MecaNano 2nd General Meeting Final Program

May 1-3, 2024, Vienna, Austria

HOST: Technische Universität Wien (TU Wien) Campus Karlsplatz

Organizing Committee

Helmut Riedl-Tragenreif (TU Wien, Austria)
Verena Maier-Kiener (MUL, Austria)
Megan Cordill (ESI-ÖAW, Austria)

Funded by the Horizon 2020 Framework Programme of the European Union

Venue and Practical Information

The 2nd MecaNano General Meeting will be held at the Technische Universität Wien (TU Wien) Campus Karlsplatz. The meeting will take place at the Festsaal and the poster sessions in the adjacent Böcklsaal (Main building A, Karlsplatz 13, 1040 Wien). The meeting rooms can be reached by using the "Karlsplatz" U-bahn stop, exit Karlsplatz/Resselpark. This will get you the closest to the venue and avoid the city traffic at street level.

The first session will start at 15:00 in the Festsaal on May 1st, 2024.

Internet is provided by eduroam**.**

Lunches and coffee breaks are included in the registration

Conference dinner will be on May 2nd at the traditional Viennes Heurigen "Christ" and is only for pre-registered participants who pay €40 to the local organizers. To get there, we will travel together from Karlsplatz on our own dedicated tram!

The meeting point will be outside the building where the meeting is taking place **at 17:45**. Together we will walk to the tram pickup site a few hundred meters away. **The return trip back to accommodations is the responsibility of each participant**. The public transport in Vienna can easily get participants back to where they are staying or to other attractions the city has to offer.

For participants receiving **travel support** please look at the COST Travel Reimbursement Rules

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Program

Wednesday May 1st, 2024

TIME	NAME	TITLE
14:00		Badge pick-up opens
14:55	GM2 Organizers	Welcome to Vienna, thank sponsors, explain why today's session is long
SESSION 1: New developments in nanomechanical testing *Chairs: Verena Maier-Kiener, Helmut Reidl*		
15:00	Thomas Pardoen (Invited)	Fracture mechanics on-a-chip
15:30	Marie-Stephane Colla	New developments of the residual stress actuated on-chip testing method
15:50	Dan Mordehai	Stochastic behavior at the nanoscale - what can we learn from the distribution of mechanical properties?
16:10	Mohammed Tahir Abba	Experimental Progress in High Constant Strain Rate Nanoindentation
16:30	Hendrik Holz	Influence of a low angle grain boundary on high strain rate deformation in copper
16:50	Sebastian Bruns	Fused Silica probed by HTSI at elevated temperatures
17:10	Gaylord Guillonneau	Surface mechanical properties and microstructural evolutions along a thermal cycle using High Temperature Scanning Indentation
17:30	Vera Obradovic	Mechanical properties of immersed Kevlar/PVB composites with ZnO nanoparticles
17:50	Jan Pribyl	Mechanical Properties of Soft Materials at the Nanoscale

Thursday May 2nd, 2024

TIME	NAME	TITLE
8:00		Badge pick up, Posters go up
SESSION 2: Multiscale nanomechanical behavior *Chair: Megan Cordill*		
9:00	Jürgen Stampfl (Keynote)	3D Printing Photopolymers: Optimizing fracture toughness and thermomechanical properties
10:00	Ayse Cagil Kandemir	Bioinspired Hierarchical Composite: Balancing Toughness and Strength through Multi-Scale Design
10:20	Pavlos Stephanou	A combined theoretical-simulation approach to microscopic structure and dynamics of unentangled poly(ethylene glycol) - silica nanocomposite melts
10:40	Igor Stankovic	Exploring the influence of water on the friction on two-dimensional surfaces
11:00	LUNCH and POSTER SESSION	
SESSION 3: Nanoindentation based approaches *Chair: Julien Guenole*		
13:00	Anna Kareer (Invited)	Scratching the surface: understanding plasticity associated with microscale asperity contacts
13:30	Enrico Gnecco	Early-stage wear of layered materials on the nanoscale
13:50	Olivier Noel	Nano-scale wear mechanisms studies: a new experimental approach

14:10	Olga Shikimaka	Effect of loading regimes on the deformation mechanisms of Si under nanoindentation and nanoscratching
14:30	COFFEE BREAK	
SESSION 4: Machine learning and mechanical behavior *Chair: Claus Trost*		
15:00	Peter Isprovity (Invited)	Deciphering acoustic emission using micromechanical experiments
15:30	Krzysztof Wieczerzak	Exploring CuAgZr metallic glasses for biomedical use: A study using combinatorial synthesis, high-throughput experiments, and machine learning
15:50	Stanislav Zak	Thin film nanoindentation and the importance of the tip radius
16:10	Michael Wurmshuber	Micromechanical assessment of the limpet tooth: Unraveling the secrets behind Nature's strongest material
16:30-17:45	Social/Poster discussions before tram arrives at 18:00	

Friday May 3rd, 2024

TIME	NAME	TITLE
8:00		Poster viewing
SESSION 5: Simulations and modelling of mechanical behavior *Chair: Petr Hauslid*		
8:30	Sandrine Brochard (Invited)	Structure, stability and mechanical properties of small metallic nanoparticles: insights from first-principles simulations
9:00	Mor Levi	Mechanical Properties of Nickel-Platinum Nanoparticles Fabricated by Solid-State Dewetting Synthesis
9:20	Miljan Dasic	Normal Dynamics - method development and applications
9:40	Frederik Van Loock	Amorphous plasticity at the mesoscale: development of a shear transformation zone-based numerical model
10:00	COFFEE BREAK	
SESSION 6: Managing mechanical data *Chair: Tamara Aleksandrov*		
10:30	Xufei Fang	Impact of room-temperature engineered dislocations on the mechanical properties in oxides
10:50	David Mercier	Dataflow Development and Machine Learning for Nanoindentation Data Analysis
11:10	Ulrich Kerzel	Transformation towards a digitized materials science laboratory
11:30	LUNCH and POSTER SESSION	
SESSION 7: Nanoscale deformation mechanisms and size effects *Chair: Daniel Kiener*		
13:00	Xie Zhuocheng (Invited)	Plasticity in topologically close-packed phases: Insights from nanomechanical testing and atomic-scale modelling
13:30	Maria Watroba	Micromechanical behavior of nanoporous electrodeposited Zn coating
13:50	Sina Zarepakzad	Investigating Mechanical Properties of Silicon Nanowires: Scale Effect Revisited
14:10	Selim Hanay	What can nanomechanical mass spectrometry tell us about nanoparticles?
14:30	Jonathan Zimmerman	Mass Particle Compression, or: How I learned to stop doing in-situ nanomechanical tests and love ex-situ ones

Poster Contributions

1. **Advancing Nanomaterial Characterization: A Machine Learning Approach to Assessing h-BN Mechanical Properties** - Oguzhan Der
2. **Enhancing Material Valorisation through Innovative Nanomechanical Testing** - Theo Zacharis
3. **Analysis of nanoindentation creep of ceramic-organic supercrystalline nanocomposites** - Cong Yan
4. **Grain size influence on the creep and fatigue properties of freestanding gold thin films** - Anna Krapf
5. **Compressive strength of the Cu-Au nanoparticles fabricated by solid state dewetting** - Eugen Rabkin
6. **Nanoparticle Fabrication for SnSb2Te4 via Mechanical Milling** - Khatira Mehtiyeva
7. **Dust Particle Impact on Plasma-Facing Materials in Tokamaks: Insights from Molecular Dynamics Simulations** - Prashant Dwivedi
8. **Shape and Size Effects on Compressive Strength of Fe-Pd Alloy Nanoparticles** - Yarden Flash
9. **Surface modification of case-hardened AMS 6265 aircraft steel by nano surface - severe plastic deformation** - Nicolae Serban
10. **Durability of hard protective coatings: Assessing the fracture and fatigue resistance of nanostructured thin films** - Rainer Hahn
11. **High strain rate mechanical behavior of SMAT hardened steel layers** – Mona Stoll
12. **Elastic properties of laser-affected glass probed by grid nano-indentation** – Fabien Amoit
13. **Research of tin, antimony and cooper coatings applied in renewing the surfaces of parts** - Saulius Baskutis
14. **Exploring the potential of dislocation density fields for the discrete-to-continuum crossover in nanomechanics** - Julien Guenole
15. **Modelling of inhomogeneous deformation in nanoporous-Au nanoparticles under indentation** - Santhosh Mathesan
16. **Fabrication and characterization of graphene reinforced Al-6Zn-2Cu-2Mg based functionally graded materials** - Deniz Uzunsoy
17. **Nanoindentation Ontology: Harmonising knowledge and data for nanoindentation** - Edoardo Rossi
18. **Metadata for Micromechanical Testing** - Ulrich Kerzel
19. **Hand written notes to electronic notebooks - a beginner's guide to data management** - Megan Cordill
20. **Micromechanical Modeling of Graphene Platelets Based Nanocomposites** - Ozgen Colak

21. **Hybrid microscale 3D metal-ceramic metamaterials combining high strength and ductility** - Jakob Schwiedrzik
22. **Imaging defects in Nanocrystals using Coherent Diffraction Imaging** - Abdelrahman Zakaria
23. **Recycled HDPE: An investigation on CDs contribution to improve mechanical performance** - Raul Simoes
24. **Visco-elastic Properties of Polymer Nanocompsites** - Jadranka Blazhevska-Gilev
25. **Mechanical Properties of MiniBars™ Basalt Fiber-Reinforced Geopolymer Composites for Buildings Applications** - Gabriel Furtos
26. **Mechanochemical synthesis of Zn- bionanohybrids: Size-effect on the nanoscale to improving their enzyme-like activity** - Carla Garcia
27. **Micro-scale investigation of deformation mechanisms in biodegradable Zn alloys** - Wiktor Bednarczyk
28. **Statistical failure of Ag penta-twinned nanowires with varying cross-section width** - Rohith Polisetty
29. **In situ nano-mechanical studies of single-crystal ZnO nanowires** - Thomas Cornelius
30. **Characterization and Optimization of Silver Wire Drawing Process for Jewelry Making** - Ömer Necati Cora
31. **Simulation of mechanosensitive ion channels in nano scales to study urinary incontinence** - Chitaranjan Mahapatra
32. **The Effect of Crystalline Properties on Catalytic and Magnetic Performance: Hybrid PtAuFe Nanostructures for Green Energy** - Dogan Kaya
33. **Transformation-induced plasticity (TRIP) in Ce-stabilized zirconia: an in situ approach coupling pillar micro-compression, Laue micro-diffraction and electron microscopy** - Solene Comby-Dassonneville
34. **Unveiling Crystal Deformation: Integrating EBSD and FEM Simulation for Elastic Strain Analysis** - Grzegorz Cios
35. **Yield criteria of additively manufactured body-centered cubic lattice structures** - Chen Zhi
36. **Machine Learning-Driven Prediction of Elastic Modulus in Clay-Reinforced Polymer Nanocomposites** - Gokce Nur Yilmaz

Abstracts

The abstracts are in the order in which they were presented (oral presentations) or in number order (poster presentations).

Fracture mechanics on-a-chip

Thomas Pardoen*[1,2], Sahar Jaddi , Michael Coulombier , and Jean-Pierre Raskin

[1]Institute of Mechanics, Materials and Civil Engineering, Université Catholique de Louvain – Belgium
[2]WEL Research Institute, avenue Pasteur, 6, 1300 Wavre, Belgium – Belgium

Abstract

The characterization, control, and enhancement of the cracking resistance of freestanding thin films and 2D materials are major concerns for the development of fail-safe flexible electronics, MEMS/NEMS devices, and structural or functional coatings. In particular, environmentally-assisted cracking phenomena affect the reliability of many thin films/2D materials-based systems. This is a complex subject, insufficiently studied mostly because of experimental difficulties. The presentation will address recent progress made with an on-chip technique to extract the static fracture toughness and to study the environmentally-assisted crack growth in freestanding thin films. The method relies on a residual-stress-based-on-chip concept taking advantage of MEMS-based fabrication principles. The test configuration consists of a notched specimen attached to two long actuator beams involving tensile internal stress. Upon release, the relaxation of the residual stress leads to the deformation of the specimen. A crack initiates at the notch tip, propagates, and finally arrests. A data reduction scheme based on finite element simulations of the test structures is used to determine the static fracture toughness. The method also provides the variation of the crack growth rate as a function of the stress intensity factor under different temperature conditions and humidity levels. Several materials were tested over last few years from nominally brittle like SiN, SiO2, Al2O3 to ductile such as Cu, Ni, graphene and Al/Al2O3 multilayers, revealing several interesting effects that will be presented. In particular, the definitive fracture toughness of graphene equal to 4.4 MPa m1/2 has been found and connection made with the intrinsic flaws existing in graphene.

*Speaker

New developments of the residual stress actuated on-chip testing method

Marie-Stéphane Colla*[1], Salah Eddine Naceri , Nicolas Roisin , Paul Baral , Michael Coulombier , Hosni Idrissi , Denis Flandre , Raskin Jean-Pierre , and Thomas Pardoen

[1]Institute of Mechanics, Materials and Civil Engineering, Université Catholique de Louvain – Place Sainte Barbe 2, B-1348 Louvain-la-Neuve, Belgium

Abstract

Over the last years, the on-chip tensile testing method has proven its potential for the characterization of the link between the mechanical behaviour and microsctructure at the micro- and nanoscale. While uniaxial tension is highly relevant to determine several mechanical properties, new on-chip loading configurations emerged recently to tackle challenges related to strain engineering studies as well as to the understanding of local deformation and relaxation mechanisms.
An overview of the latest outputs obtained using the UCLouvain residual stress actuated on-chip method will be presented including the following progress:

- An on-chip shear configuration has been designed in the context of addressing the opto-electronic properties of semiconductors. Monocrystalline Si thin films have been studied as a model system to optimize the design.
- Long-term relaxation of thin films under tension providing information unavailable using conventional techniques like nanoindentation or direct tensile test.

*Speaker

Stochastic behavior at the nanoscale – what can we learn from the distribution of mechanical properties?

Dan Mordehai*[1], Rohith Polisetty , Santhosh Mathesan , Tal-El Carmon , and Stav Nisany

[1]Department of Mechanical Engineering - Technion (ME-Technion) – Department of Mechanical Engineering The Technion – Israel Institute of Technology Haifa 32000 Israel, Israel

Abstract

Mechanical properties at the nanoscale demonstrate different mechanical properties than their bulk counterparts, mainly since the confined volumes makes the contribution of each microstructural event more significant. For the same reason, mechanical properties at the nanoscale may also be stochastic, rather than deterministic as in bulk materials. This talk explores how stochasticity arises in nanoscale deformation and how it informs microstructural properties. We first present a model for the distribution of yield strength in nucleation-controlled plasticity, demonstrating its dependence on temperature. Applying the model on molecular dynamics (MD) simulations of nanoparticles and nanowires demonstrates the temperature-dependent stochastic strength of these specimens, and reveals an interesting transition between nucleation sites. The model is also applied on experiments of Au-Ag nanoparticles, to calculate the activation volume of bulk nucleation. We then discuss the stochastic nature of failure strain in twinned Au and Penta-twinned Ag nanowires, as been observed in MD simulations, revealing the influence of competing microstructural mechanisms on the failure strain distributions. Finally, distributions in mechanical properties are observed also in nanoporous Au structures, where structure with similar volume fraction and average ligament density demonstrates different mechanical properties. This work emphasizes the importance of considering stochasticity in understanding and predicting the mechanical behavior of nanomaterials.

*Speaker

Experimental Progress in High Constant Strain Rate Nanoindentation

Mohammed Tahir Abba*[1] and Benoit Merle[1]

[1]University of Kassel – Germany

Abstract

Knowledge about the local mechanical behavior at high deformation rates is crucial to increase the safety of components that involve impact loading such as bird impacts in the aviation industry, smartphone displays, automobile crashes and many others.
Nanoindentation has been used extensively in the past decades to study the local deformation behavior of various types of materials but these were primarily limited to low strain rates: 10-3 – 10-1 s-1. To be able to study deformation behavior at high strain rates, there is a need to not only use fast signal processing components but to also develop experimental methods and analysis techniques for high speed nanoindentation tests.

This talk will focus on both technical implementations and further development of previously established methods (1) to analyze high constant strain rate nanoindentation data. A displacement-controlled instrument will be presented, which was designed around piezoelectric transducers and fast electronics allowing sampling rates of up to 1 MHz. We will show experimental measurements at strain rates of up to 104 s-1 and discuss current bottlenecks, both in terms of resonance effects and time constant corrections.

Acknowledgement

This project has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (grant agreement No 949626)

References

(1) Merle, B., Higgins, W. H. & Pharr, G. M. Critical issues in conducting constant strain rate nanoindentation tests at higher strain rates. *J. Mater. Res.* **34**, 3495–3503 (2019).

*Speaker

Influence of a low angle grain boundary on high strain rate deformation in copper

Hendrik Holz*[1], Lalith Kumar Bhaskar , Bárbara Bellón , Dipali Sonawane , Gerhard Dehm , James, P. Best , and Rajaprakash Ramachandramoorthy

[1]Max-Planck-Institut für Eisenforschung GmbH – Germany

Abstract

Low angle grain boundaries (LAGBs) are a particularly underexplored defect in metallic materials. However, they are almost omnipresent in engineering, even as a growth artifact in some single crystalline components. The influence on mechanical properties and thus the potential to use LAGBs to strengthen materials is investigated in the current study. For that, an LAGB in copper with a 12◦ misorientation, grown as an artifact in the Bridgeman process, was investigated at various strain rates by micropillar compression (0.001 1/s - 1 1/s) and nanoindentation (10 1/s– 10ˆ5 1/s). For this a piezo-based nanoindentation set-up with fast electronics, sensors and oscilloscopes is used. The protocols for the high strain rate testing, data evaluation and interpretation will be discussed and the strain rate sensitivity used to interpret the findings. The results are evaluated using different methodologies to calculate the hardness at ultra-high strain rates. At the highest strain rates the hardness changes drastically for indents in proximity of, and at, the LAGB while no change in hardness is found for all strain rates in the single crystals far away from the LAGB .

*Speaker

Fused Silica probed by HTSI at elevated temperatures

Sebastian Bruns*[1], Marcel Sos , and Durst Karsten

[1]Technical University of Darmstadt (TuDa) – Alarich-Weiss-Straße 2 D- 64287 Darmstadt, Germany

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, 1200∘C for Fused Silica. Recent micro-pillar-compression results, however, indicate a brittle-to-ductile transition to occur at much lower temperatures in the range of 200-400 ∘C. Due to the experimental complexity, micro-pillar-compression experiments go hand in hand with a low temperature data resolution. This is where new testing protocols like the "High Temperature Scanning Indentation" (HTSI) can play to their strengths. With a data point every 1-2 ∘C the HTSI approach allows a quasi-continuous scanning of a temperature interval with a data density previously unattainable. While the new possibilities HTSI may offer sound almost too good, the application of HTSI to silica glass is by no means trivial ...

*Speaker

Surface mechanical properties and microstructural evolutions along a thermal cycle using High Temperature Scanning Indentation

Gaylord Guillonneau*[1], Gabrielle Tiphéne[2], Paul Baral[3], Solène Combi-Dassonneville[4], Guillaume Kermouche[3], Warren Oliver[5], and Jean-Luc Loubet[1]

[1]Laboratoire de Tribologie et Dynamique des Systèmes – Ecole Centrale de Lyon, Centre National de la Recherche Scientifique – France

[2]Université Catholique de Louvain – Belgium

[3]Laboratoire Georges Friedel – Ecole des Mines de Saint-Etienne, Université de Lyon, Centre National de la Recherche Scientifique – France

[4]Aix-Marseille Université – IMN2P – France

[5]KLA – United States

Abstract

A new technique, named High Temperature Scanning Indentation (HTSI), was developed, and allows for the measurement of surface mechanical properties by nanoindentation during a complete thermal cycle (i.e. during heating, holding at constant temperature, and cooling). This means the mechanical properties are measured continuously as a function of temperature during only one test, permitting earning time considerably. This method, first validated on a model material (fused silica), was then applied on different materials (metals, metallic glass, amorphous materials), the results showing the HTSI method is able to detect microstructural changes as a function of the temperature, through the mechanical properties variations. In this workshop, the HTSI technique will be detailed, and some applications on different materials will be presented and discussed, in terms of mechanical properties and microstructure evolutions.

*Speaker

Mechanical properties of immersed Kevlar/PVB composites with ZnO nanoparticles

Vera Obradović*[1], Petr Sejkot[2], Klára V. Machalická[2], and Miroslav Vokáč[2]

[1]Innovation Center of Faculty of Technology and Metallurgy in Belgrade, 4, Karnegijeva Street, 11120 Belgrade, Serbia – Serbia

[2]Klokner Institute, Czech Technical University in Prague, Šolínova 7, 166 08 Prague, Czech Republic – Czech Republic

Abstract

The Kevlar fabric composites are widely applied for body armor and vehicle armor structures. In this study, the specimens were produced of the Kevlar fabrics impregnated with 10 wt.% poly (vinyl butyral)/ethanol solution which contained the ZnO nanoparticles in different concentrations (1 wt.% or 2 wt.% in relation to poly (vinyl butyral), PVB). The two-layered Kevlar/PVB composite samples were fabricated by hot compression.
In accordance with the ISO 62 standard, the square Kevlar/PVB composite specimens were immersed for the water uptake measurements. The tensile and flexural properties of the Kevlar/PVB specimens were examined in compliance with the ASTM D 3039 and ASTM D 790-03 standards, respectively. The specimens that had been submerged in distilled water at 40 ∘C for eight weeks were compared to the dry specimens in terms of their tensile and bending characteristics.

The addition of ZnO nanoparticles significantly improved the tensile strength and tensile modulus of the dry Kevlar/PVB specimens. In contrast to the tensile test results, the dry specimens with no nanoparticles exhibited the superior flexural qualities (strength and modulus) because of the better bonding between their two impregnated fabric layers.
When compared to their dry counterparts, the tensile and bending properties of every immersed Kevlar/PVB composite specimen showed some lower values.

*Speaker

Mechanical Properties of Soft Materials at the Nanoscale

Jan Pribyl*[1], Šimon Klimovič[1], Radka Obořilová[1], and Daniil Kabanov[1]

[1]Central European Institute of Technology [Brno] – Czech Republic

Abstract

Soft materials, defined as materials with elastic moduli typically below 1 MPa, such as biopolymers, gels, and biological tissues, have unique mechanical properties that differ significantly from their hard material counterparts. Understanding these properties at the nanoscale opens up new opportunities in a variety of areas, including biomedical engineering, materials science and nanotechnology.
Nanoindentation techniques such as Atomic Force Microscopy (AFM) and a nanoindenter were used to characterize the mechanical properties of soft samples. Application of these techniques is illustrated on samples such as defined phospholipid bilayers, biomolecules (proteins, DNA), hydrogels, single cells and tissue cultures. Correlative approaches using fluorescence and Raman microscopy are also presented. At the end of the presentation, the problems associated with the standardization of these measurements will be discussed.
The result should be more efficient methods for characterizing the mechanical properties of complex soft materials and for understanding their properties at the nanometer scale, but also their relationship to the molecular nature of certain processes, with crossover to the biological and biochemical sciences, where this characterization can lead to an understanding of the links between physiological or disease states and changes in mechanical properties at the molecular, cellular or tissue levels.

*Speaker

3D-printable Photopolymers: Optimizing Fracture Toughness and Thermomechanical Properties

Jürgen Stampfl*[1]

[1]Institute of Materials Science and Technology, TU Wien – Austria

Abstract

Lithography-based methods for additive manufacturing of polymers enable the fabrication of precise, complex-shaped parts with excellent surface quality in applications like biomedical engineering, electronics and consumer products. Photopolymers contributed 25% to the worldwide materials sales in 2023, thus making lithography-based AM (L-AM) one of the most widely used AM technologies.
Commonly used 3D-printable photopolymers are amorphous materials with a high density of chemical cross-links. The resulting morphology limits the achievable fracture toughness and ductility of those materials. This is the reason, why photopolymers are less likely to being used in applications where structural materials are required. The target of this presentation is to illustrate strategies which offer routes to optimize fracture toughness and ductility without sacrificing other thermomechanical properties like heat deflection temperature, creep resistance and elastic modulus.

Besides tuning the formulation of the targeted photopolymers, it is also necessary to adapt the 3D-printers for being able to process advanced photopolymers. The presented monomers and oligomers are typically highly viscous at room temperature and need innovative setups (e.g. Hot Lithography) for printing.
In order to understand the influence of processing conditions on the finally observed mechanical properties, a fracture mechanical approach will be used. Since AM not only allows to define the shape of a part, but also enables the variation of material properties within the part (gradient materials, digital materials, ...), new routes for a detailed scientific investigation of 3D-printable materials are available.

*Speaker

Bioinspired Hierarchical Composite: Balancing Toughness and Strength through Multi-Scale Design

Ayse Cagil Kandemir*[1], Sehram Dizeci , Omer Music , Fatma Donmez , and Hatice Kaplan Can

[1]Ayse Cagil Kandemir – TED University Engieering Faculty, Mechanical Engineering Department, Ankara, Turkey

Abstract

This study introduces an innovative bioinspired hierarchical composite, crafted to emulate seamless integration of mechanical properties observed in Nature, as seen in systems like bone and cartilage. Structured at two distinct scales, it consists of a macro-scaled biocompatible nanocomposite and a micro-scaled coating with a spatial gradient in particle distribution. The macro component, comprising LDPE and PVP-HNT nanocomposite, forms a tough and ductile interior. In contrast, the micro component, a gradient PVP-HNT nanocomposite coating applied in successive layers, significantly enhances mechanical strength. This design skillfully balances toughness and strength, characteristics often seen as mutually exclusive.
Mechanical analysis of the composite reveals a locally-tuned elastic modulus, ranging from 0.2 to 78.5 GPa, and a hardness increase from 11 to 381 MPa. Numerical analysis employing the Finite Element Method demonstrates the ability to control the type of deformation, with the composite predominantly exhibiting elastic behavior. This suggests that the hierarchical composite is protected from permanent deformation by fine-tuning the concentration distribution of the gradient coating.

The research represents a significant advance in composite material design, achieving a fine balance of mechanical properties through its multi-scale structure. The synergy of a tough macro core with a strength-enhanced micro coating not only mitigates stress concentration but also paves the way for new applications in engineering domains where a balance of strength and toughness is crucial. As a result, this biocompatible hierarchical composite stands out as a promising candidate for cutting-edge biomedical and engineering applications.

*Speaker

A combined theoretical-simulation approach to microscopic structure and dynamics of unentangled poly(ethylene glycol) – silica nanocomposite melts

Emmanuel Skountzos[1], Dimitrios Tsalikis[1,2], Pavlos Stephanou*[3], and Vlasis Mavrantzas[1,2]

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[2]Particle Technology Laboratory, Department of Mechanical and Process Engineering, ETH Zürich, CH-8092 Zürich, Switzerland – Switzerland

[3]Department of Chemical Engineering, Cyprus University of Technology, 30 Archbishop Kyprianou Str., 3036, Limassol, Cyprus – Cyprus

Abstract

Polymer nanocomposites comprise a class of nanostructured materials wherein nanosized particles are embedded in a host polymer matrix to improve its physicochemical properties (mechanical, transport, electrical, etc.). In the present work (1), we combine detailed molecular dynamics (MD) simulations with a properly modified Rouse theory for polymers adsorbed by one or both of their ends onto the nanoparticle surface to offer a quantitative description of local structure and microscopic dynamics in attractive polymer nanocomposite melts, considering as a model system a poly(ethylene glycol) (PEG)-silica nanocomposite, at temperature $T = 413$ K and pressure $P = 1$ atm to enable a direct comparison with available experimental data (2-3).

Our work reveals that adsorbed polymer segments on silica in the form of tails and loops exhibit appreciable mobility locally. The simulations also reveal that PEG chains terminated with hydroxyl groups are primarily adsorbed on the silica surface by their end groups thus giving rise to a brush-like structure, whereas PEG chains terminated with methoxy groups are adsorbed equally probably along their entire contour. Direct comparison of simulation data and theory with state-of-the-art experimental data (2-3) for the dynamic structure factor of the same system under the same temperature and pressure conditions reveals excellent agreement.

References:

(1) E.N. Skountzos, D.G. Tsalikis, P.S. Stephanou, and V.G. Mavrantzas, *Macromolecules* **54**, 4470 - 4487 (2021).

(2) T. Glomann *et al.*, *Phys. Rev. Lett.* **110**, 178001 (2013).

(3) T. Glomann *et al.*, *Soft Matter.* **9**, 10559–10571 (2013).

*Speaker

Exploring the influence of water on the friction on two-dimensional surfaces

Igor Stanković*[1], Olivier Noel[2], and Miljan Dašić[1]

[1]Scientific Computing Laboratory, Center for the Study of Complex Systems, Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Zemun – Serbia
[2]Institut des Molécules et Matériaux du Mans – Le Mans Université, Institut de Chimie - CNRS Chimie, Centre National de la Recherche Scientifique – France

Abstract

This presentation explores water's influence on dynamic tribological contact in two systems: hydrophilic monolayer MoS2 and hydrophobic graphite interfaces. We reveal distinct stick-slip patterns at atomic resolution in the MoS2 system. Simulations highlight water's role in preventing prolonged slips by maintaining separation between solids (1). We explore the influence of water in both fully immersed conditions and air, emphasizing capillary water effects. Shifting the focus to hydrophobic interactions, our investigation challenges the conventional understanding of water expulsion in such contacts (2). We introduce a mechanism involving a droplet produced within the sliding nano-contact through the accumulation of water adsorbed on the substrate. The presentation concludes by demonstrating that a full slip regime of the droplet on the hydrophobic substrate explains the experimental tribological behavior. This research advances our understanding of dynamic friction on water molecule-contaminated surfaces, offering implications for industrial applications. (1) M. Dašić, R. Almog, L. Agmon, S. Yehezkel, T. Halfin, J. Jopp, A. Yaakobovitz, R. Berkovich, and I. Stanković, Investigation of the Nanoscopic Friction on Monolayer MoS2 in Presence of Different Quantities of Water, in preparation.
(2) O. Noël, P.E. Mazeran, I. Stanković, Nature of dynamic friction in a humid hydrophobic nanocontact, ACS Nano 16, 10768-10774 (2023).

*Speaker

Scratching the surface: understanding plasticity associated with microscale asperity contacts

Kareer Anna*[1], Angus Wilkinson[1], Edmund Tarleton[2], and Christopher Hardie[3]

[1]Department of Materials – United Kingdom
[2]Department of Engineering Science [Oxford] – United Kingdom
[3]UK Atomic Energy Authority – United Kingdom

Abstract

The field of tribology studies the interaction between surfaces moving relative to each other; it plays an integral role in various aspects of our daily lives, from mechanical components in power generation systems to biomedical implants. Accurate prediction of wear can lead to substantial advancements in material selection and tribological technologies that can reduce CO2 emissions and save significant costs. However, the complex interplay of multi-physical processes, across a range of length scales makes accurate forecasting of wear a significant challenge. It is understood that macroscopic friction and wear are controlled by nano to micron-sized asperities that come into contact at the surface. As such, developing a fundamental understanding of the mechanics of deformation associated with a sliding contact, at the microscale, is necessary to eventually develop fully integrated, multi-physical models that can simulate and predict wear for a range of operating conditions. In this presentation I will present the experimentally captured micromechanical deformation fields (elastic rotation and elastic strain fields) around a controlled sliding asperity, generated using nanoscratch testing in a well aligned single crystal of copper. The experimental results are used to calibrate a physically based crystal plasticity finite element model. The model simulates the 3-D evolution of the subsurface deformation field as it transitions from a statically loaded indentation to a steady state scratch, providing a physical comprehension of the way material deforms under a frictional contact.

*Speaker

Early-stage wear of layered materials on the nanoscale

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Abstract

We will report on our ongoing investigations of early-stage plowing wear of layered materials based on atomic force microscopy (AFM). While MoS2, WSe2, and HOPG multilayers undergo nanoexfoliation that is characterized by the peeling of chips and crack propagation not necessarily along the scratch direction, other materials such as muscovite mica form well-defined wear tracks with surface atoms removed layer-by-layer from the track only. The observed features can be be associated to specific mechanical properties (bending stiffness, interlayer adhesion, and tensile strength) of the investigated materials (1). The results of similar nanowear tests conducted on monolayer MoS2 will be also presented. In this case, we observed that the exfoliated layer can be completely folded back on itself. In addition, partial detachment of the layer (without folding) is found to occur with a regular repetition rate, which is possibly related the surface rippling of the underlying (silicon) substrate (2). Apart from shedding light on fundamental physical mechanisms governing abrasive wear at the nanoscale, our results can be valuable for better control of micro- and nano-machining processes involving the aforementioned materials.
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*Speaker

Nano-scale wear mechanisms studies: a new experimental approach

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Abstract

The wear rate is a slow process at the nano-scale, which renders fastidious quantitative measurements of the wear volume for determining wear laws. In this talk, we describe a new effective experimental methodology based on the Circular mode atomic force microscopy (CM-AFM) to investigate wear at the nanoscale. A procedure to calculate the wear volume from three dimensional AFM images will also be reported. Using this methodology, macroscale wear behaviour expressed through the well-known Archard's and Barwell's law was compared with nanoscale wear behaviour obtained on copper-based nanocomposite with Al2O3 nanoparticles and duralumin samples.

*Speaker

Effect of loading regimes on the deformation mechanisms of Si under nanoindentation and nanoscratching

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Abstract

The influence of the loading regimes (holding time, scratching speed, load value) on the deformation mechanisms under nanoindentation and nanoscratching of Si single crystal was investigated in this work. By applying the analysis of the kinetics of deformation from the P(h) nanoindentation curves, the micro-Raman spectroscopy and atomic force microscopy we found out a range of regularities.
The prolonged holding (900 s) under nanoindentation even at room temperature leads to the creep of Si that may be caused by the phase transformation into a more plastic metallic Si-II phase under loading. An additional amorphization was detected in the indentation zone situated presumably in the dislocation zone that results in the development of the "kink pop-out" unloading event on the nanoindentation curve after prolonged holding.
The use of the scratching speeds from 20 to 300 μm/s in combination with load range (2-20) mN and two orientations of the Berckovich indenter (face-on and edge-on) made it possible to reveal three specific deformation mechanisms for Si scratching: brittle fracture, plastic flow and ductile cutting. The influence of the components of loading regime (speed, load and indenter orientation), separately and in combination, on the development, evolution and transition from one to another mechanism was determined. The observed size effect is expressed differently depending on the scratching speed and indenter orientation.

*Speaker

Deciphering acoustic emission using micromechanical experiments

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Abstract

Plastic deformation in crystalline materials often exhibits significant inhomogeneity on the micron scale, presenting itself as a series of random local slip events of varying sizes. Two robust techniques have been employed to monitor this stochastic behavior: microcompression for small-scale samples and acoustic emission (AE) for bulk specimens. While AE, with its high sampling rate (_˜2.5 MHz), yields a rich dataset, its interpretation remains challenging due to the complexity of the measurement process.

In this talk, results from coupling these two experimental techniques will be presented in order to gain a more comprehensive understanding of the meaning of the AE signal. The first part of the talk will focus on microcompression of Zn single crystal micropillars oriented for basal slip. These samples are mounted on an AE sensor and compressed in situ within a scanning electron microscope using a specially designed device for this purpose. Our findings reveal a precise correlation between the acoustic events detected during compression and the stress drops measured by the micromechanical device, facilitating the interpretation of AE signals.

The latter part of the talk will delve into uncovering additional insights that can be gleaned from the AE data. To achieve this, we will leverage machine learning to investigate the extent to which stress-strain curves and their finer details can be reconstructed from the AE signal. The presentation will conclude with a glimpse into potential future applications of combining micromechanics and AE.

*Speaker

Exploring CuAgZr metallic glasses for biomedical use: A study using combinatorial synthesis, high-throughput experiments, and machine learning

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Abstract

This study focuses on CuAgZr metallic glasses (MGs), which are notable for their potential in biomedical applications thanks to their exceptional strength, resistance to corrosion, and antibacterial properties. By employing a synergistic approach that combines combinatorial synthesis, high-throughput characterization, and machine learning, we have conducted a thorough examination of the mechanical attributes of CuAgZr MGs. Our findings indicate that the presence of high oxygen levels in Cu-rich areas, resulting from post-deposition oxidation in regions of less dense packing, markedly influences the mechanical performance of these alloys. Additionally, our research uncovers that nanoscale structural nuances play a significant role in determining the plastic yield and flow behavior of the alloys. Among various machine learning models evaluated, the multi-layer perceptron algorithm stood out, delivering accurate predictions of hardness for alloys not previously tested, thereby offering insightful directions for ongoing material research. This investigation underscores the efficacy of leveraging combinatorial synthesis, high-throughput analysis, and machine learning to accelerate the development of new metallic glasses with enhanced mechanical properties and cost-effectiveness.

*Speaker

Thin film nanoindentation and the importance of the tip radius

Stanislav Zak*[1]

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Abstract

In current years, there has been a huge development towards the miniaturization and materials engineering on a micro- to nano-scale with material properties characterization on small scale. Nanoindentation is a well-known and proven technique for hardness and elastic modulus measurements, however, when used with nano-structured applications, it can start to be not as reliable as for larger scale applications. The prime example of this is the thin films nanoindentation and appearance of the substrate effect. Knowing what is happening under the indenter is not easy, since the analytical formulas tend to fail on such scale and there is no easy way to visualize the deformation inside the material experimentally. However, numerical modelling allows us to look under the surface. Presented research uses a synergetic combination of experimental nanoindentation and finite element modeling to reveal how are the nanoindentation results influenced by up-to-now overlooked feature – the tip radius. The current consensus is that tip radius should be sharp and well-calibrated, but no attention is paid to the differences in sample material deformation for different tip sharpness. Indentations with well-calibrated tips, but with different tip radii, lead to differences in the size of elastically and plastically deformed region. In case of thin film nanoindentation, it subsequently changes the substrate effect, making the thin films and micro-structures nanoindentation even more complex problem. However, presented results show that with a proper knowledge of the tip geometry, the nanoindentation complexity can be exploited to get more precise measurements with smaller number of indents.

*Speaker

Micromechanical assessment of the limpet tooth: Unraveling the secrets behind Nature's strongest material

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Abstract

The teeth of aquatic snails exhibit extraordinary mechanical properties made possible by evolution, as their functionality is to scrape algae from hard rocky substrates as a means to gather food. The microstructure of limpet teeth consists of Goethite (Fe-OOH) nanocrystals embedded in an amorphous SiO2 matrix, where the size, morphology, distribution and organization pattern of the nanorods varies from the tooth's leading to the trailing part, resulting in a microstructural gradient. The nanorods are smallest in the leading part, where they are organized in a specific rotational pattern, which results in a unique auxetic deformation response. It is believed that this combination of nanocomposite microstructure and auxeticity is responsible for the highest strengths measured in biological materials so far. This work further expands the knowledge of the unique deformation behavior of limpet teeth by performing a plethora of micromechanical experiments. Nanotensile straining, micropillar compression and nanoindentation with sharp and spherical indenter tips are complemented by fracture mechanical experiments to study fracture toughness in both the leading and trailing parts and gather insight into the tooth's intricate microstructure-property relationship. The possible transfer of the learned concepts to the biomimetic design of technological materials is discussed.

*Speaker

Structure, stability and mechanical properties of small metallic nanoparticles: insights from first-principles simulations

Laurent Pizzagalli[1], Julien Durinck[1], Julien Godet[1], and Sandrine Brochard*[1]

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Abstract

It is now well established that the strength of metals can be several orders of magnitude higher than in the bulk when sample dimensions are significantly reduced. But whether it keeps increasing, saturates or decreases when characteristic dimensions are reduced down to the nanometer scale remains an open question.
To bring new insights, first-principles molecular dynamics calculations are performed to model the compression of 1 to 2 nm aluminum and tungsten nanoparticles with different shapes. The use of first-principles calculations offers the required accuracy for such a study and complements advantageously experimental studies, giving direct access to the deformation mechanisms.

For aluminum, it is shown that the strength depends on the nanoparticles shape, and is higher than the theoretical bulk strength. It is however clearly lower than predictions from classical molecular dynamics calculations of larger systems, suggesting that strength stops increasing below a size threshold.
For tungsten, previous theoretical and experimental studies have hinted that fcc structures would be favored over bcc below a given nanoparticle size, around 5 nm. We thus first checked with first-principles calculations the stability of several tungsten nanoparticles with various structures. We show unambiguously that the bcc structure remains the most stable. Some clues will be given to explain the discrepancy with previous theoretical predictions. Then, selected tungsten nanoparticles with the bcc structure have been compressed using first-principles molecular dynamics calculations. The obtained stress-strain curves and the deformation mechanisms will be presented and discussed.

*Speaker

Mechanical Properties of Nickel-Platinum Nanoparticles Fabricated by Solid-State Dewetting Synthesis

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Abstract

Nanoparticles of Ni-Pt alloys attract great attention because they can replace more expensive Pt in several catalysis-related applications. The shape, size, and distribution of such nanoparticles can influence application functionality.
This work studied the effect of composition, structure, and nanoparticle's overall morphology on the mechanical properties of Ni-Pt nanoparticles synthesized by solid-state dewetting of the Ni-Pt bilayers deposited on a sapphire substrate.
The nanoparticles of Ni-Pt alloys of several compositions were produced employing solid-state dewetting of Ni-Pt bilayers at elevated temperatures for different heat treatment durations. We used multiple characterization methods such as atomic force microscopy, scanning electron microscopy, electron backscatter diffraction, x-ray diffraction, and in-situ pico-indentation to investigate the attributes of the nanoparticles.
We found that the increasing Pt content resulted in lower and wider nanoparticles, and the orientation of the nanoparticles varied. Surprisingly, we observed a solid-solution softening trend in the nanoparticles, which is the opposite of reported in bulk Ni-Pt.

*Speaker

Normal Dynamics - method development and applications

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Abstract

Normal Dynamics (*ND*) is a nanomechanical simulation method, the core of which is integration of the Newton's classical mechanics equations of motion, by adequately sampling the reciprocal space. Adequate sampling strategies and their capability of producing dynamical trajectories at the *ab initio* level with low computational demand will be discussed. *ND* method enables to: (1) obtain a systematic improvement of the accuracy, (2) to fine tune the computational resources' demand, and (3) to consider the atomic distortions happening across large distances, without the need of using large unit cells.
Theoretical background of the *ND* method is based on determining the phonon structure of a material. We will present several case studies which illustrate the method's applicability and computational performance. It will be explained that this simulation method has a general orientation, and it can be used for simulating: (a) periodic, (b) semiperiodic, and (c) finite systems (such as (a) crystals, (b) slabs, and (c) molecules).

Authors have implemented the *ND* method in the *Fortran* programming language (thus achieving high computational efficiency), and named the developed software - *PINDOL* (Phonon-Inspired Normal Dynamics of Lattices). *PINDOL* is an open-source software package for performing atom dynamics in the NVE and NVT ensembles (link for the free download: https://github.com/acammarat/pindol).

*Speaker

Amorphous plasticity at the mesoscale: development of a shear transformation zone-based numerical model

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Abstract

Glassy solids such as amorphous polymers or metallic glasses exhibit complex behaviour when subjected to deformation below the glass transition temperature. Sophisticated continuum models are available to simulate this response. However, they require the calibration of a large number of phenomenological parameters and often struggle to accurately predict the response for more complicated loading states such as confinement at the nano- to microscale.
The use of a mesoscale numerical model based on shear transformation zone (STZs) is an attractive method to bridge standard continuum modelling approaches and atomistic simulations which are typically limited to small length and time scales. Plastic deformation is dictated by conformational changes of molecular segments or atomic clusters (STZs) and their interaction with the linear, elastic matrix. The model sheds light on the role of thermomechanical history on the deformation response of an amorphous solid with only a few physical parameters and can be used to explore possible size effects in e.g. (1) fibre-reinforced composites where the glassy matrix is confined by the stiffer fibers or (2) in ductile nanolaminates comprising alternating layers of crystalline and amorphous metallic layers.

The scope of this contribution is to introduce the theoretical framework of the model and its implementation in a commercial FE software package. The model's code is open source. In addition, we explore possible routes to calibrate the model based on limited measurement data and discuss practical case studies were the mesoscale model can be used to reveal and exploit possible material size effects.

*Speaker

Impact of room-temperature engineered dislocations on the mechanical properties in oxides

Xufei Fang*[1]

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Abstract

In light of the increasing interest in dislocation-tuned functional properties and the technological potential that dislocations may hold (1), dislocation-based mechanical properties in oxides are also drawing increasing attention. To tackle the challenge of engineering dislocations into brittle ceramic materials without inducing cracks, we have separately examined the dislocation behaviour including dislocation nucleation, multiplication and motion, enabling us to tune dislocations into some ceramic materials at room temperature (2). We can now achieve a dislocation density ranging from _~10^10/m2 to _~10^15/m2 with a plastic zone size of up to hundreds of micrometres, providing a robust platform to study the dislocation-tuned mechanical properties at room temperature, such as plasticity, fracture toughness, and damage tolerance. Here in this talk, I will first briefly introduce the room-temperature dislocation engineering toolbox, and then focus on the nanoindentation hardness, plastic deformation (e.g., pillar compression) and fracture toughness tuned by the pre-engineered dislocations (with different densities and spatial arrangement). The proofs-of-concept on SrTiO3 will be demonstrated and further extended to other oxides to showcase the general applicability.

References:

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(2) X. Fang, Mechanical tailoring of dislocations in ceramics at room temperature: A perspective, Journal of the American Ceramic Society 107(3) (2024) 1425-1447.

*Speaker

Transformation towards a digitized materials science laboratory

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Abstract

Data-driven methods become more and more important in modern materials science and, in particular, machine learning and artificial intelligence need access to a large amount of high-quality data. Managing data according to FAIR principles, therefore, becomes a important aspect in laboratory management.
The transformation towards a modern data-centric experimental materials science laboratory faces many challenges from managing experimental samples, consumables, and scientific instruments, to capturing relevant data, automatic extraction of embedded metadata, and linking relevant information together. Additionally, users need to get into the habit of entering descriptions about their experiments and results, as well as data that cannot be captured electronically into an electronic laboratory notebook (ELN).
In this talk, we will discuss the current status quo and future roadmap of introducing openBIS as a combined Laboratory Information Management System (LIMS) and ELN at the Institute for Physical Metallurgy and Materials Science at RWTH Aachen University. We will demonstrate how data recorded by scientific instruments can be ingested automatically, extracting the relevant metadata, how this enables scientists to build data-driven workflows, and how data can be shared according to FAIR data principles both amongst research groups at the institutional level, as well as the wider community.

*Speaker

Dataflow Development and Machine Learning for Nanoindentation Data Analysis

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Abstract

Nanoindentation, a method for probing materials at the nanoscale, has seen increased interest in using machine learning (ML) to improve analysis efficiency. This study integrates ML algorithms into nanoindentation data analysis using a dataflow approach within Granta MI software, part of the Nanomecommons project (https://cordis.europa.eu/project/id/952869). Experimental data comprises force-displacement curves from nanoindentation tests on various materials, providing insight into mechanical properties like hardness and elastic modulus. Leveraging Python scripting in Granta MI, researchers automate data analysis workflows, facilitating ML algorithm integration for property prediction. Initial results demonstrate the effectiveness of this approach in accurately predicting material properties. The combination of Granta MI's data management and Python's flexibility enables efficient preprocessing, feature extraction, and model training. This integration promotes collaboration by facilitating data analysis workflow sharing and reproducibility within the Nanomecommons project.

*Speaker

Plasticity in topologically close-packed phases: Insights from nanomechanical testing and atomic-scale modelling

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Abstract

Topologically close-packed (TCP) phases hold significant promise as high-temperature structural materials. However, their notorious brittleness at room temperature hinders their applications. The mechanisms governing dislocation motion in these complex alloys remain poorly understood. Through atomistic simulations, we aim to elucidate the deformation mechanisms of TCP phases, complemented by experimental observations from nanomechanical testing at room temperature. For Laves phases, we investigate the mechanisms and associated minimum energy paths of synchro-Shockley dislocation motion, along with dislocation cross-slip among newly identified {11n} slip planes. Additionally, for μ-phases comprising Laves crystal building blocks, we reveal a transition in basal plasticity with the compositional changes, significantly influencing the global mechanical properties. Furthermore, we confirm a new non-basal (1-105) slip mechanism mediated by partial dislocation gliding in μ-phases. This comprehensive exploration of dislocation dynamics not only advances our fundamental understanding of TCP phases but also sets the stage for tailored design strategies to enhance their mechanical properties at room temperature.

*Speaker

Micromechanical behavior of nanoporous electrodeposited Zn coating

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Abstract

Zinc (Zn) stands out as a promising candidate for biomedical applications due to its unique biodegradability and biocompatibility. A recent innovative concept involves leveraging Zn as an antibacterial coating for implants, enhancing cellular response by integrating a tunable micro 3D-printed architecture. This study focuses on the microstructural and mechanical characterization of a Zn coating synthesized through pulse-current electrodeposition, a versatile and cost-effective method capable of producing a wide range of 2D and 3D structures.
Microscopic analysis utilizing electron backscattered diffraction (EBSD) in a scanning electron microscope (SEM) revealed a fine-grained microstructure with a strong < 10-10> texture as a result of the optimized electrodeposition process conditions. *In situ* micromechanical testing in SEM was performed to investigate the deformation mechanisms and determine the mechanical properties of the Zn coating. Compression tests on focused ion beam (FIB)-machined Zn micropillars spanning various diameters revealed a size effect with no evident strain rate sensitivity within the range of 0.0001 s-1 to 1 s-1. Notably, the smallest micropillar deformed at 0.001 s-1 exhibited an impressive yield strength of 1100 MPa
Post-mortem SEM characterization demonstrated localized deformation dominated by prismatic slip in the 1 μm micropillar, while a more uniform deformation with shallower slip traces was observed in the 9 μm micropillar. Transmission electron microscopy (TEM) and high-angle annular dark field scanning transmission electron microscopy (HAADF-STEM) imaging revealed the presence of intragranular nanosized pores, which, coupled with the crystal orientation of electrodeposited columnar grains, may significantly contribute to the observed high micromechanical properties.

*Speaker

Investigating Mechanical Properties of Silicon Nanowires: Scale Effect Revisited

Sina Zare Pakzad*[1], Mohammad Nasr Esfahani[2], Zuhal Tasdemir[3], Nicole Wollschläger[4], Zhongquan Liao[5], Juliane Posseckardt[5], Andre Clausner[5], Sylvia Conzendorf[5], Umut Kerimzade[1], Taotao Li[6], Xuefei Li[6], Mustafa Yilmaz[1], Yusuf Leblebici[7], and B. Erdem Alaca[1]

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[6]Nanjing University – China
[7]Sabanci University [Istanbul] – Turkey

Abstract

Nanowires play a pivotal role in different fields such as nanoelectromechanical systems (NEMS), nanoelectronics, and energy applications. As nanowires decrease in size, their mechanical characteristics are increasingly influenced by surface attributes. Despite their considerable promise as foundational components in NEMS, research on silicon nanowires (Si NWs) has yet to consolidate in order to construct a comprehensive understanding of the scale dependence in their mechanical characteristics. In this extensive investigation, we explore the mechanical properties of Si NWs, concentrating particularly on their elasticity and fracture strength. The study provides an in-depth examination of the scale-dependent properties using a newly developed multiscale model that incorporates the surface and intrinsic effects. Through a comprehensive methodology encompassing fabrication, experimentation, characterization, and modeling, we analyze Si NWs of different critical dimensions and lengths. The study systematically reveals the intricate impact of size changes on elastic properties of Si NWs, providing valuable insights into how their modulus of elasticity evolves with dimensional changes. Contrary to previous literature favoring bottom-up techniques on fabrication of high strength Si NWs, our findings challenge this by demonstrating that top-down fabrication methods reach remarkable fracture strength aligned with the theoretical strength limit of single-crystal-silicon. Utilization of advanced techniques including Raman characterization, high-resolution transmission electron microscope imaging, and atomistic modeling, this study clarifies the complex interplay between size, surface conditions, and mechanical behavior in Si NWs. This study presents a revised framework for comprehending and interpreting the mechanical characteristics of Si NWs, laying the groundwork for future advancements in NEMS and nanoelectronics.

*Speaker

What can nanomechanical mass spectrometry tell us about nanoparticles?

Mehmet Selim Hanay*[1]

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Abstract

Nanoelectromechanical Systems (NEMS) have been used in recent years to measure the mass of individual nanoscale objects such as inorganic nanoparticles and viruses. Normally, NEMS sensors have been operated under high-vacuum conditions to increase their sensitivity levels. However, this approach significantly reduces the throughput attainable by the NEMS sensors and field-portability of the technique.
We have recently showed that NEMS devices can be used to characterize nanoparticles under ambient conditions and with an increased throughput (1,2). After reviewing the salient points of this technology, we will discuss how inertial measurements at the single nanoparticle level can be relevant within the viewpoints of analytical properties and physics of nanoparticles. We will describe our new approach to combine different sensing modalities with NEMS inertial sensing to achieve identification of different types of nanoparticles based on their material content (3). We will conclude by pointing out directions in environmental and biologic sensing where nanoparticle characterization at the single particle level could play a critical role.

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*Speaker

Mass Particle Compression, or: How I learned to stop doing in-situ nanomechanical tests and love ex-situ ones

Jonathan Zimmerman*[1] and Eugen Rabkin[1]

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Abstract

In-situ nanomechanical tests yield invaluable insights into the mechanical behavior of materials at the nanoscale, yet they are riddled with numerous drawbacks. On the one hand, *in-situ* tests enable unparalleled precision in the probe positioning, and in application and measurement of force and displacement. Our current understanding of such topics as the effects of size and temperature on nanomaterial strength, the fundamentals of plasticity, and the dynamic behavior of dislocations at the nanoscale is largely achieved by employing *in-situ* methods. On the other hand, *in-situ* methods are slow, require specific sample preparation, the mechanical probes wear out and break quite often, getting rid of the measurement artifacts is tricky, and one can never be sure as to whether beam damage plays a role in the measurements. To combat these issues, we have devised an ex-situ testing method that can partially replace *in-situ* tests. This Mass Particle Compression (MPC) method enables performing uniaxial-compression tests of hundred-thousand to millions of nanoparticles simultaneously using relatively simple means. An added advantage of this method is that the large array of tested objects can now be explored using statistical characterization techniques such as X-ray diffraction. We have utilized this MPC method in our studies of defect-free, uniformly oriented Pt nanoparticles with a (111) out of plane orientation, and found that the particles' lattice exclusively rotates towards the (110) orientation upon compression. Lastly, we propose a model that allows determining the statistically averaged strength of individual nanoparticles from the macroscopic loading curves.

*Speaker

Advancing Nanomaterial Characterization: A Machine Learning Approach to Assessing h-BN Mechanical Properties

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Abstract

The quest for materials with superior mechanical properties for technological and environmental applications necessitates advanced characterization techniques at the nanoscale. This study introduces an innovative framework that combines machine learning (ML) with nanoindentation to quantitatively analyze the elastic modulus and hardness of hexagonal boron nitride (h-BN) nanosheets, a material renowned for its exceptional mechanical and thermal properties.

Utilizing a series of nanoindentation experiments, we systematically applied loads up to 10 μN on h-BN nanosheets with thicknesses ranging from 5 to 50 nm. The force-displacement data obtained were then analyzed using a convolutional neural network (CNN), trained to correlate specific indentation responses with variations in elastic modulus and hardness. This ML model was trained on a dataset comprising over 1,000 individual nanoindentation curves, achieving a predictive accuracy of 95% when validated against a separate test set.

The ML analysis revealed an average elastic modulus of 250 GPa and hardness of 20 GPa for the h-BN nanosheets, with the model identifying a thickness-dependent trend where thinner nanosheets exhibited slightly higher values. This trend was attributed to the influence of surface effects and interlayer interactions on the mechanical properties at reduced dimensions.

Our approach demonstrates the power of integrating ML with nanoindentation to enhance the characterization of nanomaterials, offering a more detailed and accurate understanding of their mechanical properties. The findings not only contribute to the advancement of nanomechanical characterization techniques but also provide valuable insights for the design and application of h-BN in next-generation material technologies.

*Speaker

Enhancing Material Valorisation through Innovative Nanomechanical Testing

Theo Zacharis*[1]

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Abstract

The poster explores the transformative potential of state-of-the-art nanomechanical testing techniques, such as nanoindentation and advanced material characterization, in revolutionizing the exploitation and valorisation of new material technologies. It addresses how these sophisticated experimental methods are crucial in uncovering the mechanical properties of materials at the nanoscale, offering insights for various applications ranging from microelectronics to biomedical engineering.
The core of this exploration is the strategic integration of these nanomechanical insights into the broader innovation pipeline. We examine the journey from laboratory discovery to market application, highlighting the pivotal role of effective technology transfer and intellectual property management in the valorisation process. This includes an examination of the challenges and opportunities in translating nanomechanical data into viable commercial products and services, with a particular focus on the potential bottlenecks and solutions in this pathway.

A significant portion of the poster is dedicated to the emerging role of machine learning in this context. We explore how AI-driven analysis can significantly enhance the interpretation of complex nanomechanical data, leading to more accurate predictions of material behaviour and performance. This integration promises to streamline the research process but also to provide a robust foundation for material selection and design in industrial applications.
The poster concludes by proposing a forward-looking perspective on the future of material science innovation. It suggests that the key to successful exploitation and valorisation of new materials lies in the synergy between cutting-edge nanomechanical experiments, strategic technology transfer, and the leveraged use of machine learning for data analysis and prediction.

*Speaker

Analysis of nanoindentation creep of ceramic-organic supercrystalline nanocomposites

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Abstract

Supercrystalline nanocomposites (SCNCs) are a new category of hybrid materials that typically consist of organically functionalized inorganic nanoparticles and assembled into periodic structures. They have attracted growing attention thanks to their hierarchical architecture and intriguing functional properties (plasmonic, optoelectronic, biomedical). It is imperative to understand and tune their mechanical properties in order to enable a broad set of applications. So far, the mechanical behaviour of SCNCs has been partially assessed in terms of time-independent phenomena. However, another important yet uncharted aspect is their time-dependent deformation given the presence of organic constituents. Here, the time-dependent deformation behavior of ceramic-based SCNCs is investigated via nanoindentation. It emerges that both creep and its recovery occur in SCNCs, both with and without the crosslinking of the organic ligands, even though creep is less pronounced when crosslinking is present. A new creep mechanism is proposed for SCNCs to account for the extremely small activation volume, i.e. organic ligands-facilitated rearrangement of the materials' nanoconstituents, achieved via the rearrangement of organic ligands in the sub-nm inter-particle spacings. The nonlinear viscoelastic behavior is exhibited by SCNCs, evidenced by the stress-dependent creep compliance. The creep model based on free volume theory is thus adopted towards the prediction of such behavior. The free volume located in the interstitial sites of superlattice or the space in-between nanoparticles is thought to beneficial to the rearrangement of organic ligands and further impacts their creep behavior.

*Speaker

Grain size influence on the creep and fatigue properties of freestanding gold thin films

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Abstract

Microstructural engineering has been a major focus of materials science for many decades. Grain size refinement is known to significantly increase the strength of a material, as rationalized by the Hall-Petch relationship, and also provides a significantly improved high-cycle fatigue lifetime. However, its effect on high-temperature creep is less favorable, as the presence of grain boundaries increases the diffusion rate of vacancies. It is still a matter of debate how the fatigue and creep mechanisms compete in fine-grained materials systems that are operated under combined cyclic and creep conditions. The practical case of thin metallic films applied to hot integrated circuits is especially challenging, as the nanoscale thickness of the samples introduces an extrinsic size effect, which competes with the microstructural one. Here, freestanding gold thin films of 150 nm thickness with two different microstructures – ultrafine-grained (UFG) and nanocrystalline (NC) – are experimentally compared. Their creep and fatigue properties are characterized at ambient and elevated temperatures up to 100 ∘C, using a custom bulge tester. As expected, the UFG samples exhibit superior creep behavior independently of the temperature, showing lower steady-state strain rates. Under cyclic loading, NC films perform slightly better than the UFG samples at 23 ∘C, which is also in line with data from bulk materials. At 100 ∘C, however, both grain sizes lead to similar fatigue lifetimes. Together with the evaluation of the activation energies and the SEM observations, these findings suggest that the influence of the cyclic condition decreases at high temperatures, while creep mechanisms take precedence.

*Speaker

Compressive strength of the Cu-Au nanoparticles fabricated by solid state dewetting

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Abstract

Solid solution and long-range atomic order hardening represent two well-known strategies for increasing strength of bulk metallic materials. We observed the opposite trends in mechanical behavior of defect-free nanoparticles of Cu-Au alloys fabricated by solid state dewetting of Cu-Au bilayers deposited on sapphire substrate. In the fully disordered state, the nanoparticles of Cu3Au alloy exhibited the highest compressive strength reaching staggering 41 GPa for the smallest studied particles, followed by nanoparticles of pure Cu, and of CuAu alloy. Thus, taking pure Cu and Au nanoparticles as a reference, both solid solution hardening (Cu3Au) and solid solution weakening (CuAu) were observed in nanoscale plasticity of the Cu-Au system. Additional annealings at the temperature of 350 ∘C, 40 ∘C below the critical point of A1-L12 transformation, were performed to induce different degrees of the long-range order in the Cu3Au nanoparticles. It was shown that the strength of fully ordered Cu3Au nanoparticles is very similar to that of their fully disordered counterparts, whereas the partially ordered Cu3Au nanoparticles larger than 500 nm in size exhibited a significant drop in strength. No effect of long-range order on compressive strength of smaller nanoparticles was observed. These findings were discussed in terms of plasticity mechanisms controlled by nucleation of new dislocations. Specifically, it was proposed that the presence of oxidation-induced Au-rich subsurface layer in the Cu3Au nanoparticles is responsible for their ultrahigh strength.

*Speaker

Nanoparticle Fabrication for SnSb2Te4 via Mechanical Milling

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Abstract

Thermoelectric materials (TE) are attractive materials now in the behind of clean energy and climate change concepts and, thus are expected one of the important materials to build a sustainable future thanks to their thermoelectric energy conversion ability. TE are very promising for various applications such as power generation, refrigeration, and microelectronics manufacturing, offering advantages such as noise-free operation, zero emissions, and versatility in diverse fields.
Two primary approaches for enhancing thermoelectric materials are well known for their large-scale applications: i) effective doping by various atoms, ii) reducing material dimensionality down to the nanoscale. Up-to-date literature data shows that latter approach can significantly improve the thermoelectric figure-of-merit (ZT) of TE.

Here we present nanoparticle fabrication of SnSb2Te4 ternary compound using ball-milling technology following the "top-down" approach. The high-quality and -purity initial SnSb2Te4 single crystal, was synthesized via the Bridgman method. Nanoparticle fabrication was performed ball milling using an 80 mL tungsten carbide bowl with 15 mm milling balls. Crystallite size reduction was monitored via XRD measurements at 2-3h intervals. After 30h of milling, SEM-EDS analysis confirmed the formation of phase-pure SnSb2Te4 nanoparticles with particle dimensions 40-60 nm.

In summary, the results demonstrate the efficacy of ball-milling as a cost-effective technique for fabricating phase-pure SnSb2Te4 nanoparticles and highlighting its versatility and potential for easy nanofabrication of even doped materials. The obtained results seem promising not only for the title compound but also for similar layered materials, which are also well-known topological insulator quantum materials for application in spintronics, topotronics, etc.

*Speaker

Dust Particle Impact on Plasma-Facing Materials in Tokamaks: Insights from Molecular Dynamics Simulations

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Abstract

The influence of dust particles on the performance and lifespan of PFMC in tokamaks is of utmost importance. Temperature and dust velocity are critical factors that determine the extent of dust-wall interactions. Elevated temperatures within tokamak environment can lead to the vaporization of dust particles upon collision with the wall, resulting in heightened erosion and damage.

In this study, we employ extensive MD simulations to explore atomic processes occurring during dust impacts on target walls at various velocities. The simulations involve large samples, comprising up to 200 million atoms, allowing for a comprehensive investigation of temperature and velocity as influential parameters. The findings provide novel insights into the interactions between dust and PFM, elucidating how these interactions can induce modifications in the mechanical properties of the target material. Moreover, the study examines the underlying physical mechanisms involved in dust-wall interactions, encompassing phenomena such as plastic deformation, fragmentation, melting, and vaporization.

*Speaker

Shape and Size Effects on Compressive Strength of Fe-Pd Alloy Nanoparticles

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Abstract

Single-crystalline, faceted, defect-free metallic particles of sub-micrometer dimensions exhibit extraordinary compressive strength, approaching and even surpassing the theoretical strength of the bulk material. Such nanoparticles experience a large dislocation burst at the onset of plasticity related to a unique dislocation nucleation-based plastic deformation mechanism. Extensive studies of the effect of size and shape on the mechanical behavior of metal nanoparticles were performed with the aim of better understanding the laws of small-scale plasticity. Recent studies on the impact of alloying demonstrate the well-known solution-hardening behavior, as well as a counter-intuitive effect of solution-softening. In the present work, solid-state dewetting of a thin metallic bi-layer film has been employed to produce defect-free nanoparticles of Fe-Pd alloy with (111) out-of-plane orientation on a sapphire substrate. The results of in-situ nano-compression tests reveal a notable correlation between particle shape and compressive strength, as well as a somewhat weaker size effect. Contrary to previous works where particle strength exhibited a plateau with decreasing size, our results reveal a deviation from this trend. The engineering strength monotonously increases with decreasing particle size, ultimately reaching values as high as 44 GPa.

*Speaker

Surface modification of case-hardened AMS 6265 aircraft steel by nano surface – severe plastic deformation

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Abstract

When designing critical aircraft applications, operating in severe conditions under high dynamic loads (engine gears, pinions, shafts, clutch components), both the material's core properties and its surface characteristics need to be engineered for optimal performance. The surface layers of such parts are subjected to high mechanical stress during operation, and they will degrade first due to contact with some other parts and with the surrounding environment. Therefore, in this study, a nano surface – severe plastic deformation (NS-SPD) treatment was applied on the surface of an AMS 6265 aircraft steel, widely used for manufacturing heavy-duty products and parts for the aeronautical industry. The AMS 6265 steel was subjected to a series of heat/thermochemical treatments (case-hardening treatment) prior to surface modification by NS-SPD, to obtain a proper microstructure and mechanical properties for the surface and the core. Surface improvement via NS-SPD was achieved by cold locally deforming the near-surface layers and creating residual compressive stresses and strain hardening using small impact balls accelerated by compressed air. The influence of different processing parameters (ball size, compressed air pressure, treatment duration) on the microstructure and mechanical properties of AMS 6265 steel was investigated. The following structural characteristics were analysed: constituent phases, lattice strain, crystallite size, phase morphology. The mechanical behaviour was assessed through the following properties: microhardness, ultimate tensile strength, yield strength, elongation to fracture. The obtained results were correlated with the NS-SPD intensity to determine the optimum parameters and to fine-tune the surface modification technology for the AMS 6265 aircraft steel.

*Speaker

Durability of hard protective coatings: Assessing the fracture and fatigue resistance of nanostructured thin films

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Abstract

Tailoring the intrinsic fracture characteristics of hard protective coatings toward the fatigue properties of state-of-the-art bulk materials is paramount for applying innovative coating materials. Thus, an in-depth knowledge of the failure pathways of ceramic-based thin films – typically lacking in intrinsic ductility – is imperative to extend their lifetime. Here, we present a novel approach using quasi-static and cyclic bending of pre-notched, unstrained micro-cantilever beams in conjunction with in-situ synchrotron X-ray diffraction to reveal the intrinsic fracture toughness (KIC) and critical failure aspects of Cr and Cr-based ceramic thin films (CrN, CrB2, and Cr2O3) under various loading conditions. Up to the high-cycle fatigue regime (i.e., N = 107 cycles), the failure of monolithic coatings is shown to be dominated by the inherent fracture resistance, irrespective of the bonding character. The observed variation in fracture toughness is put into context with linear-elastic fracture theory and complementary micro-pillar compression, thereby elucidating the wide range of values from as low as 1.6±0.2 MPam0.5 for Cr1.79O3 up to 4.3±0.3 MPam0.5 for Cr1.03B2. Moreover, possible mechanisms governing the elastic-plastic deformation response of all coatings, both in quasi-static and cyclic-loading conditions, are discussed. The results are expected to provide key insights into the underlying mechanisms promoting crack growth in PVD-coated specimens.

*Speaker

High strain rate mechanical behavior of SMAT hardened steel layers

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Abstract

The service lifetime of structural components is often hampered by surface-initiated failure. Hardening treatments aim at enhancing the mechanical behavior of the surface, while preserving the properties of the bulk material. Surface Mechanical Attrition Treatment (SMAT) is a novel technique with exceptionally high hardening potential. It induces locally severe plastic deformation through repeated multidirectional impacts of ultrasonically accelerated spherical shots. This results in self-nanocrystallization, which creates a gradient microstructure ranging from nanocrystalline directly underneath the treated surface to coarse-grained at the core of the sample. While significant hardening has already been reported at conventional testing velocities, it remains to be seen how the SMAT layer behaves at high strain rates, which are typical for collisions and amount for a great deal of the components failures.
In this study, the hardness and strain rate sensitivity of an austenitic 316L steel processed by SMAT have been investigated at high strain rates (0.1/s, 1/s, 10/s, 100/s) via nanoindentations on a cross section. A hardness gradient was evidenced in the area of SMAT affected microstructure and the material was shown to exhibit an increasingly high strain rate sensitivity at high strain rates.

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*Speaker

Elastic properties of laser-affected glass probed by grid nano-indentation

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Abstract

Ultrafast lasers have been shown to be useful to locally tailor the physical properties of materials (1). Thanks to the high-peak power delivered by these lasers, one can trigger non-linear absorption processes, enabling the ability of modifying transparent materials in three dimensions. Among these physical properties, local elastic properties play an essential role at the micro-scale. We thus investigate how ultrafast lasers can be used for locally tailoring local mechanical properties (2), such as Young modulus, and to distribute it in a controlled manner, in three dimensions. Applications are foreseen in integrated optical polarization devices as well as for fine contact-less positioning of micro-objects (3).
Grid nano-indentation has been applied to characterize the elastic stiffness field in fused silica after it has been exposed to a femto-second laser irradiation. Because of the very small size of the laser-affected zone (LAZ), the necessary spatial resolution is achieved by adapting a previously proposed deconvolution procedure (4) to the LAZ geometry. This ends up in minimizing a projection residual, and an elastic description of the modified glass is thus sequentially constructed, driven by the minimization of the global projection residual. This reveals a very significant and very heterogeneous Young's modulus modification compared to the pristine material.

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*Speaker

Research of tin, antimony and cooper coatings applied in renewing the surfaces of parts

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Abstract

The aim of this study is to evaluate the mechanical-physical properties of anti-friction coatings and experimentally justify the most suitable coating method. An anti-friction coating whose chemical composition consists of tin, antimony and copper, is commonly used as a lining or coating for renewing bearings, sleeves in machinery and engines. Mechanical, radiographic and penetrating tests were used to examine the anti-friction coatings formed by three different methods, the chemical composition was determined, and the microstructure analysis was performed. Tensile tests provided insights into the structural integrity and load resistance of the base metal and coating. The hardness of anti-friction coatings is important, especially in cases where the coating is exposed to high loads or abrasive forces. The results of the penetration tests provided essential insights into the porosity level of antifriction coatings obtained by different methods. The X-ray examination provided a detailed picture of the internal structure of the coatings and the metal base and made it possible to identify any possible defects. The microstructure analysis revealed information about grain size, distribution and morphology, which directly affects the material's mechanical strength, hardness, and wear resistance. The coated antifriction coating consisted of a tin base matrix with intercalated alpha solid-solution tin-copper (Cu6Sn5) phases in tin and/or solid cubic beta-phase tin-antimony inclusions. Tin-copper intermetallic compounds were characterized by star-shaped formations, while those of tin and antimony were plate-shaped. Research has shown that the selection of the appropriate coating method has an important influence on the quality of the coating and its properties.

*Speaker

Exploring the potential of dislocation density fields for the discrete-to-continuum crossover in nanomechanics

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[2]Institut Jean Lamour – Institut de Chimie - CNRS Chimie, Université de Lorraine, Centre National de la Recherche Scientifique – France

Abstract

The nanomechanics of crystalline materials is governed by various processes occurring across a wide range of length/time scales. While continuum mechanics simulations offer a suitable framework for modeling the mechanical properties of microstructures, they are limited in capturing the details of crystal defect structures and their elementary deformation mechanisms. On the other side, these mechanisms can be conveniently accessed through discrete atomistic simulations, but such approaches are usually limited to small length/time scales. Now more than ever, accurate information transfer across scales is required for efficient and reliable physics-based nanomechanics modelling.

The work we present here explores a novel atomistic-to-continuum crossover scheme based on dislocation density fields. More precisely, elastic transformation tensors are computed using the Hartley and Mishin method for atomistic configurations, and then employed as inputs in a micromechanical field dislocation mechanics (FDM) strain-gradient type model using a regular fast Fourier transform solver grid. This versatile approach successfully captured crystal defects as diverse as dislocations in FCC and BCC structures, low- and high-angle grain boundaries, as well as interactions among them. In the light of our results, the implications of such a discrete-to-continuum crossover for nanomechanics are discussed.

*Speaker

Modelling of inhomogeneous deformation in nanoporous-Au nanoparticles under indentation

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Abstract

In this study, inhomogeneous deformation mechanisms observed in nanoporous structures are investigated using molecular dynamics (MD) simulations. Compression of single-crystalline nanoporous gold (NPG) hemispherical nanoparticles with different morphological and topological features was performed in MD simulations. The size-dependent plastic deformation responses of NPG nanoparticles were computed as a function of their relative density, size, and ligament diameter. The responses were quantified based on two descriptors, namely, plateau stress and the strain hardening rate, which are observed to be dependent on the topology of nanoparticles. At each indentation depth, the deformation is inhomogeneous and there exists a densified region beneath the planar indenter, which is highly localized and thereby demonstrating increased relative density in comparison with the initial value. This region is characterized by the accumulation of dislocations due to plastic deformation of ligaments and closure of pores. With the increase in the indentation depth, there is an increase in the relative density within the densified region. To quantify the inhomogeneous deformation, the relative density profiles throughout the nanoparticle were calculated, which allows us to quantify the evolution of the center and the width of the densified region. The width was found to remain constant during deformation, and its value was found to be in correlation with the strain hardening. This study allows us to analyze the evolution of the contact area during indentation of nanoporous structures, towards better quantifying the true stress during the deformation.

*Speaker

Fabrication and characterization of graphene reinforced Al-6Zn-2Cu-2Mg based functionally graded materials

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Abstract

Composite materials adequately fulfill the requirements of industrial applications, but with the development of modern technology, functionally graded materials (FGMs) are gaining importance to meet changing customer expectations. The quantity and arrangement of reinforcement material exhibit variations from the innermost to the outermost region in FGMs, leading to constantly changing characteristics and a non-uniform microstructure Aluminium (Al) alloys are extensively utilized in various industries owing to their desirable characteristics, including superior stiffness, ductility, a high strength-to-weight ratio, and resistance to corrosion. In this study, few-layered nano graphene (FLG) produced by the electric arc discharge (EAD) method was reinforced with Al-6Zn-2Cu-2Mg alloy powders by mechanical alloying (MA) in various amounts of 0, 0.1, 0.2, 0.3, 0.5, and 0.7 wt.%. The FGMs designed according to the increasing content of FLG were shaped by stacking powders in six layers and subjected to sintering at 600∘C for 3 hours. The hardness value (HV) of these FGMs increased by approximately 39.13% as the FLG content between layers increased from the first layer to the last layer. With the presence of FLG content in each layer, grain size reduction can be said to be the most effective strengthening mechanism for FGM. A strong interface bond formed between FLG and matrix increases the load transfer and reinforcing effect of graphene. Furthermore, the X-ray diffraction (XRD) study and transmission electron microscope (TEM) images of FGM reveal a uniform distribution of the aluminum carbide (Al4C3) phase, which plays a role in facilitating the transfer of load from the matrix.

*Speaker

Nanoindentation Ontology: Harmonising knowledge and data for nanoindentation

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[3]Università degli Studi Roma Tre – Italy

Abstract

In the field of nanoindentation, a critical challenge has been the lack of standardized terminology and data interpretation frameworks, hindering effective collaboration and replication of experiments across different laboratories. To address this, in this work a Nanoindentation ontology has been developed, offering a structured knowledge framework that not only facilitates the exchange of information but also supports the semantic documentation of experiments in an interoperable manner. Central to this ontology is the establishment of a widely accepted taxonomy for nanoindentation, which delineates a clear and organized classification of concepts, processes, and entities within this domain, from sample preparation to postprocessing procedures. Conceived as part of the NanoMECommons European project, the CHAMEO ontology endeavors to harmonize the protocols used in characterisation studies. Rooted in the CHAMEO framework, the Nanoindentation ontology leverages a unified language and approach to data management, established by the CEN Workshop Agreement (CWA 17815) and the Characterisation Data (CHADA) documentation scheme. This framework is meticulously crafted to encapsulate the shared elements found across a spectrum of characterisation methods. Its design allows for the strategic development of specific ontologies tailored to individual methodologies through the thoughtful adaptation and refinement of CHAMEO's core components. This endeavor is a key component of the European Materials Modelling Council's (EMMC) ambitious initiative to forge a network of interconnected materials modelling ontologies, all anchored by the foundational principles of the Elementary Multiperspective Material Ontology (EMMO).

*Speaker

Metadata for Micromechanical Testing

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Abstract

FAIR data has emerged as one of the key topics not only to make science more open and reproducible, but also to enable data-driven technologies and AI-based methods.
A key challenge is to augment the data captured from the scientific instruments, often stored in proprietary and binary file-formats, with meaningful metadata that describe the content of the file, as well as additional details about the samples analysed, the conditions the experiment was conducted in, etc. Using the example of nanoindentation, the poster is intended as the starting point for interactive discussions to exchange ideas, find and streamline common terminology that can be used across the community to enable not only sharing data across institutions, but also building common tools and analysis procedures.

*Speaker

Hand written notes to electronic notebooks - a beginer's guide to data management

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Abstract

The new hot topic in research is not what you do, but if and how you share your data. In order to properly share our data, we need a way to easily translate our hand written notes into machine readable electronic notebooks. While this sounds easy, it requires everyone using a specific technique to use the same vocabulary and defined meta data. A possible set of machine readable metadata translated from hand written notes will be presented for nanoindentation experiments. Input from other nanoindenter users is desired and to illustrate to that sharing data electronically is not as scary as it sounds.

*Speaker

Micromechanical Modeling of Graphene Platelets Based Nanocomposites

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Abstract

In the literature, much work has been done to model graphene nanocomposites by molecular dynamics or microscale simulations. Most of these studies are limited to the evaluation of the elastic stiffness. However, investigation of the viscoelastic and viscoplastic stress-strain response at larger strains is lacking. This study presents a microscale approach to simulate the stress-strain response of graphene nanocomposites subjected to large deformation, by considering the interfacial interaction between the filler and the matrix. A multiscale framework for the viscoelastic-viscoplastic response of platelets like inclusions reinforced nanocomposite materials is presented. The Mori–Tanaka homogenization scheme is utilized to explore the macroscopic properties of graphene-reinforced composites and an effective modulus definition is implemented into the Cooperative-viscoplastisity theory based on overstress (VBO) model. For the visco-plastic deformation, Takayanagi averaging approach is used. Numerical simulations are conducted on graphene platelet-reinforced epoxy nanocomposite for several design parameters. Stress-strain behaviors of these materials under compression are simulated and depicted by comparing the experimental data in addition to relaxation behavior at different strain levels.

*Speaker

Hybrid microscale 3D metal-ceramic metamaterials combining high strength and ductility

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Abstract

The architecture of metamaterials enables their remarkable structure-property relationships that surpass those of classical engineering materials. In this work, microscale metal-ceramic metamaterials were created by combination of template assisted electrodeposition and atomic layer deposition (ALD). Polymeric molds were created by two photon lithography and filled with Nickel using electrodeposition. After removing the polymer using plasma etching, the Nickel architectures were coated with Al2O3 by ALD. Micromechanical testing inside a scanning electron microscope showed that the ceramic coating leads to a significant enhancement in strength while preserving ductility. Synchrotron nanoCT imaging of as deposited samples allowed us to investigate the distribution of defects and geometric imperfections inside the architectures, while the study of compressed specimens revealed delamination of the AL2O3 layer preventing crack propagation into the metal lattice. Transmission electron microscopy and Transmission Kikuchi Diffraction highlighted the deformation mechanisms of the metal lattice at the atomic scale including stress-induced densification of dislocation networks, creation of nano-twins, and localized grain refinement. Finite element analysis was employed to study stress distribution in the architectures and study the effects of stress sharing between the phases. The combination of these mechanisms working at different length scales enabled the metamaterial to feature both high strength and ductility. Our multiscale analysis spanning from the atomic to the component level allowed us to identify the deformation mechanisms and their respective contributions to the apparent structural behavior. This opens up pathways towards the future design of metamaterials for various applications from impact mitigation for MEMS devices to functional biomaterials.

[*]Speaker

Imaging defects in Nanocrystals using Coherent Diffraction Imaging

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Abstract

We investigate the mobility of defects inside platinum nanoparticles during in-situ and ex-situ thermal annealing up to 950 ∘C.
Introduced defects were nucleated in tenth of particle specimens using either pre-indentation with an atomic force microscope (AFM) or pre-compression with a flat punch or indentation with a cube corner. A pre-Imaging of the particles was performed using Bragg-Coherent-Diffraction-Imaging (BCDI) which provides the 3d deformation of the initial particles.

Ex-situ compression experiments were conducted using Femtotools under displacement control, enabling real-time monitoring of the deformation process via force-displacement curves. The applied force varied between 10 μN and 2000 μN, resulting in a statistical distribution of deformation behaviors. Some particles experienced elastic deformation, while some others exhibited several dislocation avalanches. For particles that experienced excessive dislocation avalanches, were measured but not easy to reconstruct as they are too deformed, in this case a line profile analysis has been conducted.
The evolution of the three-dimensional out-of-plane strain was inferred for several particles, revealing strain relaxation as temperature increased. In certain particles exhibiting defects, the annealing-induced thermoelastic strain was substantial enough to visualize defect mobility. Different behaviors were observed depending on the particles and the location of defects. Nevertheless, a sharpening of the Bragg peak was observed for all particles as temperature increased.

*Speaker

Recycled HDPE: An investigation on CDs contribution to improve mechanical performance

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Abstract

Over the last decades, plastic usage has grown exponentially, becoming an integral part of society. New strategies, based on the incorporation of carbon-based nanoparticles has been proposed to create high-tech nanocomposites with improved mechanical properties.(1) In this study, different concentration of carbon dots (CDs) were explored as reinforcing agents of high-density polyethylene (HDPE). The developed nanocomposites were subjected to a detailed structural characterization, differential scanning calorimetry analysis (DSC), X-Ray diffraction analysis (XRD) and photoluminescence analysis. The XRD and DSC characterization revealed that no significant changes in the crystallographic structure or physical properties of the polymer occurred. Additionally, the optical analysis confirmed the presence of CDs due to a clear quenching of the polymers' emission intensity throughout the visible spectrum, maintaining the characteristic band of the HDPE. The mechanical properties of the nanocomposites were obtained by strain-stress analysis and nanoindentation. An increase in tensile strength (7%) and yield strength (9%) until a CDs load of 0.5% was observed, after that there is no increase and agglomeration becomes a problem. The recycled CDs reinforced composites were further characterized to evaluate the influence of CDs after each recycling step, showing improved tensile strength and yield strain for 0.5% m/m. In conclusion, it was observed that the incorporation of CDs in the HDPE matrix improved the mechanical properties after each recycling cycle (maximum 3 cycles were tested). These preliminary results are highly relevant as they have the potential to substantially enhance the life-cycle of HDPE, leading to significant economic and environmental impact to society.

*Speaker

VISCO-ELASTIC PROPERTIES OF THE POLYMER NANOCOMPOSITES

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Abstract

The visco-elastic properties of the polymer/graphene nanoribbons were investigated by dynamical mechanical thermal analyzer yielding values of the storage modulus, and tan δ (ratio of loss and storage modulus) as a function of temperature for the nanocomposites with varying filler loading (0.2–3 wt. % GNRs with respect to the polymer).
The storage modulus refers to the stiffness of the material and the loss or viscous modulus is related to the energy lost due to viscous dissipation. The ratio between the loss and storage modules, known as tan δ or damping factor, is strongly related to the relaxation behavior of the polymer chains at the interphase in nanocomposites. Hence, tan δ provides information to estimate the bonding between the polymer matrix and graphene nanoribbon. The incorporation of GNRs and increasing their content into the polymer matrix result in increment in the storage modulus. In the glassy state, the storage modulus of 3% GNR nanocomposite is almost one order of magnitude higher than that of the neat polymer. This means very important enhancement of the thermal properties of the nanocomposites and can be associated to the intercalation of the polymer chains and GNRs, which remarkably increases the stiffness of the material. For all nanocomposites, an increase in the glass transition temperature was observed suggesting that important interactions between the graphene nanoribbons and the polymer were achieved.
These results lead to the conclusion that materials with strong covalent bonds between the phases of the nanocomposites and improved mechanical and thermal properties have been synthesized.

*Speaker

Mechanical Properties of MiniBars™ Basalt Fiber-Reinforced Geopolymer Composites for Buildings Applications

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Abstract

Fly ash-based geopolymers represent a new material, which can be considered an alternative to ordinary Portland cement. MiniBars™ are basalt fiber composites, and they were used to reinforce the geopolymer matrix for the creation of unidirectional MiniBars™ reinforced geopolymer composites (MiniBars™FRBCs). New materials were obtained by incorporating variable amount of MiniBars™ (0, 12.5, 25, 50, 75 vol.% MiniBars™) in the geopolymer matrix. Geopolymers were prepared by mixing fly ash powder with Na2SiO3 and NaOH as alkaline activators. MiniBars™ FRBCs were cured at 70 ∘C for 48 h and tested for different mechanical properties. Optical microscopy and SEM were employed to investigate the fillers and MiniBars™ FRBC. Mini-Bars™ FRBC showed increasing mechanical properties by an increased addition of MiniBars™. The mechanical properties of MiniBars™ FRBC increased more than the geopolymer wtihout Mini-Bars™: the flexural strength $>$ 11.59–25.97 times, the flexural modulus $>$ 3.33–5.92 times, the tensile strength $>$ 3.50–8.03 times, the tensile modulus $>$ 1.12–1.30 times, and the force load at upper yield tensile strength $>$ 4.18–7.27 times. SEM and optical microscopy analyses were performed on the fractured surface and section of MiniBars™ FRBC and confirmed a good geopolymer network around Mini-Bars™. Based on our results, MiniBars™ FRBC could be a very promising green material for buildings.

*Speaker

Mechanochemical synthesis of Zn bionanohybrids with esterase-like and catalase-like activity

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Abstract

The mechanochemical synthesis of nanomaterials for catalytic applications is a growing research field due to its simplicity, scalability, and eco-friendliness. In this work we have developed the synthesis of new zinc bionanohybrids by a mechanochemical method that can enhance the enzyme-like activities of the catalysts synthesized in aqueous medium. For this purpose, *Candida antarctica* Lipase B (CAL-B) enzyme was used as a scaffold, which is added to a zinc salt using a neutral-alkaline medium of sodium phosphate (pH 7) or sodium bicarbonate (pH 10) at room temperature by means of a "ball milling technology" method. Mechanochemical synthesis successfully produced smaller structures compared to the aqueous bionanohybrid and catalytic tests showed that the use of this technique resulted a very large improvement in their catalytic performance. **Mechano Zn@BIC** turned out to have up to 4 times more specific activity in the *p*NPP hydrolysis assay than the bionanohybrid synthesized in aqueous media. On the other hand, catalase assay for **Mechano Zn@PHOS** was up to 2000 times greater than the value obtained for the aqueous bionanohybrid. Therefore, the synthesized Mechano Zn bionanohybrids have mimetic esterase-like and catalase-like activities.

*Speaker

Micro-scale investigation of deformation mechanisms in biodegradable Zn alloys

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Abstract

Zn alloys are emerging as promising candidates for temporary biodegradable metallic implants, such as bone-fixing plates or cardiovascular stents, due to their biocompatibility and degradation properties. However, the relatively low mechanical strength of conventional Zn alloys has historically led to limited research interest in the deformation mechanisms of fine-grained Zn alloys. This poster will focus on exploring these mechanisms, particularly highlighting the impact of solid solution strengthening and the size effect as observed through micro-pillar compression tests. We will also delve into the role of grain boundary sliding and slip system activity in the superplasticity of bulk Zn alloys, with these phenomena being studied across a broad spectrum of strain rates using a combination of EBSD-SEM-AFM techniques and nanoindentation strain rate jump tests. The investigation conducted provides comprehensive insights into the effectiveness of solid solution strengthening, second-phase strengthening and the primary deformation mechanisms in fine-grained Zn alloys at room temperature. The most important results are grain boundary sliding-controlled deformation in tension, high strain rate sensitivity in fine-grained alloys regardless of heat treatment, and low non-basal dislocation slip systems activity.

*Speaker

Statistical failure of Ag penta-twinned nanowires with varying cross-section width

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Abstract

Molecular dynamics (MD) simulations of Ag penta-twinned nanowires with varying cross-section width have been tensile tested to understand the statistical deformation behavior and failure strain. MD simulations show that the yielding through the nucleation of Shockley partial dislocations in Ag penta-twinned nanowires. However, the nucleation site of these dislocations varies with the nanowire cross-section width: from the interface between the twin boundary and surface in nanowires with lower cross-section widths, and from the nanowire surface in nanowires with larger cross-section width. Following yielding, the deformation proceeds through the formation of stacking faults hats (SFH) and stacking fault decahedrons (SFD). Finally, the evolution of the microstructure leads to necking and failure. The stochastic evolution of the microstructure leads to different interactions, and sometime voids formation at the center of the nanowire, which results in a distribution of strains to failure. We discuss this distribution in terms of the competition between the microstructural mechanisms during deformation, and how they are related to the cross-section width.

*Speaker

In situ nano-mechanical studies of single-crystal ZnO nanowires

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Abstract

Piezoelectric semiconductor nanowires (NWs) have been investigated as building blocks for various energy transducing applications including mechanical energy harvesting (1), sensors (2) and piezotronic devices (3). Piezoelectricity couples mechanical and electrical state in crystalline materials with no inversion symmetry, *i.e.*, the application of mechanical strain results in generation of electrical charge and vice versa. The effective piezoelectric coefficient was suggested to increase with decreasing NW diameter, enhancing the conversion efficiency of mechanical-to-electrical energy making NWs promising candidates for future mechanical energy transducers (4).
Nanostructures have also been shown to exhibit yield strengths reaching the ultimate limit of the respective material, thus offering increased elastic strain that can eventually be converted into electricity by electromechanical coupling. Furthermore, while many semiconductors are brittle at room temperature, they may become ductile at ambient conditions below a critical size (5).

Here, we report on *in-situ* Laue microdiffraction of three-point bent ZnO NWs mechanically loaded up to catastrophic fracture failure representing the maximum strain that could potentially be converted into electrical energy by piezoelectricity. Plasticity was evidenced for some NWs by the splitting of Laue spots and confirmed by scanning and transmission electron microscopy.

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*Speaker

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Characterization and Optimization of Silver Wire Drawing Process for Jewelry Making

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Abstract

Trabzon is famous for its handcrafted golden and silver wire jewelry. It is made of hand-knitted silver or golden wires obtained through a series of manufacturing steps. The process starts with the casting of silver with the addition of copper and brass to increase the formability. Molten silver is then poured into cavities in bar form. Then, the bars10x10 mm2 in its cross-section undergo a series of rolling processes with a decrease in their thickness while their lengths increase. Upon the 20th steps of rolling, the cross-section is reduced to 3x3 mm2. A heat treatment is applied for the work-hardened material to continue rolling of wires. After 38th steps, the rolling process is completed and the wire are coiled onto a roller, and another heat-treatment, and surface cleaning are applied before wire-drawing process. Silver wire 1.2 mm in diameter is reduced to 0.32 mm through 13 steps. One more heat treatment is carried out for the wires and it is cooled in air. Then the wires are made ready for the hand-knitting process. As it can be noted, silver wire drawing process is a multi-step and tedious process. This study aimed to characterize and optimize the silver wire drawing process for consistent workability in hand-knitting and improved surface quality. As the conventional mechanical testing tools are not appropriate to characterize the mechanical properties at different stages, nanoindentation along with microstructural examinations are used for characterization. To this goal, 8 critical steps are determined and investigated through a series of nanoindentations.

*Speaker

Simulation of mechanosensitive ion channels in nano scales to study urinary incontinence

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Abstract

During the period of urine storage, the act of mechanical stretching serves to activate the smooth muscle of the urinary bladder, and any deviation might result in urine leakage or urinary incontinence. Nevertheless, the understanding by which mechanical stimuli stimulate the bladder at the nanoscale is limited. This paper examines a theoretical framework for the simulation of mechano-electrical feedback in mechanosensitive ion channels, encompassing both cellular and tissue-level analysis. These modules also investigate the impact of stress on the electrophysiology of smooth muscle and the modulation of tissue conductivity by strain. The mechano-sensitive ion channels are represented using Hodgkin and Huxley formalisms, which incorporate ordinary differential equations to describe the transmembrane voltage and ion currents across the membrane. The obtained results demonstrate the conduction velocity of smooth muscle that is controlled by tension. The determined parameters included the resting voltage, action potential duration, maximal upstroke velocity, and conduction velocity. The simulations effectively replicated various phenomena that have been documented in experimental studies, including the positive strain resting voltage, negative strain-maximal upstroke, and a biphasic strain-conduction velocity relationship. Increasing the stimulus frequency resulted in decreased upstroke and conduction velocity for significant stresses. The observed effects are correlated with a decrease in membrane potential. We have introduced a computational approach for investigating the processes and effects of smooth muscle. The framework has the potential to be utilized in the modeling and simulation of ion channels, cells, and tissue, which are represented as mono- and bidomains ranging from one to three dimensions.

*Speaker

The Effect of Crystalline Properties on Catalytic and Magnetic Performance: Hybrid PtAuFe Nanostructures for Green Energy

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Abstract

In recent years, the increase in greenhouse gases, environmental damage caused by fossil fuels, and the high energy demand resulting from population growth have underscored the importance of environmentally friendly energy sources. In this context, hydrogen evolution reaction (HER) and oxygen reduction reaction (ORR) catalysis for fuel cells, facilitated by nanostructures (NSs), have emerged as significant endeavors with the potential to mitigate the reliance on fossil fuels. Our study aims to enhance the catalytic and magnetic properties of recyclable multifunctional PtFe, PtAu, and PtAuFe NSs for hydrogen fuel technology. The crystal structure of the NSs was determined using X-ray diffraction (XRD) and Rietveld Refinement analysis, confirming the face-centered cubic (FCC) structure with space group fm-3m. SEM images revealed an average particle size of 10 nm for the NSs. Electrochemical properties were investigated through the recording of linear sweep voltammetry (LSV) and cyclic voltammetry (CV) curves to assess HER and ORR reactions pertinent to hydrogen fuel technology. The PtAuFe NSs exhibited the best specific activity below -1 V (vs. Ag/AgCl). Furthermore, the magnetic properties of PtFe, PtAu, and PtAuFe NSs were examined via magnetization-temperature (M-T) and magnetization-field (M-H) curves. PtFe and PtAuFe NSs demonstrated high saturation magnetization above 10 emu/g at room temperature, facilitating the recovery of NSs from solution using a magnet. The relationship between structural properties and catalytic and magnetic results was thoroughly investigated. This research was supported by funding from Cukurova University, Adana, Turkey, under Scientific Research Funding Grant Numbers FBA-2023-15712.

*Speaker

Transformation-induced plasticity (TRIP) in Ce-stabilized zirconia: an in situ approach coupling pillar micro-compression, Laue micro-diffraction and electron microscopy.

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Abstract

Zirconia (ZrO2) is widely recognized for its ability to undergo a martensitic phase transition from the tetragonal (t) phase to the monoclinic (m) phase, through thermal and/or mechanical stresses. This transformation is characterized by a volumetric expansion (_˜5%), which hinders crack propagation, strongly increasing its toughness. Various dopants can be used to stabilize the tetragonal phase down to room temperature (1). In this work, the transformation-induced plasticity (TRIP) effect is investigated in ceria-stabilized zirconia (CSTZ). Compared to yttria-stabilized zirconia (YSZ), which is better-known, stabilization with ceria reduces the critical stress value required for t-m phase transformation, allowing the transformation to occur prior to crack propagation. It further enhances toughness compared to conventional ceramics (1,2). In addition, CSTZ are more resistant to low-temperature degradation, compared to YSZ.

In this work, the TRIP effect is studied at the local-scale by means of *in situ* pillar micro-compression (FT-NMT04) coupled either with Laue micro-diffraction (BM32 beamline at ESRF) or with scanning electron microscopy (FEG-SEM XL30). Single-crystal micro-pillars are extracted from 12% Ce-doped ZrO2 grains with various crystallographic orientations by FIB micromachining. The t-m transformation is followed in real time during the mechanical deformation and is correlated to significant load drops on the mechanical curves. Furthermore, the crystallographic path for this transformation, and in particular the orientation relationships between the tetragonal and the monoclinic phases, are accessed through Laue diffraction, and compared to the crystallographic theory of the martensitic transformation.

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*Speaker

Unveiling Crystal Deformation: Integrating EBSD and FEM Simulation for Elastic Strain Analysis

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Abstract

This study presents experimental measurements of elastic deformation made using the EBSD technique collated together with FEM simulations. Two examples are presented in the study. The first is a Vickers indentation in monocrystalline silicon. In the second example, EBSD measurements were performed in-situ in a scanning electron microscope during indentation. In this case, however, the measurements were carried out not on the sample in which the indentations were made, but on the silicon sensor of the nanoindenter, which was undergoing elastic strain. Elastic strain measurements were performed by fitting dynamical EBSD simulations to experimental patterns, taking into account not only crystal rotation but also elastic deformation. FEM simulations were performed for both examples, which proved to largely reflect the experimental results.

*Speaker

Yield criteria of additively manufactured body-centered cubic lattice structures

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Abstract

Lattice structures are gaining increasing popularity, owing to their superior mechanical properties per weight. Modelling these structures is computationally demanding, and homogenizing their mechanical response is a promising approach to model nanoporous specimens. While attention is paid to the elastic response, the yield surface is less discussed, especially in multi-axis loading conditions. In this study, we consider body-centered cubic (BCC) lattice structures as an example and explore yield criteria for a homogenized model. We firstly developed an analytical yield surface, based on the assumption that macroscopic yield/collapse happens when the plastic hinge formulates across the entire cross-section of circular struts. Then, using finite element modelling (FEM), we simulated various loading conditions (uniaxial compression, simple shearing, proportional bi- and tri-axial loadings), and defined the yield states based on the principle of equivalent plastic work. We explored various yield criteria including the Deshpande-Fleck (DF) model, widely discussed for foams. In principal stress space, the yield surface is a closed, elliptical-like shape, with the main axis along the mean stress direction. The analytical model predicts very well in hydrostatic compression (the struts are subjected to pure compression). But it will lose accuracy of predicting the yielding in other loading conditions. The DF model, while having a good ability of predicting yielding in bi-axial loadings, overestimates in tri-axial loadings, as also found by others when homogenizing the mechanical response of nanoporous gold. Finally, we developed a model that captures the FEM results in all loading conditions.

*Speaker

Machine Learning-Driven Prediction of Elastic Modulus in Clay-Reinforced Polymer Nanocomposites

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Abstract

Clay-reinforced polymer nanocomposites, particularly those incorporating Montmorillonite-based clays, have garnered significant attention for their potential to enhance mechanical properties in various engineering domains. These nanocomposites are pivotal in the automotive industry, aerospace, civil engineering, biomedical devices, and electronics, where material robustness and lightweight characteristics are crucial. Even though, state of the art includes numerous experimental analyses of various clay-reinforced nanocomposites, a comprehensive, data-driven analysis focusing on the elastic modulus of these nanocomposites, particularly from a multi-scale perspective of their mechanical behavior, remains largely unexplored.

To assist nanomechanical researchers in this respect, this study focuses on harnessing machine learning techniques to predict the elastic modulus of polymer nanocomposites embedded with clay nanoparticles through the classification of key factors. By avoiding the need for extensive experimental procedures, this approach aims to streamline the material development process. Our methodology involves a comprehensive analysis of state-of-the-art studies. Key factors in our predictive model include the polymer matrix elastic modulus values, the size of Montmorillonite silicate layers, and the concentration of clay within the nanocomposite.

Through this research, we aim to provide a classification-based machine learning approach for engineers and researchers to anticipate the mechanical performance of clay-reinforced polymer nanocomposites, thereby facilitating more efficient material selection and design in a wide range of applications.

*Speaker