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European Network for the Mechanics of Matter at the Nano-Scale

General Meeting – April 26-27, 2023
Book of abstracts

IMDEA, Madrid

Organizing Committee
Jon Molina-Aldareguia (IMDEA, Spain)
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Marc Legros (CNRS, France)
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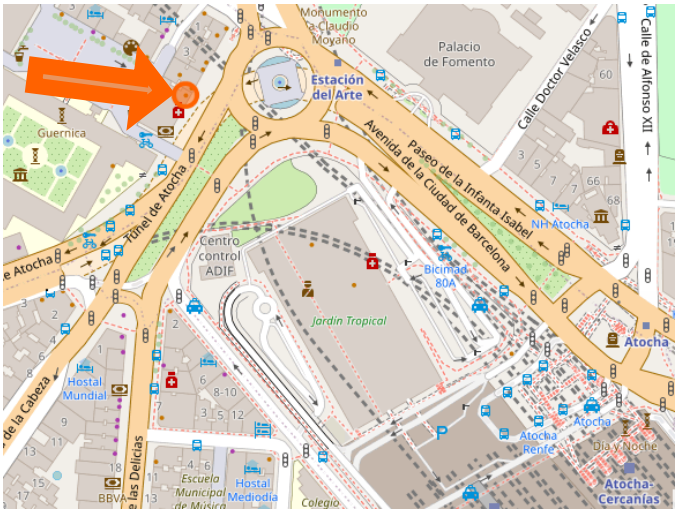
Practical informations

Shuttle bus

- Free shuttle
- For all participants, for both days
- **Morning pick-up point**: **9.15 am** at the bus stop in front of cafeteria El Brillante (near Atocha), arrival around 9.45 am at IMDEA
- **Evening return trip**: from IMDEA (departure around 17.15 pm) to Atocha bus stop (arrival around **5.45 pm**)



Meeting room

- Auditorium

Lunches

- Included in your registration

Conference dinner

- Only for pre-registered participants
- On April 26th at 8.30 pm at restaurant La Mucca del Prado
- Arrival on your own to the restaurant

Refunding

- Please have a look at the COST Travel Reimbursement Rules

Wednesday, 26 April 2023

9:15	Shuttle bus pick-up at Atocha
9:45	Registration
10:00	Welcome address
	New Processing routes – new materials *(Chair: Jon Molina)*
10:05	**Tuning the mechanical properties of steels using additive manufacturing (Invited)** Seita Matteo, University of Cambridge, United Kingdom
10:30	**Deformation of nanocomposite thin fims produced by combined gas phase aggregation and magnetron sputtering** Putz Barbara, EMPA Switzerland/Montanuniversität Leoben Austria
10:45	**Solid-solution and precipitation softening effects in defect-free faceted Nickel-Iron nanoparticles** Rabkin Eugen, Technion, Israel
11:00	**Microscale 3D printing and characterization of cellulose nanocrystal reinforced nanocomposite inks** Schwiedrzik Jakob, EMPA, Switzerland
11:15	Coffee break + group picture
	Machine learning *(Chair: Stefan Sandfeld)*
11:35	**Making the most of your indentation data using explainable machine learning** Trost Claus, Erich Schmid Insitute of Materials Science, Austria
11:50	**Challenges and opportunities of using AI technologies for design and characterization of mechanics of matter at nano-scale** Domazetovska Simona, Ss. Cyril and Methodius University, Macedonia
12:05	*Presentation of structure and activities of WG5 (Communication)*
12:15	*Presentation of structure and activities of WG3 (Open research data management)*
12:25	*Presentation of structure and activities of WG4 (Machine Learning)*
12:35	Lunch break / posters / campus tour
	Micromechanical testing *(Chair: Barbara Putz)*
14:20	**Microcast metals: processing and tensile behavior (Invited)** Mortensen Andreas, Ecole Polytechnique Fédérale de Lausanne, Switzerland
14:45	**Nanoheterogeneous Thin Film Metallic Glasses with Improved Toughness and Ductility** Özerinç Sezer, Middle East Technical University Ankara, Turkey
15:00	**Strong and ductile thin film metallic glasses through advanced nanoscale design strategies** Ghidelli Matteo, Laboratoire des Sciences des Procédés et des Matériaux, France
15:15	**Approaching second-strain gradient elasticity with soft X-rays diffraction** Amiot Fabien, femto-st, France
15:30	Coffee break
	Nanoindentation *(Chair: Solène Comby-Dassonneville)*
15:50	**Indentation size effect at shallow penetration depths (Invited)** Haušild Petr, Czech Technical University in Prague, Czech Republic
16:15	**Indenting thin films is a risky business** Cordill Megan, Erich Schmid Institute of Materials Science, Austria
16:30	**Creep-dominated fatigue of freestanding gold thin films** Krapf Anna, Friedrich-Alexander Universität Erlangen, Germany
16:45	**Effects of Radiation Damage on the Critical Resolved Shear Stresses in Zirconium Alloys for Nuclear Applications** Gibson James, University of Oxford, United Kingdom
17:00	Announcements
17:15	Bus departure to city center (arrival in Atocha at 17:45)
20 :30	Conference dinner at La Mucca del Prado [for pre-registered participants only]. Other participants have dinner on their own or in small groups at a location of their choice.

Thursday, 27 April 2023

9:15	Shuttle bus pick-up at Atocha
9:45	Registration
10:00	Welcome address
	Simulations *(Chairs: Jonathan Amodeo and Dan Mordehai)*
10:05	**Elastic and Plastic Response of FCC-Metallic Nanostructures under complex Loads (Invited)** Bitzek Erik, Max-Planck-Institut für Eisenforschung (MPIE), Germany
10:30	**Topology- and size-governed plasticity of nanoporous Au** Mathesan Santhosh, Technion – Israel Institute of Technology, Israel
10:45	**Mechanical Properties of Si/SiC Nanoparticles using Finite Temperature Ab Initio Molecular Dynamics** Brochard Sandrine, Institut Pprime, France
11:00	Coffee break
11:20	**Influence of roughness on the mechanics of nano-objects** Amodeo Jonathan, Institut des Matériaux, de Microélectronique et des Nanosciences de Provence, France
11:35	**Shape effect on mechanical properties of nanoparticles: from atomistic to continuous simulations** Gatti Riccardo, Laboratoire D'Etudes des Microstructures, France
11:50	**Failure of a brittle layer on a ductile substrate: Nanoindentation experiments and FEM simulations** Rusinowicz Morgan, University of Louvain, Belgium / SIMaP, France
12:05	**Propagation of zonal dislocations: the case of the synchroshear mechanism in Laves phases** Guénolé Julien, Laboratoire d'Etude des Microstructures et de Mécanique des Matériaux, France
12:20	Lunch break / posters
	Advanced TEM characterization *(Chair: Szilvia Kalacska)*
14:05	**Atomic scale engineering of dislocation slip and twinning in magnesium alloys (Invited)** Perez-Prado Maria Teresa, Institute IMDEA Materials, Spain
14:30	**Advanced Electron Microscopy techniques for strain evaluation in nanostructured materials at the atomic scale** Komninou Philomela, Aristotle University of Thessaloniki, Greece
14:45	**Grain boundary plastic mechanisms on polycrystals: the case of shear-coupled GB migration studied by in-situ TEM and AFM** Gauthier Romain, UCLouvain, Belgium / Cemes, France
15:00	**In-situ TEM nanomechanical investigations on a grain boundary sliding mechanism in forsterite** Ul Haq Ihtasham, Electron Microscopy for Materials Science EMAT, Belgium
15:15	*Presentation of structure and activities of WG1 (Size effects)*
15:25	*Presentation of structure and activities of WG2 (Experimental and simulation challenges)*
15:35	Coffee break
	Pillar compression *(Chair: Petr Hausild)*
15:55	**Strain rate and size dependent mechanical behaviour of a dual phase high-entropy alloy (Invited)** Kalacska Szilvia, Laboratoire Georges Friedel, France
16:20	**Room Temperature Viscous Flow of Amorphous Silica Induced by Electron Beam Irradiation** Bruns Sebastian, Technical University of Darmstadt, Germany
16:35	**Coupling micro-compression testing and Laue micro-diffraction** Comby-Dassonneville Solène, Aix Marseille Univ, Univ Toulon, France
16:50	Concluding remarks
17:15	Bus departure to city center (arrival in Atocha at 17:45)

Poster contributions

1. **DESIGN, SIMULATION AND OF AN MICRO-MANIPULATOR**
   Alionte Cristian Gabriel
2. **Study of the structure and mechanical properties of ferrous and non-ferrous metal welded joints**
   Baskutis Saulius
3. **EFFECT OF ADDITION OF GRAPHENE ON THE MECHANICAL PROPERTIES OF THE POLYMER NANOCOMPOSITES**
   Blazhevska-Gilev Jadranka
4. **Atomic Scale Simulations of Twins – Interfaces Interaction in a Nanolamellar Ag/Cu System**
   Brochard Sandrine
5. **Atomic Scale Simulations of {112} Symmetric Incoherent Twin Boundaries in Gold**
   Brochard Sandrine
6. **The extended scaling laws of the mechanical properties of additively manufactured body-centered cubic lattice structures using finite element modelling**
   Chen Zhi
7. **Viscoelastic and Viscoplastic Behavior of Graphene - Epoxy Nanocomposites: Experiments and Constitutive Modeling**
   Colak Ozgen
8. **NiTi alloys manufactured by LPBF for cardiovascular applications**
   Contreras-Almengor Oscar
9. **Mechanical Property Mapping for Dual Phase (DP) Steels**
   Cora Ömer Necati
10. **Mechanical and electronic properties of metallic nanoparticles**
    Erbi Matteo
11. **Atomistic simulations of the deformation of ultra-thin films of nanoporous gold constructed from experimental samples.**
    Godet Julien
12. **Multiscale and multifunctionality of textile structures**
    Hadj Taieb Amine
13. **Dislocations annihilation under reciprocating friction in LiF single crystals**
    Harea Evghenii
14. **Strain- and temperature-induced local dilatancy in ductile ZrNi thin film metallic glasses with nanoscale structural heterogeneities**
    Idrissi Hosni
15. **Modelling of interfacial energies and strains in GaN/AlN superlattices**
    Karakostas Theodoros

16. **Combining nano-scale digital image correlation with ACOM-TEM for unravelling plasticity mechanisms in UFG Al freestanding thin films**
    Kashiwar Ankush
17. **Size Effect on Strength of Equilibrated Copper Nanoparticles Fabricated by Solid-State Dewetting**
    Liang Zhao
18. **Thermal Stability, Microstructure, and Mechanical Properties of Cu1-X – AlX – Al2O3 nanolaminates**
    Maeder Xavier
19. **Can device performance be enhanced by designing the guide layer as a metamaterial?**
    Okyar Ali Fethi
20. **Searching for model systems to study the relationship between the structure and mechanical properties of materials.**
    Pawlyta Miroslawa
21. **Cross-sectional size-dependent stochastic deformation and ductility of Au bi-crystalline nanowires**
    Polisetty Rohith
22. **Effect of composition and nanostructure on mechanical properties and thermal stability of ZrCuAlx thin film metallic glasses**
    Poltronieri Cristiano
23. **Exploring tungsten response under small-scale compression deformation**
    Pouriayevali Habib
24. **Factors Affecting the Deformation-Relaxation Behavior of Materials under Nano- and Micro-Indentation**
    Shikimaka Olga
25. **Structured approach towards correlation of finite element models and nanoindentation measurement data**
    Srnec Novak Jelena
26. **Nanoindentation material testing using sm@rt500 and sm@rt cubes**
    Stein Wolfgang
27. **The Nanoindentation Characterisation of Biocompatible Polymer – Flexdym**
    Stojanovic Goran
28. **3C-2H Phase Transformation in Silicon and Germanium nanowires**
    Van Den Berg Theo
29. **Another Twist on Graphene – Twistronics as a Way to Engineer Superlubric Coatings**
    Vilhena J.g.
30. **Correlating microstructure and mechanical behaviour in BCC-RHEAs using nanoindentation mapping**
    Wang Jin

Oral contributions

Tuning the mechanical properties of steels using additive manufacturing

Matteo Seita*[1] and Shubo Gao

[1]University of Cambridge, Department of Engineering (CUED) – Trumpington Street, CB2 1PZ, United Kingdom

Abstract

One of the defining features of fusion-based additive manufacturing processes is the localized melting of metal by a high-energy source, which fuses the material together point by point into a 3-D part. By varying the processing parameters at any point across the build, it is possible to control the local solidification of the material and drive the formation of different microstructures at a high spatial resolution. This unique capability opens the path to designing and producing metal parts with highly tunable mechanical properties by combining dissimilar microstructures in a controlled manner. Here, I will demonstrate this strategy by focusing on laser powder bed fusion (LPBF) of stainless steel 316L. I will show that local microstructure control during LPBF enables site-specific recrystallization. By varying the volume fraction of the recrystallized and non-recrystallized regions, it is possible to fine tune the alloy's strength and ductility. Moreover, decreasing the size of the different domains gives rise to additional strengthening mechanisms, which may be exploited to produce superior steels compared to those made by conventional manufacturing processes.

*Speaker

Deformation of nanocomposite thin fims produced by combined gas phase aggregation and magnetron sputtering

Emese Huszar[1], Peter Schweizer[1], Thomas Edwards[1], Laszlo Pethö[1], Johann Michler[1], and Barbara Putz[*1,2]

[1]EMPA Mechanics of Materials and Nanostructures – Thun, Switzerland
[2]Montanuniversität Leoben (MUL) – Franz Josef-Straße 18, 8700 Leoben, Austria

Abstract

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 (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. 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 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 to study deformation mechansims at the nanoscale.

[*]Speaker

Solid-solution and precipitation softening effects in defect-free faceted Nickel-Iron nanoparticles

Eugen Rabkin*[1], Amit Sharma[2], Oz Mendelsohn[3], Raj Koju[4], Anuj Bisht[3], Johann Michler[2], and Yuri Mishin[4]

[1]Technion – Department of Materials Science and Engineering, Technion – Israel Institute of Technology, 3200003 Haifa, Israel

[2]Empa – Swiss Federal Laboratories for Materials Science and Technology, Laboratory for Mechanics of Materials and Nanostructures, Feuerwerkerstr. 39, Thun CH-3602, Switzerland

[3]Technion – Department of Materials Science and Engineering, Technion – Israel Institute of Technology, 3200003 Haifa, Israel

[4]GMU – Department of Physics and Astronomy, MSN 3F3, George Mason University, Fairfax, VA 22030, United States

Abstract

It is well known that metals are strengthened by alloying additions or finely dispersed precipitates of a second phase. We demonstrated that alloying pristine, defect-free single crystalline nickel nanoparticles with iron results in a counter-intuitive softening due to randomly distributed solute (Fe) atoms and nano-size precipitates of the ordered Ni3Fe or Fe-rich phases. The Ni-Fe particles with Fe concentration of 0-50 at.% were synthesized by solid-state dewetting of Ni-Fe bilayer thin films deposited on a sapphire substrate. Ni-27Fe and Ni-50Fe particles exhibited a bimodal size distribution with small (111) and large (100) oriented particles. The solid solution softening was observed in all particles. The precipitation softening was observed in (100) oriented Ni-27Fe particles with uniformly distributed ordered Ni3Fe (L12) precipitates. Fe-rich precipitates were found on the surfaces and near the edges of the highly alloyed Ni-50Fe particles, leading to even greater softening. Molecular dynamic simulations of particle deformation have demonstrated that the softening effect is associated with premature dislocation nucleation at sites with a local stress concentration caused by the randomly distributed solute atoms. This work illustrates how the classical hardening mechanisms operating in bulk materials can be manipulated and even reversed in defect-free single-crystalline metal nanoparticles whose plastic deformation is controlled by dislocation nucleation.

*Speaker

Microscale 3D printing and characterization of cellulose nanocrystal reinforced nanocomposite inks

Alexander Groetsch[1], Samuel Stelzl[1], Yannick Nagel[2], Tatiana Kochetkova[1], Nadim Scherrer[3], Aleksandr Ovsianikov[4], Johann Michler[1], Laszlo Pethö[1], Gilberto Siqueira[2], Gustav Nyström[2], and Jakob Schwiedrzik*[1]

[1]EMPA Mechanics of Materials and Nanostructures (Empa) – Thun, Switzerland
[2]EMPA Cellulose and Wood Materials (Empa) – Dübendorf, Switzerland
[3]Bern University of Applied Sciences (BFH) – Bern, Switzerland
[4]Vienna University of Technology (TU Wien) – Vienna, Austria

Abstract

The increasing demand for functional materials and an efficient use of sustainable resources makes the search for new material systems an ever growing endeavour. With this respect, architected (meta-)materials have attracted considerable interest. Their fabrication at the micro- and nanoscale, however, remains a challenge. This study demonstrates that it is possible to create a non-cytotoxic nanocomposite ink reinforced by a sustainable phase, cellulose nanocrystals (CNCs), to print and tune complex 3D architectures using two-photon polymerization (TPL). Micro-compression, high-resolution SEM, (polarised) Raman spectroscopy and composite modelling were used to study the structure-property relationships. A 100% stiffness increase was observed already at 4.5 wt% CNC while reaching a high photopolymerisation degree of around 80% for both neat polymers and CNC-composites. Polarised Raman and the Halpin-Tsai composite-model suggest a random CNC orientation within the polymer matrix. The microscale approach can be used to print small-scale structures with tunable CNC-reinforced nanocomposite inks. The new insights pave the way for future applications where the 3D printing of small structures is essential to improve the performance of tissue scaffolds, bioelectronics, or microscale energy-absorption devices.
References:
(1) A. Groetsch, S. Stelzl, Y. Nagel, T. Kochetkova, N. Scherrer, A. Ovsianikov, J. Michler, L. Pethö, G. Siqueira, G. Nyström, J.J. Schwiedrzik: *Microscale 3D printing and tuning of cellulose nanocrystals reinforced polymer nanocomposites.* **Small**, 19, 2202470, 2023.

*Speaker

Making the most of your indentation data using explainable machine learning

Claus Trost*[1]

[1]Erich Schmid Insitute of Materials Science of the Austrian Academy of Sciences – Jahnstrasse 12, 8700 Leoben, Austria

Abstract

Nanoindentation has developed into a high-throughput technique that can be used for various applications. This talk presents three different applications of XAI (explainable Artificial Intelligence) on indentation data.

- The possibility of extracting more parameters from single indentation experiments will be shown by predicting in-situ nanoindentation tip wear. This is performed using a complex model trained with data from finite element simulation and an experimental data set. The experimental dataset consists of self-images of the tip at various points during more than 30.000 indents in different materials.
- XAI will be used to classify different materials components in nanoindentation maps of steels, trained data extracted from indentation curves which were annotated according to SEM and AFM images of the surface. It will be shown that different phases can be differentiated, exceeding the classical evaluation of Elastic Modulus and Hardness.
- Importance of publishing nanoindentation data in databases or mining the materials data from published works will be shown in the example of finding superhard materials by adapting models from literature and making them explainable.

*Speaker

Challenges and opportunities of using AI technologies for design and characterization of mechanics of matter at nano-scale

Simona Domazetovska*[1]

[1]Ss. Cyril and Methodius University in Skopje (UKIM) – blvd. Goce Delcev 9, 1000 Skopje, Macedonia

Abstract

The field of nanotechnology is rapidly growing and is expected to have a significant impact on numerous aspects of our lives. The increasing complexity of materials and the growing demand for faster and more accurate characterization methods have led to a significant interest of using the AI technologies, as they have the potential to revolutionize the way of designing and characterizing the mechanics of matter at the nano-scale.
On one hand, the use of AI can help to accelerate the discovery and design of novel materials with tailored properties by providing a more efficient and accurate means of identifying patterns and relationships of the mechanical properties more accurately. The machine learning algorithms have shown great promise in predicting and modeling the properties of materials at the nanoscale, which is essential for understanding the complex interactions between atoms and molecules and predicting and identifying patterns and relationships that are difficult or impossible for humans to detect.

Despite the enormous potential of AI technologies, one of the biggest challenges is the lack of high-quality data sets for training the AI models that can lead to inaccurate predictions. Another challenge is the need for interdisciplinary collaborations between experts in AI, materials science, and engineering. Additionally, ethical concerns regarding the use of AI technologies must also be addressed.
In conclusion, the integration of AI technologies presents a tremendous opportunity to advance our understanding of the mechanics of matter at the nanoscale, enabling the design of novel materials with unique mechanical properties for various applications.

*Speaker

Microcast metals: processing and tensile behaviour

Luciano Borasi[1], Simone Frasca[1], Edoardo Charbon[1], and Andreas Mortensen*[1]

[1]Ecole Polytechnique Fédérale de Lausanne (EPFL) – CH-1015 Lausanne, Switzerland, Switzerland

Abstract

Shaped 2D or 2.5D structures of micrometric dimensions and made of silver or copper can be produced by combining photolithographic silicon etching with the pressure infiltration of molten metal into porous preforms at elevated temperature. Combined, these two classical materials processes merge advantages of lithography and casting to create a route for the production of monocrystalline tensile specimens that have a surface unaffected by focused ion beam milling, a diameter selected in the range from 2.5 μm to 13 μm and an aspect ratio in excess of four with a taper around 1∘. Such microtensile samples are tested under the scanning electron microscope in displacement control and at steady temperature up to 400∘C. Data are compared with bulk counterpart samples of the same metals, of diameter in the millimeter range and cast by a similar infiltration-based method. Data, which show that microcast fine-scale metal samples exhibit characteristics of confined plasticity coupled with a strong influence of crystal orientation, provide insights on the mechanisms that govern plasticity at the microscale.

*Speaker

Nanoheterogeneous Thin Film Metallic Glasses with Improved Toughness and Ductility

Sezer Özerinç*[1], Ali Behboud[1], Amir Fadaie[1], Servet Şehirli[1], and Amir Motallebzadeh[2]

[1]Middle East Technical University, Department of Mechanical Engineering (METU) – Dumlupinar Blv. No: 1 Cankaya 06800 Ankara, Turkey

[2]Koç University Surface Science and Technology Center – Rumelifeneri, 34450 Sariyer, Istanbul, Turkey

Abstract

The low ductility of metallic glasses (MG) is a major drawback that hinders their wide utilization in applications. A recent approach to solving this problem has been the design of nanoheterogeneous MGs. The nanoscale modulations in the mechanical properties provide nanoheterogeneous MGs with a unique energy landscape that stimulates shear band multiplication, enabling means for accommodating further plasticity.
This work explored the design space of nanoheterogeneous MGs by directly controlling the relevant length scales through nanolayers. Cu-Ta is selected as a model system to produce two types of nanolayers. The first type consisted of two alternating fully amorphous compositions, Cu75Ta25 / Cu40Ta60, which we refer to as A/A, and the second type combined a fully amorphous and a semicrystalline composition, Cu75Ta25 / Cu25Ta75, which we refer to as A/SC. Micromechanical measurements were performed on magnetron-sputtered films with layer thicknesses in the 20 – 100 nm range. Nanoindentation revealed the hardness and fracture toughness of the films, and tensile testing on films deposited on polyamide substrates provided strength and ductility.

The results show that the amorphous/semicrystalline (A/SC) nanolayers provide superior toughness and tensile ductility. For example, the fracture toughness of A/SC-20 nm nanolayers is 5.8 MPa·m1/2, providing a 45% improvement on Cu40Ta60. The hardness of A/SC, reaching 11.7 GPa, is also higher than that of Cu40Ta60, demonstrating a effective route for overcoming the strength-ductility tradeoff.
Nanoheterogeneous structures offer a great design space for achieving high strength and ductile MGs. Magnetron-sputtered nanolayers provide an effective tool to systematically study the underlying process-property relationships.

*Speaker

Strong and ductile thin film metallic glasses through advanced nanoscale design strategies

Andrea Brognara[1], James Paul Best[1], Thomas Pardoen[2], Hosni Idrissi[2], Andrea Li Bassi[3], Gerhard Dehm[1], and Matteo Ghidelli*[4]

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[2]Université Catholique de Louvain (UCL) – Place de lÚniversité 1 - 1348 Louvain-La-Neuve, Belgium

[3]Politecnico di Milano [Milan] - Department of Energy (POLIMI) – Piazza Leonardo da Vinci, 32 20133 Milano, Italy

[4]Laboratoire des Sciences des Procédés et des Matériaux (LSPM) – Centre National de la Recherche Scientifique – 99 avenue Jean-baptiste Clément, F-93430 Villetaneuse, France

Abstract

The synthesis of advanced thin film metallic glasses (TFMGs) with engineered microstructures capable to provide a large combination of mutually exclusive mechanical properties (i.e. high strength and ductility) is an open research topic. Here, I will present recent results involving two (2) strategies to finely tune the microstructure of TFMGs down to the atomic scale, resulting in outstanding and controlled mechanical behavior.
Firstly, I will show the potential of Pulsed Laser Deposition (PLD) as a novel technique to synthetize nanostructured Zr50Cu50 (%at.) TFMGs. Specifically, a variety of TFMG microstructures – among which amorphous nanogranular films showing large free volume interfaces and a nanolaminated self-assembled structures – have been deposited. This results in an unique mechanical behavior as shown by in situ TEM/SEM tensile/compression tests, reporting homogeneous deformation combined with a large yield strength ($>$ 3 GPa) and ductility ($>$ 9 %) product (1).

Then, I will focus on the fabrication of fully amorphous nanolaminates with nanoscale period. I will show how the control of the sublayer thickness (from 100 down to 5 nm) influences the deformation behavior, while tuning the mechanical properties. Specifically, fully amorphous (Zr24Cu76/Zr61Cu39 %at.) nanolaminates with bilayer period $<$ 50 nm limit shear band/crack propagation, while providing a good combination of large ductility ($>$ 10%) and yield strength ($>$ 1.5 GPa).

Overall, our results pave the way to the development of novel TFMGs with improved mechanical properties and wide application range.
(1) M. Ghidelli et al., Acta Mater., 213, 116955, 2021.

*Speaker

Approaching second-strain gradient elasticity with soft X-rays diffraction

Amar Chaalane[1], Frédéric Cherioux[2], Vincent Luzet[2], Eric Joseph[1], Nicolas Jaouen[3], Horia Popescu[3], Bruno Fabre[4], and Fabien Amiot*[1]

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[4]Institut des Sciences Chimiques de Rennes (ISCR) – Universite de Rennes 1, Institut National des Sciences Appliquées - Rennes, Ecole Nationale Supérieure de Chimie de Rennes, Institut de Chimie du CNRS, Centre National de la Recherche Scientifique – Campus de Beaulieu - Bât. 10 Avenue du Général Leclerc 35042 Rennes Cedex, France

Abstract

It is well established that downsizing mechanical structures make their surface-over-volume ratio much larger than for usual objects, so that their ability to interact with their environment is significantly augmented. This has been particularly used in the development of cantilever sensors, where a surface energy change on one side induces the cantilever's bending. Even though this phenomenon has been implemented for a wide range of molecules, the modeling the mechanical response of a micromechanical structure to a surface energy change has been scarcely investigated. Second-strain gradient elasticity has been shown to naturally involve the equivalent of surface tension for solids, and thus seems particularly suited to model the deformation of solids subjected to a surface energy change.
A toy model is first used to demonstrate the key role of the material in the chemo-mechanical transduction, thereby stressing the need for an adequate experimental identification procedure.
First results from an original approach are reported herein. Beams made of a material driven by second-strain gradient elasticity are expected to display short-wavelength sinusoidal components in their displacement field. In order to experimentally validate this prediction, silicon nitride cantilevers of different thicknesses have been functionalized so that the surface energy is controlled by UV illumination. The resulting deformation has been probed using a simultaneous illumination in the soft X-rays range in transmission. The sinusoidal components of the displacement are shown to act as a diffraction grating and the observed diffraction peaks yield key information on the higher-grade elastic parameters, in line with theoretical predictions.

*Speaker

Indentation size effect at shallow penetration depths

Petr Haušild*[1]

[1]Czech Technical University in Prague, Faculty of Nuclear Sciences and Physical Engineering (FNSPE CTU Prague) – Department of Materials, Trojanova 13, 120 00 Prague 2, Czech Republic

Abstract

Indentation size effect (ISE), that is, a size-dependent increase in hardness, occurs when the size of the indent approaches the critical length scale. In metals, in which the plastic deformation is mediated by the slip dislocation movement, this critical length scale is associated with the (average) dislocation spacing. The ISE makes it difficult to compare the results obtained at small loads that are needed for characterisation of, e.g. small particles or thin layers.
The most widely used model for treating ISE in metals was proposed by Nix and Gao and is based on the concept of geometrically necessary dislocations that are required to account for the permanent change of shape enforced by the indenter at the surface. There is much experimental evidence that the Nix-Gao model almost perfectly predicts the ISE for indentations at the micrometre scale but breaks down overestimating the hardness for very small indentation depths.

Some modifications to the Nix-Gao model have already been proposed based on the maximum allowable geometrically necessary dislocation density and/or an expansion of the storage volume for geometrically necessary dislocations. Despite the specific limitations (the parameters can be dependent on indenter tip geometry, penetration depths must exceed the critical pop-in event, etc.), with these models, the Nix-Gao model can be extended to submicrometric depths.
The present speech will show some examples illustrating that the information about the local elastic-plastic response is not straightforward in the regime of very shallow depths but is still contained in the measured hardness dependence on penetration depth.

*Speaker

INDENTING THIN FILMS IS A RISKY BUSINESS

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Abstract

One of the most common methods to measure the elastic modulus and hardness of thin films is to use nanoindentation and the well-known "10% rule of thumb". The general interperation of the "rule" is that the elastic modulus and hardness can be taken at 10% of the film thickness with no or little influence from the substrate. Unfortunately, the universal use of the 10% rule of thumb is not 100% accurate. Using several examples of thin film systems of various materials, microstructures, architectures, and thicknesses it will be demonstrated that the 10% rule of thumb should not be applied to evaluate the elastic modulus of thin films at 10% of the film thickness. An assessment of the hardness and elastic modulus as a function of contact depth and accurate finite element modelling of the film/substrate deformation confirms the 10% rule for hardness measurements. For elastic modulus, the indentation depths should be much smaller. A new recommended testing protocol for accurate assessment of thin film elastic modulus using nanoindentation is presented.

*Speaker

Creep-dominated fatigue of freestanding gold thin films

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Abstract

Despite their common use in microelectronics, the fatigue behavior of submicrometer metallic thin films is not yet fully understood. Unlike bulk materials, which typically exhibit persistent slip bands and extrusions as damage sites after cyclic loading, thin films exhibit surface roughening and grain boundary cracking due to their dimensional limitations. Most of the previous studies were conducted on films attached to a substrate, which influences the fatigue behavior. Here, 150-nm thick gold specimens were tested in freestanding condition. High cycle fatigue (HCF) experiments were performed in a custom bulger at temperatures between 23 ∘C and 100 ∘C and nominal stress ranges between 100 to 300 MPa. An S-N curve was generated, showing a decreasing lifetime with increasing temperature and stress amplitude. Small failure strains of 1.5 % or below were recorded. As the samples fail catastrophically, the deformation mechanisms cannot be reconstructed from post-mortem observations. Because cyclic creep is prominent in the strain data at all stresses and temperatures, a steady-state strain rate was determined. Using the stress exponent n and activation energy Q to compare the cycling data with bulge creep experiments from literature, it was found that fatigue is creep-controlled at 100 ∘C. At lower temperatures cycling effects become more pronounced. Further evaluation of the results regarding the deformation mechanisms suggests that straining due to dislocation motion is limited because of the high amount of surfaces and interfaces. Hence, diffusion processes allow further straining and the emission of new dislocations at grain boundaries.

*Speaker

Effects of Radiation Damage on the Critical Resolved Shear Stresses in Zirconium Alloys for Nuclear Applications

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Abstract

Nuclear power provides 10% of the world's electricity and is likely to expand as countries seek to provide low-carbon energy in the future. Of the current 442 commercial nuclear reactors, 96% are water cooled and thus have their uranium oxide fuel contained within a zirconium alloy cladding.
Under irradiation, like most metals, these zirconium alloys exhibit strong hardening effects. Typically, the yield stress of Zr-alloys doubles during the early stage of irradiation while a dramatic loss of strain-to-failure is observed. Irradiation hardening is currently qualitatively described by loops being barriers for dislocations during mechanical loading. This hardening is also supplemented by irradiation-induced precipitates, but their effect on irradiation hardening in Zr-alloys is currently unknown.

Like most of other hexagonal close packed (HCP) materials, zirconium deforms anisotropically via plastic slip on the basal, prismatic and pyramidal planes. As loop formation is also crystallographically influenced, a full picture of the radiation damage effects in zirconium must be gathered on a piece-by-piece basis, with the influence of damage levels, strain rate and temperature being determined on each slip system.

We present here the first steps towards painting this picture of radiation damage effects in zirconium. Nano-indentation testing using spherical and Berkovich tips correlated with indented grain orientations from EBSD has been used for initial rapid screening of irradiation hardening and strain softening effects, as required by complementary CP-FEM models. Subsequently identified "interesting" samples have been selected for more quantitative micromechanical investigation to determine critical resolved shear stresses on specific slip systems.

*Speaker

Elastic and Plastic Response of FCC-Metallic Nanostructures under complex Loads

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Abstract

Nanoscale metallic objects like thin films, nanoparticles, nanowires, or nanoporous metals receive sustained attention due to their size-dependent mechanical properties, which can include changes in deformation mechanisms, pseudoelastic behavior, and increased yield strength compared to the bulk material. In particular, fcc metallic nanowires (NWs) are regarded as promising building blocks for a variety of applications e.g., in flexible and stretchable electronics. While NWs are mostly studied in tension, these applications subject them to bending loads, and also buckling can take place, e.g., due to Poisson contraction of an NW containing film under tension. Bending and buckling are also common for struts in nanoporous metals. Here we present recent results of atomistic simulations as well as finite element simulations (FEM) on single crystalline NWs (SCNW) and nano struts, bi-crystalline twinned NWs (BTNW) as well as fivefold twinned NWs (FTNWs) subjected to tension, bending, and buckling. Dislocation-free nanostructures are known to withstand large elastic stresses without plastic deformation, which can lead to strong non-linear elastic effects and changes in defect energies. Additionally, twin boundaries are shown to also significantly affect the elastic response, resulting in a complex stress state in bent nanostructures. The complex stress state directly affects dislocation nucleation and dislocation-twin boundary interactions. The results are compared to twin-free nanostructures to highlight the impact of twins on the failure of nanowires under conditions typically found in stretchable electronics and the effect of nanostructure size on dislocation microstructure and subsequently plasticity is discussed.

*Speaker

Topology- and size-governed plasticity of nanoporous Au

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Abstract

In this study, the plasticity in nanoporous structures is addressed using molecular dynamics (MD) simulations of nanoporous gold (NPG) nanopillars. MD simulations involve uniaxial compression of single-crystalline NPG nanopillars with different ligament diameters to investigate the topology and size-dependent mechanical characteristics. The computed size-dependent stress-strain relation displays different deformation stages, namely, elastic, plateau, and strain-hardening. The ligament size-effect is insufficient to explain the elastic size-dependency in nanopillars due to the limited number of connected load-bearing ligaments. We implemented a topological analysis technique, named skeletonization, to estimate the average number of load-bearing ligaments along the loading direction, which act as a topological parameter. A modified scaling law is proposed to address the elastic size-dependency which includes both the size-effect of ligaments and the topological input. We combine the skeletonization and the common neighbor analysis algorithms to demonstrate that the ligaments yield before the plateau. As the plateau region is initiated, there is no abrupt drop in the stress as observed in nucleation-controlled plasticity in nanowires because of the three-dimensional network structure that retains the resistance to deformation. Despite the existence of 60% unyielded ligaments, the stress ceases to increase because the scaled genus density of unyielded ligaments decreases to zero. Strain hardening is characterized by the change in the topology due to the coalescence of ligaments and closure of pores. The size effect in plasticity is projected as the earlier strain hardening in lower ligament diameter NPG. Thus, the topology- and size-dependent plasticity in NPG nanopillars are demonstrated.

*Speaker

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

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Abstract

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. 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. 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 a dislocation embryo 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.

*Speaker

Influence of roughness on the mechanics of nano-objects

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Abstract

Surface roughness plays a key role in several fields of applications including friction, lubrication, machining and polishing. At the atomic scale, surfaces and surface defects are also known to be at the roots of major physical phenomena as *e.g.*, in the field of catalysis 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, drawing a correlation between degrees of roughness and the fractal dimension. In this study, we first present *Pyrough,* a tool we have recently developed to design rough virtual samples for atomistic and finite-element modeling simulations based on the classical roughness theory. *Pyrough* is a Python code that constructs 3D virtual objects with the ability to manage surface height distribution of isotropic and Gaussian random surfaces. It produces both rough 3D meshes compatible with most FEM programs and atomic files as being fully coupled with the Atomsk atomistic library. Then, we use *Pyrough* and molecular dynamics simulations to investigate the influence of surface roughness on the mechanical response of metal nanoparticles. Our results show that surface roughness has a major impact on the mechanical properties of nanoparticles and several regimes are identified. Yield stress and Young's modulus variations as function of roughness parameter are studied performing statistical analysis on hundreds of MD simulations. Additionnal investigations on the role of surface steps on the dislocation microstructure evolution during plastic deformation are also carried out.

*Speaker

Shape effect on mechanical properties of nanoparticles: from atomistic to continuous simulations

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Abstract

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.

To this end, we investigate the elastic and plastic properties of metallic (Au, Cu, and Pt) and alloy NPs as a function of different sizes and shapes (for fcc single crystalline structure). We use a multi-scale and multi-physical approach combining atomic-scale and continuous methods such as 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 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.

*Speaker

Failure of a brittle layer on a ductile substrate: Nanoindentation experiments and FEM simulations.

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Abstract

The cracking of brittle layers deposited on ductile substrates is a difficult subject to describe because of the complex response of the system: film-on-substrate geometry, substrate plasticity, possible delamination of the layer, etc. However, understanding the cracking process in such systems is of particular interest from both a fundamental and an application point of view, for example to anticipate and prevent fracture in functional devices.
In this context, the cracking of a Si3N4 silicon nitride layer deposited by Plasma-Enhanced Chemical Vapour Deposition (PECVD) on an AlSiCu metallic substrate has been studied by combining nanoindentation experiments and numerical simulations using the eXtended Finite Element Method (XFEM) including Cohesive Zone Models (CZM). An energy-based approach using pop-in features on the loading curves was developed to determine the fracture strength of the brittle layer and the complete cracking process (crack location, crack size, ...). This methodology was fully validated by comparing the numerically predicted crack pattern with that observed experimentally by electron microscopy.

*Speaker

Propagation of zonal dislocations: the case of the synchroshear mechanism in Laves phases

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Abstract

Initially introduced in the context of twinning, zonal dislocations are seen nowadays as key dislocation in few complex intermetallics, such as MAX phases and Laves phases. Combining shear with shuffling, such dislocation propagates thanks to the mechanism of synchroshear, which remain to date debated.
By focusing on Mg2Ca Laves phases, we propose a numerical exploration at the atomic-scale of mechanisms responsible for the propagation of zonal dislocations (1). In particular, we demonstrate that nucleation and propagation of kink pairs is the energetically favorable mechanism for the motion of the synchro-Shockley dislocation (2). Additionally, we investigated how vacancies and antisite defects assist kink nucleation and propagation. Ultimately, we explore the thermally activated nature of synchro-Shockley dislocations and demonstrate the crucial role of thermal assistance on the propagation of such a zonal dislocation.
By the thorough investigation of the synchroshear mechanism in Mg2Ca Laves phases, our work aims to advance the understanding of the mechanisms of motion of zonal dislocations in complex crystals.

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*Speaker

Atomic scale engineering of dislocation slip and twinning in magnesium alloys

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Abstract

This work describes novel mechanisms of interaction between dislocations and twin boundaries with nanoscale precipitates and with engineered matrix-precipitate interfaces, in magnesium alloys. A combined approach including micromechanical testing of pillars milled by focused ion beam and high resolution transmission electron microscopy, is put in place to unveil such mechanisms at the atomic scale. It will be shown that atomic scale engineering is useful to tackle some pending issues related to the macroscale mechanical behavior of these alloys.
We will target, first, the problem of basal slip localization, which is a well known cause of premature fracture. It will be shown that introducing a dispersion of nanoscale precipitates (3 atomic layers thick) by alloy design, might be very beneficial to enhance diffuse slip. In particular, it will be demonstrated that basal dislocation movement within such a precipitate dispersion leads to the dissolution of the ultrathin particles and to room temperature solute diffusion towards the active slip planes, which thus become hardened. This, ultimately, promotes the activation of additional slip planes, thus preventing localization(1).

Second, the talk will tackle the problem of mechanical anisotropy, caused by the impossibility to prevent twinning. It will be shown how atomic scale segregation of selected species at matrix-particle interfaces of Mg-Al alloys leads to a reduction of the interface energy and severely limits the possibility of twin renucleation at such interfaces, thus drastically reducing twin propagation(2).

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*Speaker

Advanced Electron Microscopy techniques for strain evaluation in nanostructured materials at the atomic scale

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Abstract

Local atomic structure of nanomaterials plays a crucial role in the mechanisms responsible for new phenomena observed and new properties measured. Interfacial structures, defects and strain are considered as the key factors.
Quantitative atomic resolution transmission and scanning/transmission electron microscopy (aHRTEM and qHRSTEM) have become increasingly important to elucidate the correlation between growth/synthesis and structure of nanomaterials and to understand nanomechanisms that tailor properties.

Several -Nitride semiconducting heterostructured nanostructures in which HRTEM/HRSTEM is employed to study the abruptness and the local atomic interfacial structure, the coincidence or not of the structural and chemical interfaces, the role of the interfaces in the introduction of defects, will be presented. qHRTEM and qHRSTEM are applied to quantify strain-composition coupling and deformation fields around defected structures and interfaces. Correlation of the quantified experimental results to simulated energetically relaxed atomistic models will be shown.
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*Speaker

Grain boundary plastic mechanisms on polycrystals: the case of shear-coupled GB migration studied by in-situ TEM and AFM

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Abstract

The Hall-Petch relationship describes the proportional evolution of the yield strength of a metal with the inverse of its grain size. Dislocation pile-up can explain this phenomenon but reaches its limit for nanometric grain size, generally dislocation free. Plastic deformation, remaining at this scale, is generally attributed to grain boundaries themselves with mechanisms like grain rotation, intergranular sliding and/or shear-coupled grain boundary migration. Even if numerous observations of this mechanisms are reported in the literature, few are quantified. Cahn, Mishin, Suzuki and Taylor (CMST) (1) proposed a predictive model linking the coupling factor (ratio of shear displacement over the migration distance) with the misorientation of tilt grain boundaries. This conservative model has been partly validated on bicrystals experiments (2) but remains unsure on polycrystals where lower coupling factors were measured (3).
The aim of this study was to bring a statistical study of coupling factors on ultrafine grain polycrystals of aluminum. The coupling factor study have been conducted by in-situ TEM, to consider the in-plane shear, and by AFM to consider the out of plane component. Compared to the CMST model, the ones based on disconnections are the most likely to explain the lack of correlation between misorientation and coupling that we measured but are still far from being predictive.

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*Speaker

In-situ TEM nanomechanical investigations on a grain boundary sliding mechanism in forsterite

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Abstract

Olivine is the most abundant (> 60 % in volume) and weakest phase in the Earth's upper mantle of which it controls the rheology. The lack of slip systems in this crystal leads to the activation of other intergranular deformation mechanisms to accommodate a general strain. Our study focuses on the grain boundary sliding mechanism, based on grain boundary amorphization which was reported recently (1). For this elementary deformation mechanism, quantitative investigations are carried out on a bi-crystal forsterite tensile specimen by in-situ TEM test with a Push-to-Pull device. This work uses synthetic forsterite (the magnesium-rich end member of the olivine solid solution) samples. We show that specimens deform exclusively by grain boundary sliding. Detailed microstructural investigation shows direct evidence of stress-induced amorphization in the sliding grain boundaries. We provide for the first time the mechanical signature of this phenomenon as well as direct evidence of the underlying elementary mechanisms. Furthermore, in-situ digital image correlation (DIC) in the TEM was used to get an enhanced spatial resolution for mapping the small localized strain onset of the grain boundary sliding. (1) Samae V. Cordier P., Demouchy S., Bollinger C., Gasc J., Koizumi S., Mussi A., Schryvers D. & Idrissi, H. "Stress-induced amorphization triggers deformation in the lithospheric mantle," *Nature*, vol. 591, 2021, doi: 10.1038/s41586-021-03238-3

*Speaker

Strain rate and size dependent mechanical behaviour of a dual phase high-entropy alloy

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Abstract

High-entropy alloy design has been in the spotlight of materials engineering, because the mechanical behaviour can be tuned by the composition and by varying the heat treatment procedure. Modern multicomponent alloys consist of more than one phase, often having distinct mechanical characteristics. Individually probing each phase in these complex materials require microscale experiments to be performed. Here, a series of micropillars were prepared and deformed by compression. Sample deformation was limited to the micro-scale while dislocation – phase/grain boundary interactions were evaluated on the atomic scale. A NiCoFeCrGa alloy was chosen with dual phase (BCC and FCC) structure. The microstructure goes through a spinodal-like decomposition when subjected to slow cooling from a high temperature, creating cuboid shaped precipitates inside the BCC grains. In order to separate the mechanical behaviour of the constituent phases, micropillars (diameters ranging between _˜500–3000 nm) fabricated by focused ion beam were deformed. Two samples having different microstructures (BCC with and without precipitates) were compared. Selected pillars were lifted out and studied by cross-sectional high (angle) resolution electron backscatter diffraction (HR-EBSD) and scanning / transmission electron microscopy (S/TEM) to characterize dislocations at the phase- and precipitation boundaries. Pillars deformed at quasi-static and high strain rates were also prepared to look at the effect of the deformation speed on the evolution of dislocations. STEM-based energy dispersive spectroscopy mapping showed that the precipitates are mainly Cr-rich cuboids that globally modify the strength of the alloy.

*Speaker

Room Temperature Viscous Flow of Amorphous Silica Induced by Electron Beam Irradiation

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Abstract

The increasing use of oxide glasses in high-tech applications illustrates the demand of novel engineering techniques on nano- and microscale. Due to the high viscosity of oxide glasses at room temperature, shaping operations are usually performed at temperatures close or beyond the point of glass transition Tg. Those treatments, however, are global and affect the whole component. It is known from the literature that electron irradiation facilitates the viscous flow of amorphous silica near room temperature for nanoscale components. At the micrometer scale, however, a comprehensive study on this topic is still pending. In the present study, electron irradiation inducing viscous flow at room temperature is observed using a micropillar compression approach and amorphous silica as a model system. A comparison to high temperature yielding up to a temperature of 1100 ∘C demonstrates that even moderate electron irradiation resembles the mechanical response of 600 ∘C and beyond. As an extreme case, a yield strength as low as 300 MPa is observed with a viscosity indicating that Tg has been passed. Those results show that electron irradiation-facilitated viscous flow is not limited to the nanoscale which offers great potential for local microengineering.

*Speaker

Coupling micro-compression testing and Laue micro-diffraction

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Abstract

White beam Laue micro-diffraction is a powerful technique to probe the crystalline structure of a material and its orientation. It also gives access to local crystal deformation and can evidence the activation of specific slip systems thanks to the shape analysis of individual Laue spots (1). The monitoring of Laue diffraction spots as a function of time also allows to detect structural changes such as phase transitions. Thus, Laue micro-diffraction is well adapted for *in situ* mechanical testing. In this communication, we will present two original studies based on the coupling between micro-compression testing, using a FT-NMT04 nanoindenter equipped with a diamond flat punch, and Laue micro-diffraction performed at BM32 ESRF synchrotron beamline.

The first case study is based on the investigation of transformation induced plasticity in ceria-doped zirconia single crystalline micropillars with different orientations. During *in situ* experiments, the micropillars were compressed and deformation was followed by Laue micro-diffraction to monitor the crystal orientation before and after the phase transformation. Regarding the effect of the crystal orientation, a competition between fracture and transformation was observed. The second case study relies on the investigation of the plastic deformation in ferromagnetic Heusler alloys, which is important to understand how magnetic order is modified by the introduction of defects, and thus by plasticity.

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*Speaker

Posters

DESIGN, SIMULATION AND OF AN MICRO-MANIPULATOR

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Abstract

Because the micromanipulation of micro parts (as a whole), biological cells in microsurgery, and microparticles in materials science are of great interest to scientists and engineers, we developed an electrothermal operated microgripper for handling cells and other biological particles. This paper presents some of the results, namely, the design and operation simulation for a micromanipulator.

*Speaker

Study of the structure and mechanical properties of ferrous and non-ferrous metal welded joints

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Abstract

This study describes the investigation of the microstructure and mechanical properties of ferrous and non-ferrous metal butt welds. Mechanical properties of welded joints were evaluated in respect of tensile strength, bend strength and microhardness under different welding modes. In order to identify defects in the fusion and thermal effect zones of the weld, the microstructure was analysed using an optical microscope. In order to evaluate the strength of the welding joints, both in the seam and in the heat-affected zone, tensile and bending tests of the specimens were performed in the longitudinal and transverse directions, respectively. Microhardness tests were performed on each specimen by moving the indenter away from the weld axis through the heat-affected zone until the microhardness of the base material was reached. Microhardness of aluminium samples were tested and also their relation with aging time was assessed. The seams of pure titanium welded specimens were additionally examined using liquid penetrant test and radiographic inspection. The localization of the defects in the hardox steel weld seams was determined using the ultrasound method. Studies were conducted using TecScan fully automated immersion ultrasonic testing system. In addition, the quality of weldability of samples of different types of metal was investigated. Recommendations have been made on suitable welding parameters to weld metals because the proper selection of welding current, filer road, welding speed, shielding gas has a huge influence on the quality of welding.

*Speaker

EFFECT OF ADDITION OF GRAPHENE ON THE MECHANICAL PROPERTIES OF THE POLYMER NANOCOMPOSITES

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Abstract

The exceptional mechanical properties of graphene nanoribbons allow its incorporation into a wide range of polymeric nanocomposites materials. The quasi one-dimensional nature of graphene nanoribbons may significantly change the mechanical percolation threshold in the polymer composites. In our research work miniemulsion polymerization was select as most promising synthesis method for hybrid dispersed systems as the present one. The polymer was joined with graphene nanoribbons stable dispersion in order to produce 0.2 - 1.0 wt. % of graphene nanoribbons in relation to polymer. The monomers used for the synthesis were methyl metacrylate/butylacrylate /hydroxyethyl methacrylate. As a result stable in situ hybrid dispersions were obtained.

The aim of this research work was to investigate the mechanical properties of polymer based nanocomposites. In situ miniemulsion polymerizations of poly(methyl methacrylate co- butyl acrylate-2-hydroxyethyl methacrylate) with weight ratio 49.5/49.5/1 in the presence of GNRs were performed in batch emulsion system. The composite films were formed by water evaporation under controlled temperature and humidity conditions and further characterized by means of tensile test measurement and DMTA for studying the mechanical, thermal and viscoelastic properties of the nanocomposites.

The nanocomposites are distinguished with improved mechanical and thermal properties compared to the neat polymer and this effect increased with higher loading of graphene nanoribbons. This is likely due to improved interaction between the polymer chains and the graphene nanoribbons that offer an important interface on the edges, reach in oxygen functional groups. The presence of these edges facilitates the interactions with polymer chains, resulting in important reinforcing effect.

*Speaker

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

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Abstract

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.

*Speaker

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

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Abstract

Nanotwinned materials are the subject of many researches because they show mechanical properties that are usually antagonistic. We performed in-situ tensile tests on gold thin films with nanotwins, and we observed an increase of the twins volume in the crystal. Atomistic simulations are a useful complementary tool to better understand the deformation mechanisms. We first focused on < 110> {112} 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. 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 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 discuss the width of the 9R phase in ITBs.

*Speaker

The extended scaling laws of the mechanical properties of additively manufactured body-centered cubic lattice structures using finite element modelling

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Abstract

Additively manufactured lattice structures are porous light-weight structures with mechanical properties that are dictated both from the topology and the parent material properties. When printed from metals, these structures can withstand large continuous plastic deformation. In this study, we perform a systematic study using finite element modelling (FEM) to find how both material properties and lattice structures are affecting the effective mechanical properties of body-centered cubic (BCC) lattice structures under compression. Based on this analysis we propose relations between the slenderness ratio of struts and the following mechanical properties: Young's modulus, yield strength, hardening rate of the structure and the densification strain. The scaling laws can be explained as an extension of the Gibson-Ashby power law relations for bend-dominated structures with non-slender beams. Additionally, the yield strength and the densification strain were found to depend also on the ratio between the hardening rate and the yield strength of the parent material. We show that rounding the connections between the struts using fillets does not affect much the volume fraction, but can improve greatly Young's modulus, the yield strength and the hardening rate, while decreasing only slightly the densification strain. We discuss the reasons for this behavior and how it can be used to absorb plastic energy.

*Speaker

Viscoelastic and Viscoplastic Behavior of Graphene – Epoxy Nanocomposites: Experiments and Constitutive Modeling

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Abstract

Improvement of the interfacial bonding between nanofiller and matrix and homogenous dispersion of nanofiller on the matrix are two main issues in the manufacturing of polymer matrix nanocomposites. To get an improved mechanical properties, first, graphene nano flakes (GNF) are functionalized using Triton X-100. Then, the f-GNF-epoxy nanocomposites are manufactured by three roll milling for two different graphene fractions (0.1 and 0.5 wt %). Thermogravimetric analysis, X-ray diffraction tests, Raman Spectroscopy and Fourier Transform Infrared Spectroscopy (FT-IR) were performed for the structural characterization of graphene. The viscoelastic – viscoplastic behavior of nanocomposites are investigated by performing Dynamic Mechanical Analysis (DMA), creep and compression tests. Rate dependency in compression and stress dependency on creep were modeled by using cooperative-viscoplasticity theory based on overstress (C-VBO) for nanocomposite model. In the recently developed nanocomposite material model, the unified state variable VBO theory which consists of two tensor valued and one scalar state variables with a flow law is taken as base. This material model which covers the total time, temperature and nanofiller fraction has been developed over the years by Colak. The Mori-Tanaka homogenization scheme is used in order to define modulus values as a function of nanofiller fraction. For stiffening effect of graphene in viscoplastic region, Takayanagi averaging approach is used as well. All behaviors mentioned above are simulated and good agreement with the experimental results is obtained.

*Speaker

NiTi alloys manufactured by LPBF for cardiovascular applications

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Abstract

Shape memory alloys offer unique shape memory (SME) or superelastic (SE) effects that have attracted the interest of different industrial sectors, such as aerospace, automotive, robotics, and biomedical devices. NiTi, also referred to as nitinol, is the most extensively used SMA in the biomedical field due to its excellent biocompatibility, corrosion resistance and mechanical properties, especially to manufacture self-expandable devices for cardiovascular applications. However, current methods for manufacturing NiTi-based cardiovascular devices only allow for simple geometries and prevent the manufacturing of patient-specific personalized devices. In recent years, laser powder bed fusion (LPBF) is emerging as an additive manufacturing technique that should allow both the production of complex-shaped and custom-made NiTi devices. In order to manufacture different devices for cardiovascular applications, two types of NiTi composition have been used to achieve the two properties of superelasticity and shape memory. To do this, the process parameters were optimized to obtain the maximum density of the parts. In addition, heat treatments were carried out that helped improve the mechanical and shape memory properties of the pieces and were tested by tensile and compression tests. Due to the high roughness obtained by LPBF, different surface treatments were carried out, such as chemical etching, electropolishing or a combination of both, and samples were characterized in terms of surface chemistry, oxide layer formation, roughness or corrosion resistance, among others. Furthermore, the biological interactions of these surface-treated and non-treated nitinol samples with endothelial and smooth muscle cells were studied in terms of viability, proliferation or gene expression.

*Speaker

Mechanical Property Mapping for Dual Phase (DP) Steels

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Abstract

Advanced high strength steels (AHSS) offer various benefits for automotive applications including lightweighthing through use of thinner sheet blanks without compromising strength, and safety. Among different AHSS grades, dual-phase steels offer improved strength and ductility thanking to their ferrite matrix (provides ductility) and martensite (provides strength). This study aimed to reveal the effect of deformation on the mechanical properties of two DP steel grades, namely DP 1000, and DP 1200 by employing maximum load-controlled indentation with a Berkovich type of indenter. The maximum indentation loading of 6 mN was employed and 400 indentations (20x20) were performed in matrix form and with 10 μm spacing. The loading scheme was loading for 5 s, holding it for 2 s, and then unloading at 5 s. To reveal the effect of deformation, the DP 1000 and DP 1200 materials in plate form were subjected to 3-point bending test that surpassed the yield point of the material. Then, two samples were extracted from the most deformed, and undeformed (or significantly less deformed) zones. The nanoindentation was applied both to deformed and undeformed sections of the investigated dual-phase steels. Hardness and modulus of elasticity values obtained are mapped for the investigated area. In addition, EBSD measurements were performed to estaliblish microstructure-property relation. It was revealed that the hardness values were relatively in a narrow range denoting the overall response of the microstructure rather than the ones for individual phases. In addition, the effect of deformation is more pronounced for DP 1000.

*Speaker

Mechanical and electronic properties of metallic nanoparticles

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Abstract

At the nanoscale, physical properties change with size, including electronic and mechanical properties. This study aims to engineer new nano-objects with targeted mechanical and electronic properties by examining the interplay among shape, size, and composition of nanoparticles (NPs). We investigate the elastic and plastic properties of metallic and alloy NPs using a multi-scale and multi-physical approach that combines atomic-scale and continuous methods, Molecular Dynamics (MD), and Finite Elements (FE).

From our study on mechanical property we can highlight two different results: the validity and limits (5nm) of the FE solution at the nanoscale, and the contribution of shape to elasticity and plasticity. Our analysis shows that the elastic response of NPs is highly dependent on their shape, with different shapes exhibiting distinct elastic behavior. The different stress distribution in the elastic field is what determine the size effect and shape effect.

In addition to mechanical properties, we also study the electronic properties of plastically and elastically deformed NPs using a tight-binding formalism and Density Functional Theory (DFT) calculations. We propose an investigation of electronic local properties and the influence of different parameter's such as size shape and deformation.

*Speaker

Atomistic simulations of the deformation of ultra-thin films of nanoporous gold constructed from experimental samples.

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Abstract

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 fusioning as well as deformation mechanism will be presented. The influence of topology (ligaments diameter, length and orientation) on plastic deformation will also be discussed.

*Speaker

Multiscale and multifunctionality of textile structures

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Abstract

This paper is dedicated to insights into the multifunctionality of advanced textile and various contributing microstructural length scales, followed by a motivation to characterize the mechanical properties from the application's point of view. In the midst, the mechanical behavior of Advanced textile materials and related mechanical characterization techniques (from mesoscale to nanoscale) are highlighted. The last part summarizes current challenges, future perspectives, and important observations.

*Speaker

Dislocations annihilation under reciprocating friction in LiF single crystals

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Abstract

The effect of friction on surfaces differs considerably depending on the unidirectional or reciprocating sliding mode was applied. The reciprocating motion reduces the yield stress at the start of reverse deformation and play an important role in depreciation of stress induced hardening of materials. For example, it was found that unidirectional friction test of metal alloy caused more wear loss than in reciprocating one. The strain-hardening effect decreased under reciprocating sliding, suggesting that the dislocations annihilation plays an important role under these worn conditions.
At the microscopic level, dislocations annihilation could be attributed to the local reversible dislocations' movement. Annihilation of dislocations is accompanied by a decrease in the rate of dislocation accumulation and, consequently, it lowers the strain hardening.

Single crystals are widely used for the analysis of the dislocation motion. In particular, the aim of the present work was the comparison of the dislocation structure of LiF single crystals in unidirectional and reciprocating friction. The experimental evidence of the dislocations around the wear tracks in both unidirectional an reciprocating friction was presented.

*Speaker

Strain- and temperature-induced local dilatancy in ductile ZrNi thin film metallic glasses with nanoscale structural heterogeneities

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Abstract

Although extensive experimental and simulation researches have been devoted in the past to study the mechanical behaviour of metallic glasses, the elementary deformation mechanisms in these complex systems are not well documented and still a subject of open debates. The determination of the relationship between the macroscopic deformation and the atomic strain phenomena in metallic glasses is essential towards unravelling some fundamental deformation mechanisms and hence their link with their mechanical properties. Thin film metallic glasses constitute exemplary systems in this context owing to their larger ductility compared to bulk counterparts, providing rich information on the elastic and plastic phenomena. However, probing specimens at the sub-micron scale with dedicated tools still remains a difficult challenge. Here, we present complementary results obtained with high resolution X-ray synchrotron scattering and in-situ annealing transmission electron microscopy (TEM) measurements on ZrNi thin freestanding films with giant strength/ductility balance. Surprisingly, the evolution of the first maximum of the structure factor in reciprocal space shows that local dilatancy involving massive generation of free volumes can take place upon loading in tension at room temperature as well as upon thermal annealing. The link of such unexpected behaviour with the out-of-equilibrium microstructure of the films involving

*Speaker

nanoscale chemical/density heterogeneities, with complex atomic phase transition as well as the exceptional mechanical properties of these films is discussed. This study brings new insights on the role of complex local atomic relaxation and deformation mechanisms on the mechanics of sputtered thin film metallic glasses.

Modelling of interfacial energies and strains in GaN/AlN superlattices

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Abstract

In this contribution, we present density functional theory calculations of the strain partitioning and energy contribution on heteroepitaxial interfaces in a series of structures comprising different m and n layers of mGaN/nAlN superlattices, with m = 1 ÷ 16 and n = 16. The excess interfacial energy is obtained by the difference *Einterface = Ebicrystal-Ecryst1 - Ecryst2 - Estrain*, and the perturbations of (0001) planes due to the presence of interfaces separating the two compounds are investigated by computing the interplanar distances, d(0001) and strains as functions of the plane position. The strains are defined as: ϵi = (di-d(i-1)/d(i-1) where, ϵi is refered to the zi- coordinate of the ith (0001) plane of the superlattice.

The strain partitioning is studied using ϵi through the whole thickness of the bicrystal after relaxation towards the z direction, normal to the interfaces. The strain has different values in the interfacial areas compared to those in the bulk. From the displacement profiles it is depicted that for the thicker strained layers (i.e. more than 2 layers), the two interfaces are separated by the biaxially compressed layers in between, while for the ultra-thin layers (1 & 2 layers) the two adjacent interfaces collapse into a deformed interfacial area.

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*Speaker

Combining nano-scale digital image correlation with ACOM-TEM for unravelling plasticity mechanisms in UFG Al freestanding thin films

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Abstract

Nanocrystalline (nc) and ultrafine-grained (UFG) metals with grain sizes in submicron regimes exhibit outstanding mechanical strength and fatigue properties compared to their coarse-grained counterparts. Thin films of nc or UFG metals are promising candidates for hard coatings on bulk components, structural components in MEMS/NEMS, and conductive layers in microelectronic devices. However, their applicability is often restricted by the limited ductility exhibited by them due to low dislocation storage capacity within small-sized grains. Besides dislocation-based processes, the complex interplay of grain boundary (GB) mechanisms is well-known to control their plasticity. In the present work, elementary plasticity mechanisms are studied in UFG Al freestanding thin films with exceptional ductility (up to 20%). The deformation processes are unraveled using a novel combination of nanomechanical lab-on-chip testing with nano-scale digital image correlation (n-DIC) followed by a correlative investigation by automated crystal orientation mapping in TEM (ACOM-TEM). n-DIC allows for high-resolution quantification of small in-plane shear strains along with the rotational behavior of the grains across the specimen. These measurements captured a detailed spatial distribution of strains in a deformed specimen at GBs as well as within the grains. ACOM-TEM results showed a clear correlation between the majority of shear strains with the GBs in the specimen enabling a quantitative understanding of shear displacements at GBs and these were further linked with the GB character, orientation, and defects. The combination of n-DIC and ACOM-TEM is demonstrated as a method for developing a closer link between localized strains and the microstructure of polycrystalline materials at nano-scales.

*Speaker

Size Effect on Strength of Equilibrated Copper Nanoparticles Fabricated by Solid-State Dewetting

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Abstract

It is now well established that mechanical properties of metal samples of nanometric dimensions are very different from those of their bulk counterparts. Strong size effect in mechanical strength has been reported for many face centered cubic (FCC) metals and alloys, yet the dislocation nucleation-controlled plasticity mechanisms are still poorly understood. In the present work, solid state dewetting technique was employed to produce defect-scarce copper nano- and microparticles of various sizes exhibiting equilibrium crystal shape. The results of in-situ microcompression tests revealed two clear size-related regimes, where large copper particles exhibit a strong size effect in strength with size exponent comparable to other FCC metals, while their smaller counterparts show weak size dependence of strength, which saturates at about 10 GPa. Our experimental results were in good quantitative agreement with the results of atomistic molecular dynamic simulations of Cu nanoparticles compression. We related the two different size effect regimes to the high probability of dislocation nucleation event at the corner of the particle facets, and increasing probability of finding crystal structure defects inside the particles with increasing particle size.

*Speaker

Thermal Stability, Microstructure, and Mechanical Properties of Cu1-X – AlX – Al2O3 nanolaminates

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Abstract

Metal multilayer composites can show an enhancement of both strength and ductility related to the structure and properties of the interfaces between the layers, as well as the thicknesses and properties of the individual layers. However, nanolaminate structures often suffer microstructural instability during annealing and extreme deformation conditions. It is well known that the alloying addition in bulk nanocrystalline materials can significantly improve the microstructural stability and mechanical properties by grain boundary pinning, secondary phase precipitation and other segregation related mechanisms. In this context, we present experimental data on the fabrication and mechanical behaviour of nanolaminate alloy thin films of varying interlayer thicknesses (40 to 120nm). The layers are separated by atomic layer deposition of 2 nm amorphous Al2O3 layers in the same chamber without breaking the vacuum. As a model system, Cu1-x – Alx (X: 0, 5 and 10 at.%) layers with a total thickness of 3 microns is deposited on Si (100) substrate by magnetron sputtering and subsequently tested by micro compression and nanoindentation experiments. The mechanical response of the multi-layered structures is also compared with single-layer counterparts. This material system leverages grain boundary solutes to stabilize the single phase nanograined Cu microstructure, maintaining stability even after elevated temperature exposure. Moreover, the multilayered microstructure takes advantage of multiple small-scale mechanisms such as Hall-Petch, solid solution, and Orowan precipitate strengthening for enhanced mechanical properties compared to bulk. The post-mortem electron microscopy investigation provides insight into deformation mechanisms in the individual layers.

*Speaker

Can device performance be enhanced by designing the guide layer as a metamaterial?

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Abstract

Surface acoustic waves (SAW) is an interesting phenomenon which seem to have been heavily utilized in interdigitated transducer (IDT) technology during the last fifty years or more. Love waves for example, which arise when a guiding layer is deposited on a relatively hard piezoelectric substrate are most useful in microfluidic sensor applications because of their shear-horizontal nature. A high sensitivity is one of the key performance indicators for such a sensor which is conventionally attained by material selection and geometry optimization. With the advent of metamaterials more innovative ways to optimize the layer for higher device performance seems to be possible. The thickness of the layer and the conventional means to produce it, however, hamper the possibility of experimenting with new microstructural unit cell geometries. To circumvent this difficulty, we propose to print the guide layer in an IDT-SAW device using a two-photon polymerization printer. With this new printing technology a structural accuracy on the order of 170 and 550 nm in-plane and out-of-plane, respectively can be achieved. The effect of various unit cell geometries can be studied by solving the electro-elastodynamic wave equations using open-source finite-element software FENICS. Upon achieving a desirable behavior by manipulating the internal meso-structure, the layer will be produced in the facilities provided by the Uppsala University. The produced device will be tested and the output will be used to validate the numerical results.

*Speaker

Searching for model systems to study the relationship between the structure and mechanical properties of materials.

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Abstract

Understanding the relationship between the structure and properties of materials helps to create the materials we need. Understanding these relationships requires conducting appropriate experiments and comparing the results of simulations and real measurements. The difficulty of this task depends on the size of the tested objects and how much the real system differs from the ideal model. The material for testing is a layered system - made of layers with a thickness of single nanometers, differentiated in terms of crystal and/or electronic structure. The first group of structures was produced by Metalorganic Chemical Vapor Deposition (MOCVD). The process of deposition of individual semiconductor layers takes place at temperatures of 680-700 C in a hydrogen atmosphere. During the process, the rate of layer growth, gas flows and organometallics as well as the temperature of the substrate are precisely controlled. Layer thicknesses range from 0.4 to 5 nm. The second group of structures is made of layers with a thickness of several tens of nanometers. These are alternating metallic and ceramic layers. In this case, the ALD (Atomic Layer Deposition) technique was used. Confirmation of receipt of the designed systems are high-resolution Scanning Transmission Electron Microscopy images (HR STEM) with simultaneous spectroscopic analyzes (EDS, EELS). The next stages of the conducted research will include measuring the mechanical properties of the produced systems, modeling their mechanical properties and comparing the obtained results. We also plan to study how the structure of these materials changes during deformation.

*Speaker

Cross-sectional size-dependent stochastic deformation and ductility of Au bi-crystalline nanowires

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Abstract

Molecular dynamics (MD) simulations have been performed to understand how the deformation mechanisms and ductility of Au bi-crystalline nanowires depend on their cross-sectional size. In the present investigation, a longitudinal twin boundary (LTB) has been introduced to create the bi-crystalline nanowire. Different cross-sectional aspect ratios and volume ratios of grain sizes have been constructed in the MD simulations and tensile loaded. The simulation results indicate that all nanowires exhibit a similar elastic regime till peak yield stress, and yielding occurs through nucleation of $1/6< 112>$ Shockley partial dislocations from nanowire edges. Upon the interaction of the nucleated defect structures with the LTB, plasticity can be favored either of two dominating scenarios, or both: detwinning of the LTB with reorientation of the crystal, and dislocation slip. For a given shape of nanowire, we found that the competition between these two operating mechanisms is stochastic and results in a distribution of detwinned volume fractions and strain to failures. Based on the simulation results we found that the average extent of detwinning is in correlation with the volume ratio of the grains. Also, the average extent of detwinning is in linear relation with the average strain to failure, which suggests that the LTB affects the ductility of the nanowire. We concluded from the results that the more symmetric are the grains that composes the nanowires, the smaller is the ductility.

*Speaker

Effect of composition and nanostructure on mechanical properties and thermal stability of ZrCuAlx thin film metallic glasses

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Abstract

Thin film metallic glasses (TFMGs) are characterized by a disordered atomic structure, leading to extraordinary mechanical properties such as large elastic limit (> 2%), high hardness and yield strength (> 2 GPa). Nevertheless, the relationship between the atomic structure - mechanical properties - thermal stability is still not well understood and only few studies aimed at further improving the plasticity by introducing nonstructural design concepts such as multilayers or nanocomposites, which still remains an open challenge.
In this context, ZrCuAlx TFMGs (x = 0, 6, 8, 9, 12 %at.) and multilayered structures of ZrCu/ZrCuAlx with different bilayer period (L = 50, 100, 200 nm) were analyzed extensively. The addition of Al showed a moderate monotonic increase of elastic modulus (from 100 up to 115 GPa, measured by optoacoustic techniques) and thermal stability (from 420 up to 510 ∘C). Tensile test on polymeric substrate revealed a maximum of 2% in crack initiation strain for 9 at.% Al, reporting the maximum of shear-resistance due to a less covalent nature of Zr-Al bonds as predicted by *ab initio* molecular dynamics simulations. Moreover, preliminary results of micropillar compression on multilayered structures demonstrated the crucial role of interface density on the deformation behavior, limiting the shear band propagation especially for a bilayer period equal to 100 nm, while maintain a yield strength values > 1GPa.
In conclusion, we report the design of novel TFMGs with tailored composition and nanostructure with large potential for industrial applications.

*Speaker

Exploring tungsten response under small-scale compression deformation

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Abstract

This study presents a rate-dependence continuum crystal-plasticity theory to investigate the mechanical response of tungsten single crystals under compressive loading. The experimental data corresponding to single-crystal micropillars is collected from the literature, and the micro-sized pillars are simulated. Then, the parameter values are employed to investigate the deformation of tungsten single crystal under nanoindentation. This study discusses the magnitude of the microscopic rate sensitivity parameter with macroscopic counterparts obtained from micropillar compression and nanoindentation. A comparison between numerical and experimental data shows the strength of the proposed framework in predicting tungsten behavior under small-scale deformations.

*Speaker

Factors Affecting the Deformation-Relaxation Behavior of Materials under Nano- and Micro-Indentation

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Abstract

The deformation behavior of any material under very non-uniform gradient stress field created under point-contact deformation (nanoindentation, microindentation and scratching) depends on the possibility of a specific inherent structure to dissipate external mechanical energy for the relaxation of induced internal stresses. The relaxation of internal stresses begins just at the loading stage by dissipating the stored elastic energy onto irreversible plastic deformation or fracture. This dissipation takes place through various "channels", i.e. mechanisms of deformation: translation mechanism (dislocation movement), rotation mechanism (disclinations, twinning), densification (phase transition, polyamorphism, interstitial plasticity) and fracture. Which of these mechanisms will be involved for the relaxation of the internal stresses depends on several main factors. The first one is *structure* of material, the second one is *strain* created by the indenter depending on its geometry and load applied. The third group of factors can be identified as *time-dependent* ones, which include loading rate and holding under the peak load. The fourth factor is *temperature of deformation.* The relaxation of material continues during the unloading stage, when the external stresses are being removed. This stage is accompanied by the elastic recovery, restructuring of the plastic zone and, in case of brittle materials, crack growth and fracture development. On the example of a range of crystalline and vitreous materials the influence of these mains factors on the development of one or another mechanism of deformation is presented in this work.

*Speaker

Structured approach towards correlation of finite element models and nanoindentation measurement data

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Abstract

The rapid development of production technologies and new materials, whose material parameters cannot be determined by conventional macroscale experiments due to their geometry, size or heterogeneous microstructure, is evident in recent years. In such cases, the nanoindentation technique can be used to experimentally assess material properties such as Young's modulus and hardness. The possibility of reproducing the load vs. indentation depth curves of the performed nanoindentation tests by means of finite element (FE) models is discussed in this work. The experimental nanoindentation measurements are herein performed on wrought as well as on AISI 316L samples attained via additive manufacturing by employing a Keysight G200 nanoindenter with a standard Berkovich tip, while applying the standard depth-controlled loading - unloading method. Since, however, the numerical simulations of nanoindentation entails a nonlinear elasto-plastic contact problem, the Young's modulus and the hardness are not sufficient to properly and completely characterize the material behaviour observed in the experimental tests. Simulations are thus performed by adopting a numerical model optimized in terms of its dimensions (i.e., the radius and the height of the model with respect to the nanoindentation depth) and employing an elasto-plastic material model. The influence of the geometrical and elasto-plastic material parameters on the quality of the simulated results is therefore systematically investigated, allowing correlations of FE and experimental data to be established.

*Speaker

Nanoindentation material testing using sm@rt500 and sm@rt cubes

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Abstract

The sm@rt 500 nanoindenter is designed to offer a broad range of force, speed and travel. The sensor has a low noise floor in the sub μN range and a max. force of 800 mN using a highly linear electromagnetic actuator. 100 μm displacement range is standard, a wider range is customized. The motorized z-drive allows an easy adaption to the actual sample height. Bidirectionally sesors enabling tensile testing with the same hardware.
Quasi-static and dynamic modes are included in the system - usuable over the full range of +/- 800 mN. The demodulation of the current displacement amplitude and phase is done by digital signal processing with no external hardware. High speed testing and properties mapping are included.
The tests are following ISO standards or customized procedures and are executed hardware near by a multicore microcontroller for realtime control of the testflow. Advanced users can generate XML based scripts to create specific test procedures. The usage of the high-end microcontroller for the test execution allows to integrate other testing hardware using digital interfaces. The fully integrated high resolution video microscope guaranty the perfect optical sample view.
SURFACE nanometrology has been a distributor for nanoindenters and add-on equipment for more than 25 years. The new SURFACE sm@rt500 reflect this long time experiance and is modular designed to allow an individual system set-up. Optional available sm@rt cubes adding additional features to the basic system: lateral force measurement, heating/cooling/humidity variation, 4" wafer stage, tensile testing, SEM module are available.

*Speaker

The Nanoindentation Characterisation of Biocompatible Polymer - Flexdym

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Abstract

Mechanical characterization is important for polymers because it allows us to understand how they will behave under different mechanical stresses and loads. Nanoindentation is an important technique for the mechanical characterization of polymers at the nanoscale. The mechanical properties of polymers may be affected by factors such as chain entanglement, crystallinity, crosslinking, and the presence of defects. This is important because the local properties can have a significant impact on the overall performance of a polymer in a given application. For example, the failure of a polymer may be initiated by a defect or stress concentration, so understanding the local mechanical properties can help to identify potential failure mechanisms and improve the design of polymer-based materials. Polymers are commonly used in microfluidic applications, where they may be subjected to a wide range of mechanical stresses, such as tension, compression, bending, and torsion. The Polydimethylsiloxane (PDMS) is one of the most common polymers used in microfluidics, but recent studies have introduced Flexdym as a promising biocompatible polymer. Therefore, the mechanical characterization of Flexdym on Nanoindenter G200 under various loads is introduced in this paper. Extruded sheets of Flexdym polymer (Eden Microfluidics SAS, Paris, France) of 3 mm thickness were cut with scalpel to the size of 1 cm x 1 cm and cleaned with tape to remove any large dust particles and characterized by means of Nanoindenter G200. Graphs for Load vs Displacement curves, Young modulus and Hardness changes of Flexdym in dependence on load are presented and appropriate conclusions made.

*Speaker

3C-2H Phase Transformation in Silicon and Germanium nanowires

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Abstract

We have developed a process of phase transformation in silicon and germanium nanowires, https://doi.org/10.1021/nl502049a. The process is very simple and benefits from size effects of nanowires. The transformation results in the formation of hexagonal 2H domains along the cubic diamond (3C) structure. The nanowires are embedded in a resist and stress is applied on the nanowire by thermal densification of the resist. The combination of shear stress and heating allows the formation of 2H bands observed for zone axis with {115} habit planes inside the -axial cubic 3C nanowires. For other axial orientations the same orientation relationships are found but the different orientation prevents organized bands to be formed (figure 1). On top of that other stress release systems like twinning are becoming dominant. This study focusses on an experimental understanding of the underlying mechanism of transformation. First of all, the densification process of the resist has been investigated to have a better estimation of the stress in the nanowires. The different resists allow us to play with the amount of stress and the densification temperatures. Playing with different nanowires/fins and their diameter/pitch, we aim at giving more insight in: (1) the difference between , and $< 100)>$ - oriented nanowires, (2) the origin of the two stable habit planes {115} and {100} between the 3C and 2H phase, (3) the diffusionless nature of the underlying process, (4) statistics showing trends between e.g. nanowire diameter and transformed material and a link between experiments and simulation/theory

*Speaker

Another Twist on Graphene – Twistronics as a Way to Engineer Superlubric Coatings

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Abstract

Friction control and technological advancement are intimately intertwined. Concomitantly, two-dimensional materials occupy a unique position for realizing quasi-frictionless contacts. However, the question arises of how to tune superlubric sliding. Drawing inspiration from twistronics, we propose to control superlubricity via moiré patterning. Friction force microscopy and molecular dynamics simulations unequivocally demonstrate a transition from a superlubric to dissipative sliding regime for different twist angles of graphene moirés on a Pt(111) surface triggered by the normal force. This follows from a novel mechanism at superlattice level where, beyond a critical load, moiré tiles are manipulated in a highly dissipative shear process connected to the twist angle. Importantly, the atomic detail of the dissipation associated with the moiré tile manipulationi.e., enduring forced registry beyond a critical normal loadallows the bridging of disparate sliding regimes in a reversible manner, thus paving the road for a subtly intrinsic control of superlubricity. Reference:
Moiré-Tile Manipulation-Induced Friction Switch of Graphene on a Platinum Surface.
Zhao Liu*, J.G. Vilhena*, Antoine Hinaut,Sebastian Scherb, Feng Luo, Junyan Zhang, Thilo Glatzel, Enrico Gnecco, and Ernst Meyer*
Just accepted in Nano Letters – featured in cover (https://doi.org/10.1021/acs.nanolett.2c03818

*Speaker

Correlating microstructure and mechanical behaviour in BCC-RHEAs using nanoindentation mapping

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Abstract

Body-centered-cubic (BCC) high-entropy alloys (HEAs) exhibit improved high temperature resistance compared to many other conventional alloys. Most BCC refractory HEAs (RHEAs), however, are brittle at room temperature, which limits their applicability. The equimolar NbMoCrTiAl RHEA was reported to have little ductility at the millimeter scale from room temperature up to 600 ∘C. The brittleness of this material at lower temperatures is believed to be attributed to its ordered BCC structure (B2-type) and the complex intermetallic precipitates at the alloy's grain boundaries. In contrast, the equimolar TaNbHfZrTi alloy has been shown to exhibit notable ductility at room temperature, which is uncommon in BCC-RHEAs. To understand the role of microstructure, particularly the grain boundaries and the local precipitates, and their effect on mechanical behaviour at the macroscale, we conducted a series of nanoindentation experiments on the NbMoCrTiAl and TaNbHfZrTi samples. Nanoindentation mapping covering different grains and grain boundaries exhibits a significant increase of hardness at the grain boundaries and the precipitates in the NbMoCrTiAl alloy, while the hardness values in the TaNbHfZrTi alloy are comparable in grains and at the grain boundaries. The pop-in behaviour of the two BCC-RHEAs was also statistically characterized and compared, and a clear strengthening effect was observed at the grain boundaries of NbMoCrTiAl alloy due to the local precipitates, which was confirmed by EBSD and EDX analysis.

*Speaker