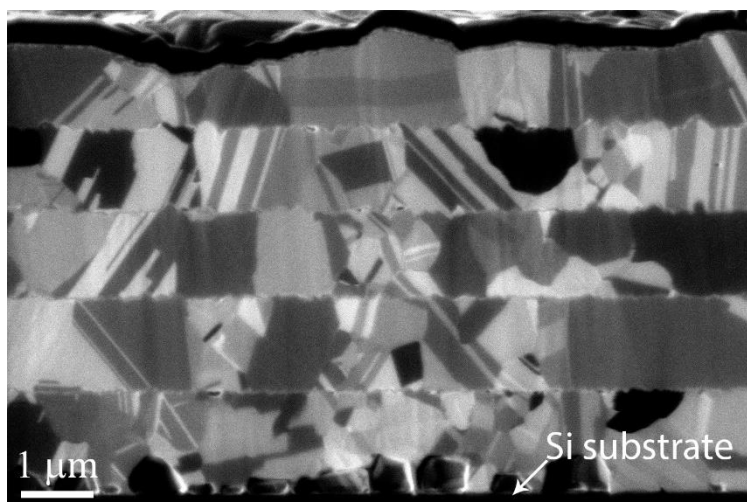


Figure 1. Cross-sectional ion channelling contrast image of the Cu-Al<sub>2</sub>O<sub>3</sub> multi-layered sample (before deformation). The grain size stabilized after 4 hours of heat treatment at 800°C.

#### References:

- [1] T. Xie, T.E.J. Edwards, N.M. della Ventura, D. Casari, E. Huszár, L. Fu, L. Zhou, X. Maeder, J.J. Schwiedrzik, I. Utke, J. Michler, L. Pethö, Synthesis of model Al-Al<sub>2</sub>O<sub>3</sub> multilayer systems with monolayer oxide thickness control by circumventing native oxidation. *Thin Film Solids*, 711 (2022) 138287.
- [2] S. Kalácska, J. Ast, P.D. Ispánovity, J. Michler, X. Maeder, 3D HR-EBSD characterization of the plastic zone around crack tips in tungsten single crystals at the micron scale. *Acta Materialia*, 200 (2020) 211-222.

#### Acknowledgment:

This research was funded in whole or in part by the French National Research Agency (ANR) under the project No. "ANR-22-CE08-0012-01" (*INSTINCT*) and No. "ANR-20-CE08-0022" (*RATES*).

**Keywords:** Metallic glasses, Thin films, Micro-mechanics.

**Disciplinary fields involved:** Materials science, Physics, Engineering

## Nanoengineering the glassy state: toward novel thin film metallic glasses with outstanding combination of mechanical properties

Francesco Bignoli<sup>1,3</sup>, Andrea Brognara<sup>2</sup>, Philippe Djemia<sup>1</sup>, Damien Faurie<sup>1</sup>, Andrea Li Bassi<sup>3</sup>,  
Gerhard Dehm<sup>2</sup>, Matteo Ghidelli<sup>1,2</sup>

<sup>1</sup>Laboratoire des Sciences des Procédés et des Matériaux (LSPM), CNRS, Villetaneuse, France.

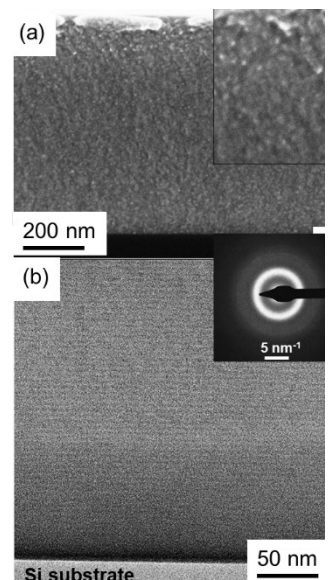
<sup>2</sup>Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany.

<sup>3</sup>Micro- and Nanostructured Materials Laboratory, Politecnico di Milano, Milan, Italy.

Thin film metallic glasses (TFMGs) are emerging materials characterized by a unique combination of mechanical involving large yield strength ( $\sim 3$  GPa) and large ductility ( $>10\%$ ) [1]. Nevertheless, the synthesis of advanced TFMGs with engineered microstructure and the understanding of their mechanical properties are barely tackled. Here, I will present recent results involving two (2) strategies to develop nanoengineered TFMGs with a controlled microstructure down to the atomic scale, resulting in outstanding and tunable mechanical properties.

Firstly, I will show the potential of Pulsed Laser Deposition (PLD) as a novel technique to synthesize nanostructured  $Zr_{50}Cu_{50}$  (%at.) TFMGs. I will show how the control of PLD process parameters enables to synthesize a variety of film microstructures, e.g. compact fully amorphous and amorphous nanogranular, showing large free volume (Fig. a) [2]. This results in unique mechanical behavior as shown by *in situ* TEM/SEM tensile/compression tests, reporting homogeneous deformation for nanogranular TFMGs combined with large yield strength ( $>3$  GPa) and ductility ( $>9\%$ ) [2].

In the second case, I will focus on the fabrication of multilayers with nanoscale period alternating either fully amorphous or amorphous/crystalline sublayers (Fig. b). I will show how the control of the sublayer thickness influences the deformation behavior affecting shear bands formation and tuning the mechanical properties. As an example, alternating CrCoNi (crystalline)/TiZrNbHf (amorphous) nanolayers results in an ultrahigh compressive yield strength (3.6 GPa) and large homogeneous deformation ( $\sim 15\%$ ) [3].



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**Keywords:** Thin films, Interlayer, Atomic Layer Deposition, Biaxial tensile testing

**Disciplinary fields involved:** Materials Science

**Sustainable Development Goals\* eventually involved in your research:** Industries, Innovation & Infrastructure, (Goal 9), Responsible Consumption & Production (Goal 12), Climate Action (Goal 13)

## **Influence of ALD interlayers on mechanical and interfacial properties of Al thin films on polyimide**

**Johanna Byloff<sup>1,4</sup>, Pierre-Olivier Renault<sup>2</sup>, Damien Faurie<sup>3</sup>, S. Altaf Husain<sup>2</sup>, Thomas E. J. Edwards<sup>1</sup>, Ralph Spolenak<sup>4</sup>, Barbara Putz<sup>1,5</sup>**

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2. *Université de Poitiers, Département Physique & Mécanique des Matériaux, 86073 Poitiers, France*
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4. *ETH Zürich, Department of Materials, Zurich, Switzerland*
5. *Montanuniversität Leoben, Department of Materials Science, 8700 Leoben, Austria*

Metal thin films on polymers serve a variety of applications in industry, medicine and space travel. The Al-Polyimide (PI) system investigated in this study offers high temperature resistance and good adhesion properties between substrate and coating. Previous studies<sup>1, 2</sup> attributed the favorable adhesive properties to the natural formation of a thin amorphous Al-O-C interlayer<sup>3</sup> (IL, 5 nm thick) between metal film and PI substrate. Through a combined atomic layer (ALD) and physical vapor deposition (PVD) setup, we are uniquely able to mimic interlayers artificially over a wide thickness range to study their mechanical and interfacial benefits. Using this setup, Al films (150 nm) with different Al<sub>2</sub>O<sub>3</sub> interlayer thicknesses (0.12-25 nm) were deposited on a polyimide substrate. These bi-layer samples were subjected to equi-biaxial tensile loading<sup>4</sup> and unloading with *in-situ* X-ray diffraction and electrical resistivity measurements at Synchrotron SOLEIL. Thus, the evolution of Al film stress, width of the Al diffraction peak and electrical resistivity as a function of the strain and IL thickness could be determined. Additionally, post-mortem SEM images were analyzed to obtain crack density and spacing, and correlate well to observed differences in the shape of the stress-strain curves. Significant embrittlement was observed only in the 25 nm interlayer sample. The comparison of 5 nm artificial versus natural interlayer shows similar resistivity but a difference in yield strength in tension and compression. Ongoing work includes thorough analysis of the Al microstructure, interlayer chemistry and high-resolution cross-sectional FIB/TEM analysis of the local interface structure.

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## Acknowledgment:

SOLEIL is gratefully acknowledged for the beam time allocation (Proposal 20220220). Further funding was obtained from the Swiss National Science Foundation under the Ambizione grant agreement No. PZ00P2\_202089. T.E.J.E. acknowledges funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No. 840222.



**Keywords :** Sputtering, X-ray, multilayer thin films, *in-situ* biaxial

**Disciplinary fields involved :** Physics

## Link between cracking mechanisms of trilayer films on flexible substrates and electro-mechanical reliability under biaxial loading

**S. Altaf Husain<sup>1,2</sup>, P. Kreiml<sup>3</sup>, P.-O. Renault<sup>2</sup>, C. Mitterer<sup>4</sup>, M.J. Cordill<sup>3,4</sup>, D. Faurie<sup>1</sup>**

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<sup>2</sup> Pprime Institute, CNRS-University of Poitiers, Département de Physique et Mécanique des Matériaux, 11 Bd Pierre et Marie Curie TSA 41123, 86073 Poitiers, France

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Flexible electronics is a technological innovation that involves the use of flexible polymer substrates as the basis structure for the assembly of electronic circuits [1]. Currently, flexible electronic devices have new emerging applications, especially for foldable displays and even in biology for integration on skin [2]. Flexible polymeric substrates show the advantages of low cost, light weight, mechanical compliance and bendability [3]. Nonetheless, these systems suffer from limited durability, both mechanically and electrically due to the multi-cracking phenomenon during loading [4]. Many works have studied the mechanical behavior of multilayers in order to profit from interfaces and mechanical contrasts (ductile/brittle, stiffness) between each layer to improve the durability [5].

In this work, the propagation of cracks from a top layer in trilayer systems (Cr/Cu/Mo) on a polyimide substrate is studied experimentally by *in situ* synchrotron X-ray diffraction under equi-biaxial loading (see figure 1). The results show that depending on the thickness of the ductile Cu middle layer (100 nm or 500 nm), the propagation can be a direct vertical path through all layers or a more complex path. These effects are analyzed by monitoring the individual stresses of each layer along with electrical resistance and resulting crack patterns. Cracks starting from the upper Cr layer propagate instantaneously through the whole system for a 100 nm Cu layer, but are strongly deflected in a 500 nm Cu layer, thus delaying the global fracture of the system measured by the increase of electrical resistance.



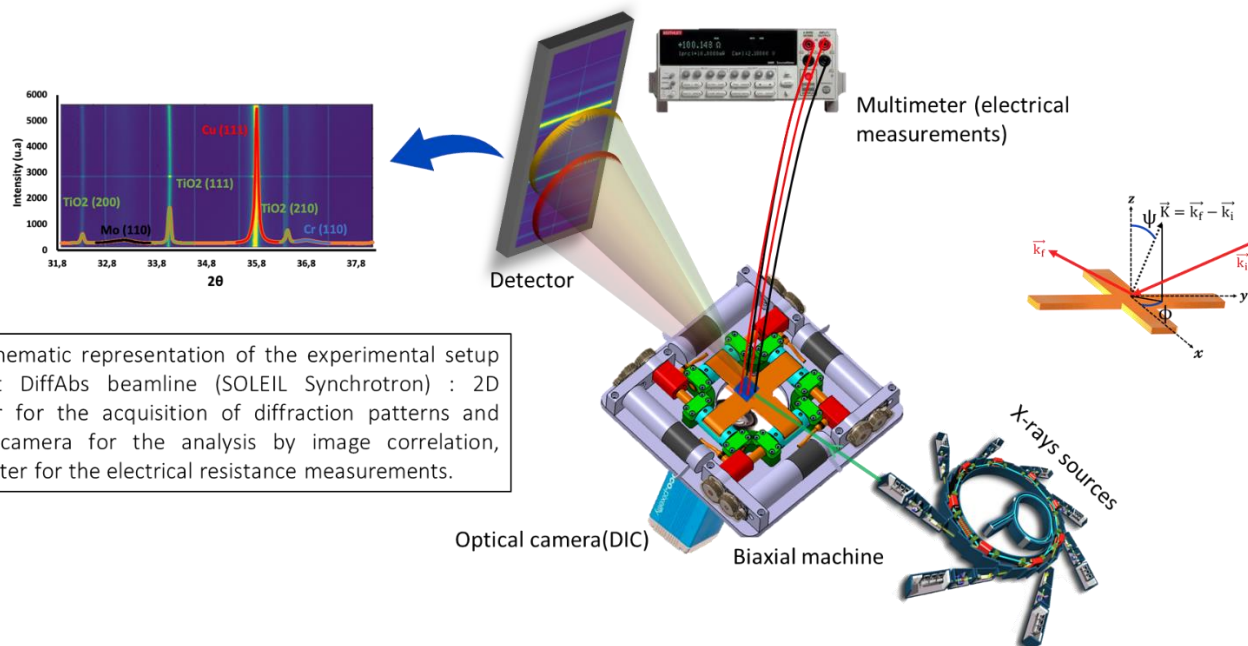


Fig : Schematic representation of the experimental setup used at DiffAbs beamline (SOLEIL Synchrotron) : 2D detector for the acquisition of diffraction patterns and optical camera for the analysis by image correlation, multimeter for the electrical resistance measurements.

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## Acknowledgment:

SOLEIL is gratefully acknowledged for the beam time allocation (Proposal 20210224) as well as the support of D. Thiaudiere. This work was in part supported by the French National Research Agency (ANR, project number ANR-20-CE91-0010) and the Austrian Science Fund (FWF, project number I 4913-N) within the framework of the project: Nanoarchitected films for unbreakable flexible electronics (NanoFilm). V.L. Terziyska from the Montanuniversität Leoben is also acknowledged for deposition of the samples.

**Keywords:** Gold nanomesh, plasticity, fracture, atomistic simulation

**Disciplinary fields involved :** Physics

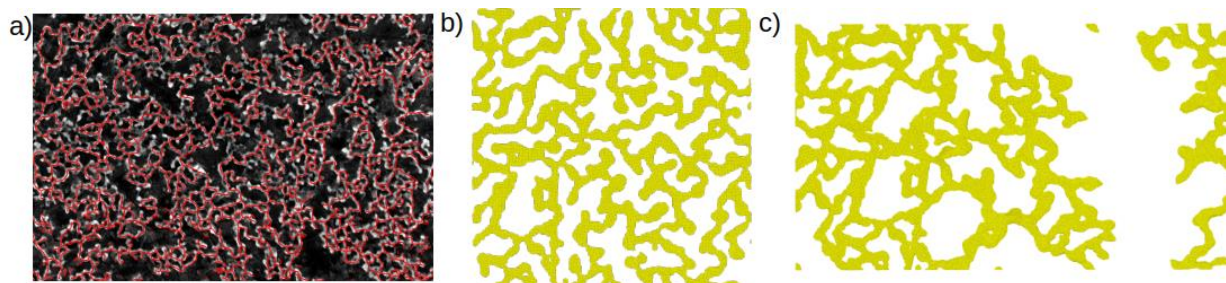
## Mechanical properties of realistic nanoporous gold ultra-thin film for flexible electronics, investigated by Molecular dynamics simulations

Gwénaél Massé<sup>1\*</sup>, Laurent Pizzagalli<sup>1</sup>, Lorianne Vernisse<sup>1</sup>, Hadi Bahsoun<sup>1</sup>, Maryline le Granvalet<sup>2</sup>, Issraa Shahine<sup>2</sup>, Quentin Hatte<sup>2</sup>, Pierre-Yves Tessier<sup>2</sup>, Julien Godet<sup>1</sup>

<sup>1</sup> Institut Pprime, dept. of Physics and Mechanics of Materials, UPR 3346 CNRS - University of Poitiers, SP2MI, BP 30179, 11 Boulevard Marie et Pierre Curie, 86962 Chasseneuil Futuroscope Cedex, FRANCE

<sup>2</sup> Institut des Matériaux Jean Rouxel, IMN, Université de Nantes, CNRS, 2 rue de la Houssinière B.P. 32229, 44322 Nantes cedex 3, FRANCE

Nanoporous gold ultra thin film is an interesting material due to its specific morphology [1]. Its large surface-to-volume ratio, large transmittance and electronic conductivity lead to potential applications in catalysis and flexible electronics. For the latter, gold nanomesh should support large deformations without failure under bending. Yet only a few mechanical studies were done. Molecular dynamics simulations were made on realistic models based on experimental images to determine the mechanical behavior in traction. Experimental images were obtained by SEM, AFM and STEM. The topology was extracted by a homemade code, revealing ligaments with 20 nm average diameters. Models were created from scaled experimental images, leading to 1.4 million atoms systems with 3 nm ligaments. Tensile tests up to 50% at 300K and 1K were made to determine the strength of the nanomesh. Strain-stress curves, ligaments breaking and fusing as well as deformation mechanism will be presented. The influence of topology (ligaments diameter, length and orientation) on plastic deformation will also be discussed.



**Figure 1:** a) Experimental SEM image with skeleton in red. b) 100 nm x 100 nm numeric sample with 3 nm ligaments, c) same sample after a traction test of 50 % at 300 K

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**Keywords:** Thin films, Nanoparticles, Nanocomposites, Nanomechanics

**Disciplinary fields involved:** Materials Science

**Sustainable Development Goals\* eventually involved in your research:** Good health and well-being (Goal 3), Affordable and clean energy (Goal 7)

## Nanoparticle morphology and stress evolution in metallic nanocomposite thin films produced by combined gas phase aggregation and magnetron sputtering

Emese Huszar<sup>1</sup>, Peter Schweizer<sup>1</sup>, Amit Sharma<sup>1</sup>, Thomas E.J. Edwards<sup>1</sup>, Laszlo Pethö<sup>1</sup>, Johann Michler<sup>1</sup>, Barbara Putz<sup>1,2</sup>

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2. Montanuniversität Leoben, Department of Materials Science, 8700 Leoben, Austria

Gas aggregation cluster sources can tailor the chemistry, size and shape of nanoparticles (NP). We investigate the influence of the type of power source (direct current vs. high-power impulse magnetron sputtering) and the method of nucleation source addition (1 SCCM air, continuous vs. periodic) on the morphology of tungsten NPs. Controlled addition of foreign nucleation sources is used to counteract depletion of active nucleation seeds and stagnation of the NP flux<sup>[1]</sup>. High-resolution transmission electron microscopy (HR-TEM) shows significant differences in the deposition rate and the average size of W NPs (3.8-6.7 nm), depending on the combination of power and nucleation source. Combining the NP gun with magnetron sputtering<sup>[2][3]</sup> enables fabrication of unique nanocomposite thin films with tailored NP distribution and volume density without precipitation-related restrictions concerning phase diagrams and solubility. We fabricated ductile thin films (Au, Cu, 50-200 nm) with and without incorporated W NPs (max. 0.034 vol%) to study deformation mechanisms as a function of nanoparticle concentration. The microstructures and NP concentrations were confirmed and characterized by TEM. Stress evolution in the nanocomposites was studied with X-ray diffraction during in-situ tensile experiments on flexible polymer substrates, whereby the observed particle influence strongly depends on the film thickness. Post mortem scanning electron imaging of the deformation pattern, as well as electrical resistance measurements recorded in-situ during straining, indicate that no significant embrittlement was introduced by NP addition. In summary, the novel manufacturing approach and resulting nanocomposites are promising candidates for model materials and multifunctional thin films in next-generation nano-devices.



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## Acknowledgment:

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**2023**

**Friday March 17<sup>th</sup>**

**2 pm – 3.45 pm**

**Amphi 150**

**Program of the session**

**Chairs: Julien GODET & Barbara PUTZ**

**NANOMECHANICS**

<b>14:00</b>	<b>When more is less: the effect of grain boundaries on the mechanical properties of metal nanoparticles</b>	<b>Jonathan AMODEO • CNRS – IM2NP, Toulon – France</b>
<b>14:30</b>	Shape controlling mechanical properties in nanoparticles: from atomistic to continuous	<b>Matteo ERBI • ONERA - LEM, France</b>
<b>14:45</b>	Atomic Scale Simulations of {112} Symmetric Incoherent Twin Boundaries in Gold	<b>Yen Fred WOGUEM • Univ.Poitiers - Inst. Pprime, France</b>
<b>15:00</b>	Mechanical Properties of Si/SiC Nanoparticles using Finite Temperature Ab Initio Molecular Dynamics	<b>Laurent PIZZAGALLI • CNRS - Inst. Pprime, France</b>
<b>15:15</b>	Pyrough : a new tool to model rough samples in atomistic and finite element simulations	<b>Hugo ITENEY • CNRS - IM2NP, France</b>
<b>15:30</b>	Plasticity and strain-hardening of glassy polymers: a microscopic theory	<b>Didier LONG • CNRS - MatéiS, France</b>



**Keywords:** core-shell nanoparticle, nanocompression, SEM, molecular dynamics, dislocations

**Disciplinary fields involved:** Mechanics, Physics

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

## When more is less: the effect of grain boundaries on the mechanical properties of metal nanoparticles

J. Amodéo<sup>1</sup>, A. Sharma<sup>2</sup>, N. Gazit<sup>2</sup>, O. Thomas<sup>1</sup>, E. Rabkin<sup>3</sup>

<sup>1</sup> Aix Marseille Univ., Université de Toulon, CNRS, IM2NP, 13397 Marseille, France

<sup>2</sup> Department of Materials Science and Engineering, Technion – Israel Institute of Technology, 3200003 Haifa, Israel

We present recent experimental and numerical data on the compression behavior of single crystalline and core-shell metal nanoparticles. Single crystalline samples deform elastically up to very high level of stresses approaching the theoretical shear strength. The following catastrophic plastic collapse is characterized by multiple dislocation nucleation events in the pristine nanoparticles. In the experiment, depositing an ultrathin (15 nm) nanocrystalline overlayer of Au on single crystalline Ag particles of hundreds of nanometers in diameter changes their deformation mode from that characteristic of single crystalline nanoparticles (high strength, wild strain burst) to a lower flow stress and strain hardening regime. Thus, paradoxically, adding more load-bearing material to the particles by coating them with a nanopolycrystalline phase drastically decreases their strength. This behavior is confirmed by molecular dynamics nanocompression simulations. Indeed, the mechanics of single crystalline core – polycrystalline shell Ag-Au nanoparticles under compression is investigated and compared to single crystalline samples. The results confirm the important role played by the dislocations nucleation process in the nanocrystalline shell (prior to the crystalline core) in which the large amount of grain boundaries promotes strain hardening.

**Keywords:** Nanoparticle, Molecular Dynamics, Finite Element

**Disciplinary fields involved:** Physics

## Shape controlling mechanical properties in nanoparticles: from atomistic to continuous

Erbi' Matteo<sup>1</sup>, Amara Hakim<sup>1,2</sup>, Gatti Riccardo<sup>1</sup>

1. Laboratoire d'Étude des Microstructure, ONERA-CNRS, UMR104, Université Paris-Saclay, Chatillon, 92322, France

2. Université de Paris, Laboratoire Matériaux et Phénomènes Quantiques (MPQ), F-75013, Paris, France

Physical properties at the nanoscale change as size scales. For instance, it is well known that the electronic properties pass from those of bulk material to those of a potential well. These changes are also seen in mechanical properties. The motto "Smaller is stronger" expresses the increase in strength associated with growing smaller nanostructures. The current contribution aims to study the interplay among shape, size, and composition of nanoparticles (NPs), with the ultimate goal of engineering a new class of nano-objects with targeted mechanical properties.

We investigate the elastic and plastic properties of metallic (transition metals: Au, Cu, and Pt) and alloy NPs as a function of different sizes and shapes (fcc single crystalline structure). We use a multi-scale and multi-physical approach combining atomic-scale and continuous methods, Molecular Dynamics (MD), and Finite Elements (FE). From this study, two key results were highlighted. Firstly, thanks to the comparison with MD simulations, we show the validity and the limits (5nm) of the FE solution at the nanoscale. Secondly, the shape's contribution to elasticity is analyzed both locally and globally: to control the shape means to control the elastic response of the NPs. Finally, size and shape are used to characterize the onset of plasticity (yield stress), and the origin of the size and shape effect is analyzed.

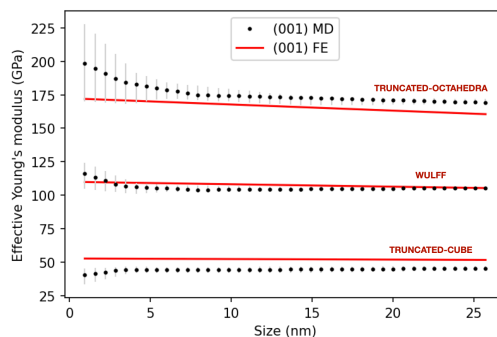


Figure 1 (001) Effective Young's modulus on gold NPs. Comparison between FE and MD.

**Keywords:** Twin boundary, Atomistic simulations, Excess volume, 9R phase, gold

**Disciplinary fields involved:** Physics

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

## Atomic Scale Simulations of $\{112\}$ Symmetric Incoherent Twin Boundaries in Gold

Y. F. Woguem<sup>1</sup>, J. Durinck<sup>1</sup>, P. Godard<sup>1</sup>, S. Brochard<sup>1</sup>

1. *Pprime Institute, Department of physics and mechanics of materials, University of Poitiers, ISAE-ENSMA, CNRS Poitiers, France*

Nanotwinned materials are the subject of many researches because they show mechanical properties that are usually antagonistic, namely high yield strength and good ductility [1]. We performed tensile tests on gold thin films with nanotwins, in-situ under X-ray diffraction, and we observed an increase of the twins volume in the crystal [2]. Atomistic simulations are a useful complementary tool to better understand the deformation mechanisms occurring in these materials. We first focused on  $\Sigma 3$   $[\bar{1}10](\bar{1}12)$  incoherent twin boundaries (ITBs). These ITBs can be described by a set of three Shockley partial dislocations where two of these dislocations are mixed and one is a pure edge [3]. The structural relaxation of such an ITB is induced by the slip of the pure edge dislocation of each set; this slip leads to the formation of a new crystalline phase, the 9R phase, whose width determines the relative lateral displacements between the two grains separated by the ITB. We have estimated the extension of the 9R phase in gold with molecular statics (with four commonly used potentials) and with density functional theory computations. The elastic deformation produced in the system to ensure consistency between the 9R phase and the fcc phase, and the formation energy of the 9R have also been computed. We have used the intrinsic stacking fault energy, the elastic deformation and the formation energy to discuss the width of the 9R phase [4]. This helps in understanding the stability of nanotwinned materials.

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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).

**Keywords:** Nanoparticles; Compression; Strength; Ab initio molecular dynamics

**Disciplinary fields involved:** Physics

## Mechanical Properties of Si/SiC Nanoparticles using Finite Temperature Ab Initio Molecular Dynamics

**L. Pizzagalli, J. Godet, J. Durinck, and S. Brochard**

*Institut Pprime, Dpt Physics and Mechanics of Materials, CNRS, Université de Poitiers, France*

The last decades have witnessed an extensive study of the mechanical properties of nano-sized systems, the main outcome being that decreasing the dimensions of a system increases its strength. Such a trend has been verified both experimentally and theoretically for characteristic dimensions as low as a few tens of nanometers. However it is totally unclear whether this is true at lower scales down to a few nanometers. Various conflicting scenarios have been proposed but with no supporting data [1]. Such conditions are out of reach of the current experimental capabilities, and classical molecular dynamics calculations are probably not reliable enough to be useful. To overcome this issue, we recently succeed in investigating the mechanical properties of 1-2nm Si and SiC nanoparticles, by modelling finite temperature compression using ab initio molecular dynamics [2]. These calculations yield several original and interesting results. First, very high compression stresses are reached, with maximum values up to 30GPa for Si, and in the range 100-120GPa for SiC. This suggests that "smaller is stronger" remains verified up to the nanometer scale for Si/SiC nanoparticles. A Schmid factor analysis shows that the theoretical bulk shear strength can be reached and even exceeded in specific cases. Second, we found that the models yield mainly by amorphization. Only in one case the formation of an embryo of 90° partial dislocation loop is observed. The hindering of dislocation formation/propagation in Si/SiC nanoparticles is discussed in relation with different hypotheses such as size or surface effects, quantum confinement, and non-Schmid behavior.

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**Keywords:** Roughness, Modeling, Surfaces, Nanocompression, Molecular Dynamics **Disciplinary fields involved:** Physics, Computer science

## Pyrough : a new tool to model rough samples for atomistic and finite element simulations

Hugo Iteney<sup>1\*</sup>, Javier Gonzalez<sup>2</sup>, Christophe Le Boulrot<sup>2</sup>, Thomas W. Cornelius<sup>1</sup>, Olivier Thomas<sup>1</sup>, Jonathan Amodeo<sup>1</sup>

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2. MATEIS, Université Lyon 1 CNRS INSA-Lyon, F-69621 Villeurbanne, France

Surface roughness has a fundamental impact on the mechanical properties of materials. It is investigated at the macroscopic scale in several fields of applications including friction and lubrication, machining or polishing. At the atomic scale, surface and surface defects are also known to play a key role as *e.g.*, in catalyses or nanomechanical engineering.

From a general point of view, surfaces can be characterized according to their chemical composition, roughness and height distribution. Mathematical formulations of rough surfaces are widely reported in the literature including the linear transformation, 2-D filters or time series approaches [1].

In this study, we introduce a new numerical tool called Pyrough developed to design rough virtual samples for atomistic (MD, DFT) simulations and finite-element modeling (FEM). Pyrough is a Python code that constructs 3D objects with the ability to manage surface height distribution of isotropic and Gaussian random surfaces. From a parameter file that includes the main aspects of the targeted 3D sample (material, shape, dimensions, orientations, crystal structure, etc.), a 3D perfect mesh is generated and roughened based on the classical roughness theory [2]. This first outcome is compatible with most FEM programs. Then, Pyrough fills the sample mesh with atoms as being fully coupled with the atomistic AtomsK library [3] providing a sample with rough surfaces designed for atomistic simulations. Several 3D shapes are currently available in Pyrough including classical particle shapes (cubes, spheres, Wulff shapes), cylindrical or faceted wires as well as plates or thin films. In this presentation, we will first introduce the main ingredients of the Pyrough workflow. Then, examples of applications related to the influence of rough surfaces on the mechanical properties of nano-objects including nanoparticle compression and nanowire tensile tests will be presented.

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**Keywords:** polymer physics; glass transition; plasticity

**Disciplinary fields involved:** Physics; Materials science; Mechanics

**Sustainable Development Goals\* eventually involved in your research:** durability of materials

## Plasticity and strain-hardening of glassy polymers: a microscopic theory

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Over the past twenty years empirical evidence has shown that the dynamics in liquids close to the glass transition temperature is strongly heterogeneous, on the scale  $\xi$  of order 3-5nm. A model for the dynamics of non-polar amorphous polymers, based on percolation of slow domains, has been developed and solved by 3D numerical simulations, succeeding in reproducing many features of polymers, from the linear regime up to yield and the onset of plastic flow [1,2]. We extend this model to large strain amplitudes [3]. We propose that local deformation induces monomer orientation at the monomer scale analogous to nematic order. We calculate the free energy barriers for  $\alpha$ -relaxation and propose that they are modified by the sum of two contributions: one, which scales as  $-\sigma^2$  where  $\sigma$  is the stress and corresponds to the elastic energy stored on scale  $\xi^3$  which leads to plastic flow, and a second one which is positive and proportional to  $\text{Tr}(q^2)$ , where  $q$  is the tensorial order parameter. The latter slows down the dynamics. This contribution relaxes very slowly far below  $T_g$  and is responsible for the Bauschinger-memory effect of polymer glasses. This model proposes a consistent description with other features such as Stokes law violation,  $T_g$  shifts in confinement, ageing and rejuvenating kinetics upon heating observed in supercooled polymer glasses.

### References:

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