COST Action MecaNano General Meeting 2025

19-21 May 2025, AGH University of Krakow, Poland

Academic Centre for Materials and Nanotechnology, Kawiory 30, 30-055 Krakow, Poland

Local organizers: Wiktor Bednarczyk (bednarczyk@agh.edu.pl), Grzegorz Cios, Piotr Bała, Anna Smyk

Monday, May 19th	
13:00	**Welcome reception**
14:00	**Opening talk**
Chairman: Marie-Stéphane Colla	
14:10	**Keynote Talk - Urszula Stachewicz, *AGH University of Krakow, Poland***
	Structure-properties relationship in electrospun polymer and composite fibers
14:50	**Aleksija Djuric, *University of East Sarajevo, Bosnia and Herzegovina***
	Influence of Adhesive Type on the Tensile-Shear Strength of CFRP-DP500 Steel Joints
15:10	**Sophie Vanpee, *UCLouvain, Belgium***
	Nanoindentation Analysis of individual phases in model Carbon Fiber-Reinforced PEEK composite
15:30	**Johanna Byloff, *EMPA - Swiss Federal Laboratories for Materials Science and Technology***
	Thin Film Interface Engineering using Atomic Layer Deposition: Improved Electromechanical Properties and Adhesion
15:50	**Coffee break**
Chairman: Julien Guénolé	
16:20	**Francesco Maresca, *University of Groningen, Netherlands***
	Multi-scale modelling of fracture from atomistics to micromechanics
16:50	**Laurent Pizzagalli, *Institut Pprime, l'Université de Poitiers, France***
	Molecular dynamics calculations of the mechanical properties of nanopillars made of pyrocarbons
17:10	**Konrad Perzynski, *AGH University of Krakow, Poland***
	Prediction of crack evolution in thin films and coatings based on the digital material representation concept
17:30	**Ashish Chauniyal, *Ruhr University Bochum, Germany***
	Using data-based methods for microstructure characterization
17:50	**Bal Burak, *Abdullah Gül University, Turkey***
	Molecular dynamics based mobility laws
18:10	**Social networking**

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Tuesday, May 20th	
Chairman: Benoit Merle	
9:00	**Marc Legros, *CEMES-CNRS, Toulouse, France***
	In situ TEM straining: old tricks and new artefacts. An intrinsically small-scale testing method
9:30	**Vivek Devulapalli, *EMPA - Swiss Federal Laboratories for Materials Science and Technology***
	Fracture behaviour in Cu-Al multilayer thin films with amorphous AlO interlayers: Insights from in-situ TEM tensile testing
9:50	**Pierre Godard, *Institut Pprime, Université de Poitiers, France***
	[110] tensile testing of single crystalline gold thin films with nanotwins: in situ TEM and XRD studies
10:10	**Luke Hewitt, *United Kingdom Atomic Energy Authority, United Kingdom***
	In-situ strain measurement of micro-mechanical specimens using DIC
10:30	**Tijmen Vermeij, *EMPA - Swiss Federal Laboratories for Materials Science and Technology***
	In situ Transmission Kikuchi Diffraction (TKD) Tensile Testing
10:50	**Coffee Break**
Chairman: Maria Wątroba	
11:20	**Martina Freund, *RWTH Aachen, Germany***
	Plasticity of Ca-Mg-Al C14 and C15 Laves Phases and its Temperature and Chemistry Dependency
11:50	**Sang-Hyeok Lee, *RWTH Aachen, Germany***
	Dislocations in Laves phases: Atomistic Mechanisms of Motion and Reaction
12:10	**Kamila Hamułka, *EMPA - Swiss Federal Laboratories for Materials Science and Technology***
	Strain rate dependence of slip vs. twinning in c-axis compression of α-titanium
12:30	**Hannah Howard, *University of California, Santa Barbara, USA***
	Dislocation-localized phase evolution in FCC alloys and the resulting dislocation mechanics evaluated by spherical nanoindentation
12:50	**Stefan Zeiler, *Montanuniversität Leoben, Austria***
	A versatile electrochemical charging cell for studying hydrogen-related effects in materials
13:10	**Lunch break (organized locally)**
Chairman: Xavier Maeder	
14:40	**Edoardo Rossi, *Università degli Studi Roma Tre, Italy***
	Decoding Microstructures: Machine Learning for High-Speed Nanoindentation Mapping
15:10	**Pedro Camanho, *University of Porto, Portugal***
	Physically recurrent neural networks for micromechanical analyses of composite materials undergoing plasticity and distributed damage
15:30	**Laia Ortiz-Membrado, *Universitat Politècnica de Catalunya, Spain***
	Deep Learning Mechanical Properties Classification of Metal-Ceramic Composites Using Nanoindentation Curves
15:50	**Ruomeng Chen, *Forschungszentrum Jülich, Germany***
	Understanding microstructure-property correlation of pearlitic steel by nanoindentation and machine learning-based modeling
16:10	**Hanna Szebesczyk, *Wrocław University of Science and Technology, Poland***
	Application of high-throughput materials science methods for rapid screening and optimization of ultra-strong light-weight alloys for automotive
16:30	**Coffee break**
16:50	**Poster session**
19:00	**Official Dinner (Paid separately) - *Klub Studio, Witolda Budryka 4, 30-072 Kraków, Polska***

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Wednesday, May 21st	
Chairman: Marc Legros	
9:00	**Bo-Shiuan Li, *National Sun Yat-sen University, Taiwan***
	Small-Scale Mechanical Testing of Semiconductor Materials
9:30	**Roozbeh Neshani, *UCLouvain, Belgium***
	Lab-on-a-chip nanomechanical study of annealing and stress-induced grain growth effects on plasticity and time-dependent deformation in sputtered Pt thin films.
9:50	**Muhammad Muzammil, *Koç University, Istanbul, Turkey***
	MEMS Platforms for Automated and High-Throughput Micromechanical Testing of Silicon Nanowires
10:10	**Gaurav Mohanty, *Tampere University, Finland***
	High strain rate nanoindentation up to 10,000/s and associated deformation mechanisms
10:30	**Hannah Lichtenegger, *Montanuniversität Leoben, Austria***
	Hardness values as a function of the degree of deformation for tungsten and doped tungsten fine wire
10:50	**Coffee Break**
Chairman: Grzegorz Cios	
11:20	**Fatima-Zahra Moul-El-Ksour, *École Centrale de Lyon, CNRS, France***
	High Temperature Scanning Indentation: Latest Results On Amorphous Selenium
11:40	**Francesc Barbera Flichi, *Universitat Politècnica de Catalunya, Spain***
	Small scale deformation of cemented carbides at high temperature
12:00	**James Gibson, *United Kingdom Atomic Energy Authority, United Kingdom***
	Irradiation Hardening in Advanced Reduced Activation Ferritic-Martensitic Steels for Future Fusion Applications
12:20	**Chunli Wu, *Technion - Israel Institute of Technology, Izrael***
	The Effect of Oxidation on the Compressive Strength of Ni Nanoparticles: a Nano-Mechanics Perspective
12:40	**Anastasiia Walrave, *Aix Marseille Université, CNRS, Marseille, France***
	Small-Scale Plasticity in ZnO: Combined Experimental and Computational Insights
13:00	**Lunch - The end of the Meeting**

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Poster list		
Poster session: Tuesday 16:50		
1	Mohammed Tahir Abba	Toward High Strain Rate Spherical Nanoindentation Testing
2	Fabien Amiot	Second strain-gradient elasticity for centro-symmetric cubic materials
3	Muhammet Anıl Kaya	Mechanical Characterization of Hazelnut Shell Powder-Reinforced Epoxy Composites for Sustainable Applications
4	Tizian Arold	Nitrogen-Doped PVD MoS2 Coatings: Enhanced Wear Resistance and Tribological Performance in Rolling-Sliding Contact
5	Saulius Baskutis	Investigation of the Potential of PTFE Coatings for Journal Bearings
6	Samuel Bojarski	High-strength and non-brittle crystalline-amorphous PVD-ALD nanolaminates of amorphous alumina and AlCoCrFeNi high-entropy alloy
7	Jaroslav Cech	Nanoindentation study of NiTi shape memory alloys
8	Grzegorz Cios	Orienting grains for nanomechanical testing without EBSD
9	Özgen Ümit Çolak Çakır	Machine Learning in Thermoset Polymer Creep Modeling
10	Diego Cruañes	Understanding nanoindentation statistical dispersion in ceramic - metal cemented carbides by numerical simulation and FIB tomography
11	Arjun Bharath Curam	Defect-driven microstructural evolution and mechanical characterization of CoCrNi, Fex(CoCrNi)100-x and CoCrNi/Fe nanolaminate complex compositional alloy thin films
12	Miljan Dašić	Selecting Protein Crystal Structure for Optimal Scoring of Protein-Ligand Interactions
13	Emine Özlem Dengiz	Investigation of the Mechanical Behavior of Graphene-Reinforced Magnesium via Experimental and Finite Element Method
14	Cengiz Görkem Dengiz	Investigation of the Mechanical Behavior of Graphene-Reinforced Magnesium via Experimental and Finite Element Method
15	Oğuzhan Der	Quantitative Analysis of Nanoscale Mechanical Behavior in Hybrid Materials Through Nanoindentation and FEM Simulations
16	Francisco Javier Dominguez–Gutierrez	Nanoindentation and Defect Dynamics in Irradiated Fcc NiFe Alloys: Insights from Experiments and Atomistic Modeling
17	Marco Ezequiel	Suppressing shear band instability for strong and ductile crystal/glass nanolaminates
18	Lala Gahramanli	Analysis of the physical properties of CdxZn1-xS-based nanocomposites synthesized through sonochemical and SILAR methods
19	Julien Guénolé	Interfaces as dislocation density fields for bridging length scales in nanomechanics
20	Amine Haj Taieb	Review of Auxetic properties of textile structures
21	Evghenii Harea	Comparative Analysis of the Gao-Nix Model and Multifractal Scaling Law Model for Indentation Size Effect
22	Petr Hausild	Temperature and strain rate dependent indentation size effect at shallow indentation depths
23	Benedykt Jany	Integrating Machine Learning and Data Mining Techniques with Surface Texture Analysis to Explore Wetting and Optical Properties of CuAg Alloys
24	Piotr Jenczyk	Modification of the matrix-reinforcement interface in Ni-SiC composites

25	Cihan Kaboglu	Investigation of Mechanical and Physical Properties of Polyphenylene sulfide (PPS) Matrix Composite Reinforced with GNP and MWCNT
26	Tomas Kacinskas	Investigation of the Potential of PTFE Coatings for Journal Bearings
27	Hesam Khaksar	A comparative study on the nanotribological properties of amorphous and polycrystalline forms of MoS2 using Nano-Indenter and AFM.
28	Rana Khankishiyeva	Effect of Chitosan Particle Size on the Mechanical Performance and UV Degradation of Low-Density Polyethylene-Chitosan Composites
29	Philipp Kroeker	In-Situ TKD Tensile Testing Reveals Complex Nanoscale Deformation Twinning in Rhenium
30	Valeria Lemkova	Scale-Bridging Nanoindentation to Probe Structural Heterogeneity in Amorphous Metals
31	Feitao Li	Room-temperature recrystallization of Mo induced by nanoindentation
32	Xavier Maeder	Metal-Ceramic Nanolaminate Design for Enhanced Thermal and Mechanical Properties
34	Lukasz Maj	Micro-mechanical evaluation of coatings produced by micro-arc oxidation of titanium
35	Bakhtiyar Mammadli	Prediction of Mechanical Properties using DIC analysis and Machine Learning
36	Sevinj Mammadyarova	Effect of Ag-doping concentration on the structural and optical properties of NiO nanoparticles
37	David Mercier	Unsupervised Machine Learning for Nanoindentation Mapping Analysis and Microstructural Correlation
38	Yannis Missirlis	Regulation of relevant gene expressions in cells and bacteria by dynamic mechanical conditioning
39	Tuğba Mutuk	Hybrid Composite production for Defense Industry
40	Paolo Nicolini	Nanowear in molybdenum disulfide studied by molecular dynamics simulations
41	Olivier Noel	Contact mechanics and tribological properties on polymers: An experimental approach.
42	Krzysztof Pajor	Comparative analysis of plastic deformation in Zr-Cu-Ag metallic glasses: insights from micropillar and bulk sample compression tests
43	Miroslawa Pawlyta	Structure of Ta/TaN nanolayered systems investigated by Transmission Electron Microscopy
44	Tatiyana Petrova	Optimal safety loads and design of polymer nanocomposites under static loading
45	Barbara Putz	Improved thermal stability of Cu nanoparticle thin films via atomic layer deposition
46	Chaofeng Qin	Phase Stability and Mechanical Properties of Cobalt Nanoparticles
47	Monika Rejek	Advanced characterization of metal-oxide-metal interfaces produced by combined ALD/PVD deposition
48	Nicolae Serban	Influence of temperature and impact energy on microstructural evolution and deformability of Inconel 925 nickel-based superalloy
49	Raul Simões	HDPE reinforced with CDs with enhanced processing lifespan and improved recyclability traceability
50	Igor Stankovic	Analytical Modeling of Wear Mechanisms in Nanocontacts: Influence of Applied Load and Material Composition
51	Wolfgang Stein	Advanced tools for G200 nanoindenter: motorized tilt correction stage to optimize flat punch measurement - motorized 8" wafer vacuum chuck allows full size wafer measurement

52	Pavlos Stephanou	Use of non-equilibrium thermodynamics to derive a variable entanglement density constitutive model for entangled polymer melts
53	Mona Stoll	Abusing the Sink-In Coefficient to Quantify Pile-Up in Nanoindentation
54	Aleksandra Szczupak	Colorimetry and Tribology of Ultrapure Copper Micromodification
55	Claus Trost	Unlocking Micromechanical Insights: Explainable Machine Learning and Feature Engineering applied to Nanoindentation Data
56	Ahmed Uluca	2D spherical nanoindentation reveals nanoscale roughness of microscopic contacts
57	Deniz Uzunsoy	Characterisation of Titanium Matrix Composites with Hybrid Reinforcements of Al2O3 and Functionalised Graphene Nanoplatelets
58	Maria Watroba	Microstructure-Property Relationships in Template-Assisted Electrodeposited Zinc Micropillars: A Comparative Study with FIB-Milled Specimens
59	Krzysztof Wieczerzak	Systematic exploration of refractory high entropy alloys using high-throughput techniques and machine learning
60	Zhuocheng Xie	Grain Boundary Segregation Landscape in Mg Alloys: From Solute Decoration to Clustering and Structural Transitions
61	Stanislav Zak	Road to Failure: AFM Indentation of Polymers
62	Sina Zarepakzad	Machine Learning-Driven High-Throughput Analysis of Damping Effects in Silicon-Based Cantilever Resonators with Metallic Coating
63	Wen Zhao	Materials Informatics in Academia: Challenges and Opportunities

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Book of Abstracts

Invited speakers

Oral presentateion

Poster presentations

Structure-properties relationship in electrospun polymer and composite fibers

Urszula Stachewicz*[1]

[1] AGH University of Krakow, Krakow, Poland

Abstract

Electrospinning enables the production of polymer fibers with unique properties by applying an electric field between a nozzle fed with the polymer solution and a counter-electrode. As the jet forms and the solvent evaporates, solid fibers are produced. The electric field not only aligns polymer chains to create supramolecular structures with enhanced mechanical or piezoelectric properties but also reorients functional polymer groups, modifying surface chemistry and potential. Furthermore, nanoparticles or other fillers can be incorporated into the polymer solution to produce composite fibers with synergistic properties, such as improved mechanical resilience or enhanced electrical and thermal conductivity. Advanced characterization techniques, including atomic force microscopy (AFM), Kelvin probe force microscopy (KPFM), piezoresponse force microscopy (PFM), and in situ tensile testing, allow for precise analysis of the structure-property relationships in both individual fibers and fiber meshes. These insights enable the design of fibers with tailored properties for diverse applications, including tissue engineering, drug delivery, and water and energy harvesting.

* Speaker

Multi-scale modelling of fracture from atomistics to micromechanics

Francesco Maresca*[1]

[1] University of Groningen - Netherlands

Abstract

Fracture is a multiscale process that originates from atomic scale debonding, propagates across microstructural features and results into macroscopic failure at the engineering scale. Predicting the nano- and micro-scale mechanisms that control this phenomenon is crucial to addressing technological problems such as hydrogen embrittlement, liquid metal embrittlement and other environmental fracture phenomena. Here, by extending a 2D discrete dislocation dynamics framework, we first show the importance of crack-tip dislocation emission on enhancing fracture toughness in body-centered-cubic (BCC) metals. Next, we focus on the accurate prediction of the competition between emission and crack propagation by atomistic simulations. Modelling crack propagation is beyond reach of quantum-mechanical simulations (e.g. density functional theory, DFT). To overcome this bottleneck while retaining accuracy, we train and benchmark an array of state-of-the-art machine learning potentials (ML-IAPs) for ferromagnetic BCC iron, including the recent Atomic Cluster Expansion potentials. We use uncertainty quantification to assess the DFT-accuracy of the predicted dislocation structures and glide mechanisms, as well as active learning to predict the crack propagation mechanism. The ML-IAP is extended to model embrittlement e.g. due to hydrogen.

* Speaker

In situ TEM straining: old tricks and new artefacts. An intrinsically small-scale testing method

Marc Legros*[1], Frédéric Mompiou[1], Stephan Sandfeld[2], and Daniel Caillard[1]

[1] CEMES-CNRS, 31055 Toulouse – France
[2] Forschungszentrum Jülich, 52425, Jülich - Germany

Abstract

The mechanical properties of metals and alloys are dictated by the individual and collective behavior of dislocations but very few techniques allow to observe them dynamically. In situ TEM straining is among those, and surprisingly, its use has remained rather confidential over the last 6 or 7 decades.

The recent advent of in situ TEM nanoindentation holders in conjunction with the renewed interest in micro-and nanoscale plasticity have shed light on the possibilities of this technique, sometimes at expenses of the legitimate doubts cast on the artifacts linked to in situ methods (sample size, image forces, electron beam interaction…)

Being able to measure a force and a deformation on tiny or complex-shaped samples has also become a stand-alone goal of such in situ studies, often missing the real opportunities that represent a detailed analysis of the dislocation behavior. Here, we will show that such analysis, either using classical elasticity theory or by taking advantage of more recent machine learning can lead to significant advances either in high entropy alloys, pure metals, and revive some old-fashioned metallurgy in small volumes.

* Speaker

Plasticity of Ca-Mg-Al C14 and C15 Laves Phases and its Temperature and Chemistry Dependency

Martina Freund*[1], Zhuocheng Xie[1], Pei-Lin Sun[1], Sandra Korte-Kerzel[1]

[1] Institut für Metallkunde und Materialphysik, RWTH Aachen University – Germany

Abstract

Understanding dislocation motion is essential for predicting materials behaviour and being able to manipulate properties. For standard crystal structures there is plenty of literature on how dislocations move through the lattice and how they can be influenced. For more complex phases there are little known, limited by the fact of its inherent resistance against dislocation motion at ambient temperature due to the topologically closed packed structure. This leads to a huge gap of knowledge regarding the dislocation behaviour below the brittle ductile transition temperature. One of the most common intermetallic phases are the Laves phase coming up to more than 1400 different compounds, for all three prototypes. The fact that these are built with similar building blocks, just slightly rearranged, suggests that the dislocation behaviour is transferable within its prototype, but also between the different prototypes.

We aim to understand the key fundamental principle of the dislocation behaviour of the forming hexagonal C14 CaMg2 and cubic C15 CaAl2 Laves phases and how this is affected by changes in chemistry and deformation temperature. With nanomechanical methods such as nanoindentation and micropillar compression testing, plasticity can be introduced locally and analysed quantitatively by evaluating the resulting slip planes and their activation frequency, and qualitatively by determining the critical resolved shear stress of specific systems. In addition, transmission electron microscopy helps to unravel the plasticity beneath the indentation by determining the dislocation Burgers vectors and confirming the slip planes. A deeper understanding of the dislocation behaviour is gained by varying the influencing factors such as chemistry and deformation temperature.

Mechanical properties, such as hardness and indentation modulus, are found to remain constant for the hexagonal C14 Laves phase in its studied range up to 250°C, but dislocation motion appears to be facilitated by temperature, as indicated by the decrease in the number of serrations with increasing temperature. On the other hand, the change in chemistry, and therefore the deviation from the stoichiometric composition, results in a decrease in hardness and indentation modulus for both Laves phases. In contrast to the macroscopic test above the BDTT the majority of the observed dislocation motion is on the non-basal planes. Especially for the cubic C15 Laves phase additional planes, the {11n}, are found to be the favoured planes for dislocation slip, which seems to facilitate their motion additionally by cross-slipping from one {11n} to another {11n}. Atomistic simulations explaining these motion by calculation the minimum energy paths for these planes.

The analysis of the resulting plasticity at room temperature and that due to changes in deformation temperature and chemistry will lead us to a better understanding of the fundamental principle of dislocation motion in these complex phases. Initial results have provided new insights into possible slip systems, dislocation motion and mechanical properties.

* Speaker

Decoding Microstructures: Machine Learning for High-Speed Nanoindentation Mapping

Edoardo Rossi*[1]

[1] Università degli Studi Roma Tre - Italy

Abstract

High-speed nanoindentation mapping generates vast datasets that capture mechanical property variations across complex microstructures. However, effectively interpreting these large-scale maps requires advanced data-driven approaches. This talk explores how machine learning techniques, including clustering and deep learning, can be leveraged to deconvolute mechanical maps, revealing distinct micro-constituents, phases, and structural features. By integrating nanoindentation data with complementary characterization methods, such as EBSD and EDX, we uncover hidden correlations between mechanical properties and material heterogeneity. Machine learning accelerates phase identification and trend extraction, pushing the boundaries of high-throughput materials characterization and paving the way for data-driven materials design.

* Speaker

Small-Scale Mechanical Testing of Semiconductor Materials

Bo-Shiuan Li*[1]

[1] National Sun Yat-sen University - Taiwan

Abstract

Vertical integration and compound semiconductor materials are emerging research areas in Taiwan's semiconductor industry. Both require good understanding of its mechanical strength at the device length scale to prevent failure during service. In this talk, the role of small-scale mechanical testing in these areas will be discussed. Case studies on the small-scale mechanical behavior of direct bonded interfaces and 4H-SiC and its relevance to processing optimization will be demonstrated. Lastly, aspects on future developments of small-scale mechanical testing for semiconductor research will be point out.

* Speaker

Influence of Adhesive Type on the Tensile-Shear Strength of CFRP-DP500 Steel Joints

Aleksija Djuric*[1]

[1]University of East Sarajevo, Faculty of Mechanical Engineering – Bosnia and Herzegovina

Abstract

This study experimentally investigated the tensile-shear behavior of adhesively bonded joints between carbon fiber-reinforced polymer (CFRP) sheets and Dual-phase steel 500 (DP500). The primary objective was to evaluate the impact of different structural adhesives on the joint's mechanical performance. Five epoxy adhesives were examined: SikaFast 555, SikaPower 880, SikaPower 1200, SikaPower 1277, and LOCTITE® EA 9466. Experimental results demonstrated a significant influence of the adhesive type on the tensile-shear strength of the CFRP-DP500 joints.

*Speaker

Nanoindentation Analysis of individual phases in model Carbon Fiber-Reinforced PEEK composite

Sophie Vanpée*†[1], Bernard Nysten[2], Jérémy Chevalier[3], and Thomas Pardoen[1]

[1]Institute of Mechanics, Materials and Civil Engineering, iMMC, UCLouvain – Belgium
[2]Institute of Condensed Matter and Nanosciences (IMCN), UCLouvain – Belgium
[3]Material Science Application Center (MSAC), Syensqo – Belgium

Abstract

In the context of the energy transition, the transportation sector faces the double challenge of producing light but high-performance structural parts while improving their recyclability. Thermoset-based composite materials allow the manufacturing of light structures with excellent mechanical properties, but are hardly recyclable and can only be processed via liquid molding techniques or prepreg consolidation. Moreover, high-rate composite processing is impossible with such matrices, as the necessary curing step often lasts few hours at a high temperature. Transitioning from thermoset to thermoplastic polymer matrix composites overcomes these shortcomings. However, the successful transition requires an understanding of the influence of processing conditions on the microstructure of the thermoplastic matrix and the mechanical performances of the composite. Among thermoplastic polymers, semi-crystalline polymers like polyetheretherketone (PEEK) offer superior mechanical properties. However, their mechanical behavior is related to the amount and characteristics of the crystalline phase, which depend on the processing conditions. In this work, the effects of crystallization conditions (processing conditions and fiber proximity) on the microstructure and mechanical properties of 'model' carbon fiber-reinforced PEEK samples and of UD composite samples are investigated. The degree of crystallinity and crystalline phase morphology are first assessed. The mechanical properties of the PEEK matrix processed in different conditions and its resulting phases (amorphous phase, spherulites and transcrystalline zones) are then evaluated via nanoindentation (NI) and atomic force microscopy (AFM). In addition, the deformation and damage mechanisms occurring in the matrix at the micro-scale during transverse compression are studied using nano-digital image correlation (nano-DIC).

*Speaker
†Corresponding author: sophie.vanpee@uclouvain.be

Thin Film Interface Engineering using Atomic Layer Deposition: Improved Electromechanical Properties and Adhesion

Johanna Byloff*[1,2], Claus Trost[3], Vivek Devulapalli[4], Pierre-Olivier Renault[5], Thomas Edwards[6], S. Altaf Husain , Damien Faurie , and Barbara Putz†

[1]Laboratory for Mechanics of Materials and Nanostructures [Thun] (EMPA) – Switzerland
[2]Laboratory for Nanometallurgy [ETH Zürich] – Switzerland
[3]Erich Schmid Insitute of Materials Science of the Austrian Academy of Sciences – Austria
[4]EMPA - Swiss Federal Laboratories for Materials Science and Technology – Switzerland
[5]Université de Poitiers, ISAE-ENSMA, CNRS, PPRIME – CNRS, Université de Poitiers, ENSMA – France
[6]National Institute for Materials Science – Japan

Abstract

In the Al-Polyimide (PI) system, an amorphous Al-O-C interlayer (5 nm) forms at the interface between metal film and polymer substrate. We mimic this interlayer artificially (Al2O3, 0-25 nm) through combined atomic layer (ALD) and physical vapor deposition (150 nm Al), to uncover fundamental mechanisms behind reported mechanical and adhesive benefits. As-deposited and annealed (400 ∘C, 90 min) samples were loaded in uni- and equi-biaxial tension, with in-situ film stress and electrical resistivity measurements tracking the deformation behavior as a function of interlayer thickness. Adhesion energies were determined using the tensile induced delamination (TID) method. Al films with an artificial ALD-Al2O3 interlayer $<=5$ nm exhibit shorter and more angled cracks compared to PVD Al films, which results in 30% higher electronic failure strain and can be attributed to higher adhesion energy provided by the ALD interface. Above 10 nm ALD thickness, embrittling effects start to outweigh the adhesive benefits, likely related to a ductile to brittle transition in the deformation of the interlayer itself. This results in an optimum ALD interlayer thickness of 5 nm for enhanced mechanical and interfacial performance, offering a transferrable approach to control interface quality in other metal-polymer thin film systems.

*Speaker
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Molecular dynamics calculations of the mechanical properties of nanopillars made of pyrocarbons

Julien Durinck[1], Laurent Pizzagalli*[2], Paul Lafourcade[3], and Jean-Marc Leyssale[4]

[1]Institut Pprime (PPRIME) – Centre National de la Recherche Scientifique : UPR3346, Université de Poitiers, ISAE ENSMA, Poitiers – France

[2]Institut Pprime – Université de Poitiers, Centre National de la Recherche Scientifique, ENSMA, Université de Poitiers : UPR3346, ENSMA : UPR3346, Centre National de la Recherche Scientifique : UPR3346 – France

[3]DAM Île-de-France – CEA DAM DIF, F-91297 Arpajon – France

[4]Institut des Sciences Moléculaires (ISM) – Bordeaux Université, Bordeaux INP,CNRS – France

Abstract

Pyrocarbons are synthetic carbon-based materials whose properties make them ideal for use in a wide range of applications in spatial, nuclear, or medicine. They are made up of disordered stacks of graphene sheets, the latter being characterized by a preferential orientation of the 002 directions and an average size, and partially connected together by point and linear defects. There is a large variety of possible configurations usually collected in different families. Because of this structural complexity and diversity, the relation between structure and mechanical properties at large deformations remains largely unexplored.

To fill the gap, we perform molecular dynamics simulations of the uniaxial compression of nanopilars made of pyrocarbons, with realistic models built using the polygranular image guided atomistic reconstruction method (1). We consider three types of pyrocarbon and three compression orientations. The variations as a function of deformation of quantities like the applied load or the energy are analyzed with respect to structural modifications during compression. In particular we monitor the average orientations of the graphene sheets, the evolution of coordination defects population, and the local shear and volumetric strains. Our investigations reveal a wealth of behaviors depending on the compression orientation, such as buckling of the graphene sheets and the formation of shear and kink bands. These results are discussed in relation to the influence of finite size and surface termination.

(1) F.Polewczyk, P.Lafourcade, JP. Da Costa, G.Vignoles, JM.Leyssale, Carbon 212, 118109 (2023)

*Speaker

Prediction of crack evolution in thin films and coatings based on the digital material representation concept

Konrad Perzynski*†[1], Grzegorz Cios[2], Barłtomiej Kowal[1], Mariusz Werminski[1], Mateusz Sitko[1], Aleksandra Fiołek[1], Tomasz Moskalewicz[1], and Lukasz Madej[1]

[1]AGH University of Krakow, Faculty of Metals Engineering and Industrial Computer Science – Poland
[2]AGH University of Krakow, Academic Centre of Materials and Nano technology – Poland

Abstract

The primary objective of this work is to numerically simulate fracture development in thin films and coatings deposited using the Pulsed Laser Deposition (PLD) and Physical Vapour Deposition (PVD) methods. The developed numerical model is based on the digital material representation concept, integrating two fracture approaches: cohesive elements and the extended finite element method (XFEM). This approach enables an explicit consideration of the influence of complex film and coatings morphology, including all its heterogeneities, on fracture initiation and propagation under loading. As a case study, thin films deposited on various substrates were selected for investigation. All samples were first investigated with nanoindentation tests and electron microscopy to evaluate local material properties and film morphology. Then, a finite element method, supported by inverse analysis, was employed to transform the measured load-displacement curves from nanoindentation into stress-strain characteristics for further numerical simulations. Fracture initiation and propagation parameters in both fracture models were also determined using the inverse analysis technique, incorporating the geometrical aspects of the film after loading into the goal function. The proposed approach demonstrates the ability to take into account local inhomogeneities that can affect the overall mechanical properties of thin films as a result of fracture formation.
Acknowledgements: This research was funded in part by National Science Centre, Poland 2024/53/B/ST8/00808 and the "Excellence Initiative – Research University" program for the AGH University of Krakow are acknowledged. We gratefully acknowledge Polish high-performance computing infrastructure PLGrid (HPC Center: ACK Cyfronet AGH) for providing computer facilities and support within computational grant no. PLG/2024/017298.

*Speaker
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Using data-based methods for microstructure characterization

Ashish Chauniyal*[1]

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Abstract

Material characterization using electron backscatter diffraction (EBSD) requires indexing the orientation of each scanned pixel based on a Kikuchi pattern. Several approaches to indexing are available like Hough Indexing (HI) which transforms the pattern to a Hough space and Dictionary Indexing (DI), where a library of simulated Kikuchi patterns is compared to the test pattern revealing a closest match. The advent of artificial intelligence and data driven material science has further led to the development of trained machine learning models which are shown to be very effective in indexation and segmentation. However, such methods are computationally expensive and require large datasets and extensive training time. Furthermore, robustness remains an issue as models trained for one type of dataset are not easily transferable to other. An effective way to circumvent these issues is the use of unsupervised data-based methods, which are easy to use and robust to deploy. There is a lot of scope in applying such methods, in innovative ways, to characterize microstructures. Principal component analysis (PCA) and non-negative matrix factorization (NMF) have been used to denoise and segment a microstructure effectively. In this work we showcase the latest data-based methods used for microstructure segmentation as well as solving specific tasks, such as pattern overlaps at grain boundaries. We describe an application of a constrained non-negative matrix factorization scheme to segment low angle grain boundaries (LAGB) effectively, which is on par with high resolution EBSD techniques. This approach allows to resolve the location of a grain boundary at the pixel level. Finally, we introduce the concept of Embeddings-EBSD and showcase its applications in segmentation and detecting accumulation of localized strains. Together with the two approaches we present some illustrative applications in material characterization.

*Speaker

Molecular dynamics based mobility laws

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Abstract

The study focuses on a phenomenological mobility law for hydrogen-induced edge dislocations in body-centered cubic (bcc) iron, derived from molecular dynamics simulations. The findings explore the impact of hydrogen on dislocation motion and plasticity in bcc Fe, providing insights into hydrogen embrittlement mechanisms at the atomic scale. The developed law could enhance the understanding of hydrogen's role in material degradation, potentially guiding the design of more resilient materials in hydrogen-rich environments.

*Speaker

Fracture behaviour in Cu-Al multilayer thin films with amorphous AlO interlayers: Insights from in-situ TEM tensile testing

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Abstract

In-situ transmission electron microscopy (TEM) enables direct observation of deformation mechanisms in advanced materials, offering valuable insights for the development of tougher nanostructured systems. This study explores the fracture behavior of Cu-Al multilayer thin films with ultrathin amorphous AlO interlayers. Using in-situ TEM tensile testing, we observed the dynamic interaction between crack propagation and microstructural evolution in real time. The multilayer system, composed of 30-120 nm thick Cu-10% Al layers separated by 2 nm AlO interlayers deposited by atomic layer deposition (ALD), exhibited exceptional toughness through multiple mechanisms. Our observations showed that void nucleation occurred primarily at the interfaces between the ALD layer and high-angle grain boundaries, which caused cracks to follow tortuous paths, enhancing material toughness. Several concurrent deformation mechanisms were identified ahead of the crack tip, including dislocation glide, grain boundary sliding, detwinning, and grain rotation. Notably, twin fraction decreased from 30% to 20% during crack growth, suggesting partial accommodation of plasticity through detwinning. Remarkably, the amorphous AlO interlayers demonstrated unprecedented ductility, thinning from 2 nm to approximately 500 pm before failure. This exceptional behavior, combined with complex crack propagation and multiple deformation mechanisms, contributes to the enhanced mechanical performance of these multilayer systems. These findings offer key insights for designing damage-tolerant metallic thin films and highlight the potential of engineered interfaces in achieving superior mechanical properties in multilayer materials.

*Speaker

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(110) tensile testing of single crystalline gold thin films with nanotwins: in situ TEM and XRD studies

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Abstract

Keywords: nanotwins, gold, thin film, in-situ transmission electron microscopy, in-situ X-ray diffraction, pole figures

Abstract:

Tensile tests on 50 nm thick gold thin films are studied with an association of two *in situ* techniques, to combine the quantitative descriptions of X-ray diffraction (XRD) and the nanoscale imaging capability of transmission electron microscopy (TEM). The films have a (001) single crystalline matrix and contain four families of nanotwins – a twin family has an orientation obtained by a reflection through a matrix {111} plane. Before straining, the typical thickness and length of the twins are 5–20 nm and 30–100 nm, respectively. The films are strained along the matrix (110) direction.

The XRD experiments (performed at the DiffAbs beamline of the SOLEIL synchrotron

*Speaker

radiation source) give the texture evolution as a function of the applied stress and strain in the film. In particular, an impressive _˜500% increase in the twin volume occurred for two favorably twin orientations at an applied strain of only 4.0%. Furthermore, the twin volume increase is accompanied by a twin rotation. The sub-micron scale TEM observations show that the increase in volume is correlated with the glide of partial dislocations, either along the coherent twin boundaries (TB) or at the incoherent TBs, or close to microstructure imperfections. In the last case, twins coalesce and acquire a micrometer size. An intense dislocation activity occurs in these large twins, still increasing the strain concentration and resulting in crack expansion. The twin rotation is also observed post-mortem in TEM.

In-situ strain measurement of micro-mechanical specimens using DIC

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Abstract

UKAEA is building a prototype fusion power plant, STEP (Spherical Tokomak for Energy Production), and the performance of materials under the harsh environments anticipated within the tokamak will be key to its success. In the absence of a representative environment such as a fusion energy spectrum neutron source, the traditional methods of materials assurance through empirical testing are not possible and alternatives must be sought.
Design by Fundamentals is a project to develop mechanistically informed, physically justified crystal plasticity models to link microstructure to mechanical properties, and predict the behaviour of materials in untestable environments. It relies on analysis of samples subject to surrogate irradiations such as in materials test reactors or with charged particles, which are typically not in the correct geometry for conventional, standardised mechanical testing and require the use of miniaturised specimens or micro-mechanical testing. Here we present work on the development of high fidelity micro-mechanical experiments to provide data for model calibration.
It is well known that micro-pillar compression samples can suffer from compliance issues, where the deformation of the substrate below the gauge results in a lower measured stiffness. This affects the strain measurement, which is important for determining the elastic and strain hardening behaviour. This talk will present the use of Digital Image Correlation (DIC) to track displacements during testing of micro-pillar compression specimens inside an SEM, enabling accurate strain measurement to correct for compliance issues. Mapping of strain to quantitatively compare effects of microstructure, size, and irradiation damage on deformation will also be presented, as well as showing applicability to other sample geometries.

*Speaker

In situ Transmission Kikuchi Diffraction (TKD) Tensile Testing

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Abstract

We present a novel methodology for *in situ* Transmission Kikuchi Diffraction (TKD) tensile testing that enables nanoscale characterization of the evolution of complex plasticity mechanisms. By integrating a modified *in situ* Scanning Electron Microscope (SEM) nanoindenter with a microscale push-to-pull device and a conventional Electron Backscatter Diffraction (EBSD) detector, we achieved TKD measurements at high spatial resolution during mechanical deformation. A dedicated focused ion beam procedure was developed for site-specific specimen fabrication, including lift-out, thinning, and shaping into a dog-bone geometry. The methodology was demonstrated on several case studies: (i) a metastable β-Ti single crystal, on which we quantified the initiation and evolution of nanoscale twinning and stress-induced martensitic transformation, (ii) an HCP Re single crystal loaded along the c-axis showing complex nanoscale twinning and twin-to-twin interactions, and (iii) a CuAl/AlO nanolaminate, which exhibited nanoscale plasticity and twinning/detwinning in a complex microstructure. Furthermore, we explore the possibilities for performing elastic and plastic strain measurements using HR-TKD and SEM-DIC, respectively, alongside regular TKD mapping. Overall, this approach provides a robust alternative to *in situ* EBSD and transmission electron microscopy testing, with the potential of providing local stress-strain data, facilitating detailed analysis of deformation mechanisms at the nanoscale.

*Speaker

Dislocations in Laves phases: Atomistic Mechanisms of Motion and Reaction

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Abstract

In Laves phases, as in other materials, the plastic deformation is mediated by dislocation motion. Recent studies have revealed new slip mechanisms in Laves phases and highlighted the thermally activated nature of partial dislocation glide, indicating that unexplored mechanisms remain. In this study, we investigated dislocation core structures and locking mechanisms in C15 NbCr2 Laves phases through high-angle annular dark field scanning transmission electron microscopy. Direct observations enabled the reconstruction of core structures, while atomistic simulations provided insights into mechanisms of dislocation motion and reaction. Through this combined framework, we characterized individual partial dislocations forming intrinsic stacking faults and their reaction products, both in-plane (extrinsic stacking faults) and out-of-plane (dislocation locks). Burgers vector analysis identified three unique types of partial dislocations, with lock structures corresponding to Lomer-Cottrell and Hirth locks. Additionally, per-atom segregation energy mapping around the core structures revealed a strong tendency for antisite defect decoration in Lomer-Cottrell locks and vacancy decoration in Hirth locks, offering a possible explanation for serrated flow in Laves phases. Finally, nudged elastic band calculations captured local events during dislocation motion and the formation of intrinsic and extrinsic stacking faults.

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Strain rate dependence of slip vs. twinning in c-axis compression of α-titanium

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Abstract

Deformation twinning plays a crucial role in governing the plastic behavior of hexagonal close-packed (HCP) metals, primarily due to the limited availability of easily activated slip systems. Twinning is often associated with reduced ductility and the generation of high residual stresses, which can contribute to material failure through cracking. Understanding the nucleation and propagation of twinning in HCP metals is essential for optimizing their mechanical properties and enhancing their performance in various engineering applications. In this study, we explore the strain rate sensitivity of deformation twinning and non-basal slip systems.
In-situ uniaxial compression tests were performed on micro-pillars in single crystal pure alpha-titanium over sever orders of magnitude of strain rates (up to 1000 s^1). All experiments were conducted with the (0001) crystal orientation aligned with the loading axis. The crystallographic orientation, active slip systems as well as the distribution of the geometrically necessary dislocation (GND) within the deformed volume of the material were analyzed using post-mortem cross-sectional transmission Kikuchi diffraction (TKD) of the deformed pillars. Additionally, post-mortem transmission electron microscopy (TEM) is used to characterize the activated dislocations and twin plane features under different deformation conditions.

A transition from slip-dominated to twin-dominated deformation is observed as the strain rate increased. At low strain rates ($\epsilon < 10^2$ s^1), plasticity was primarily governed by dislocation slip, with twinning remaining inactive. In contrast, at high strain rates ($\epsilon > 10^2$ s^1), plasticity was predominantly accommodated by $\{1122\}\langle 1123\rangle$ deformation twinning.
By combination of post-mortem TKD and TEM techniques, our work adds new pieces towards the fundamental comprehension of deformation twinning in HCP metals at the micron scale and at high strain rates.

*Speaker

Dislocation-localized phase evolution in FCC alloys and the resulting dislocation mechanics evaluated by spherical nanoindentation

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Abstract

Dislocations and the microenvironments surrounding them play a key role in the plastic deformation of crystalline solids. Recently, it has been discovered that local stresses surrounding a dislocation can induce and stabilize the formation of nanoscale phases, termed *dislocation phases*. Due to the local ordering, these dislocation phases can impact plastic deformation and alter macroscale material properties, but their behavior is still not well understood. Guided by atomistic simulations, we fabricate several bulk FCC alloys that host distinct forms of dislocation-localized ordering. This presentation will discuss spherical nanoindentation methods used to evaluate both incipient plasticity and strain rate sensitivity in these dislocation phase-containing Ni-Al and Al-Cu systems. Namely, samples containing dislocation phases in Ni-Al show a 40% increase in max shear stress at pop-in compared to samples containing no linear complexions. In Al-Cu, spherical nanoindentation at constant strain rates reveals markedly higher strain rate dependence in samples containing dislocation phases than what would be expected for more traditional strengthening mechanisms. Additionally, the combination of specific processing pathways and advanced TEM methods confirm a unique relationship between dislocation content and the formation of nanoscale ordered domains. These methods together advance understanding of the fundamental mechanisms of dislocation phase formation and elucidate the connections to macroscale properties.

*Speaker

A versatile electrochemical charging cell for studying hydrogen-related effects in materials

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Abstract

Understanding hydrogen embrittlement is crucial for the transition towards renewable energy. Beyond economic impacts, safety considerations are important, requiring robust methods to evaluate the mechanical response of materials under hydrogen influence. While macroscopic testing is widely used, in situ electrochemical nanoindentation and micromechanical testing have emerged as promising techniques. The conventional front-side charging approach introduces hydrogen on the same surface where indentation is performed. In the recently introduced back-side charging approach hydrogen is introduced on the opposite side of the indent location.

In this study, a novel side charging cell was developed and compared to the conventional front-side charging method by testing a coarse-grained ferritic steel with high chromium content, ensuring nanoindentation experiments within a single grain of similar orientation. The side charging cell demonstrated a 60% improvement in system stiffness compared to the front-side charging design. Mechanical testing revealed consistent Young's moduli before, during, and after hydrogen charging for both approaches. Hardness increased during charging, likely due to a Cottrell-like hydrogen atmosphere near dislocation cores, and returned to pre-charging values several hours post-charging. The presence of hydrogen was confirmed by in situ X-ray diffraction measurements employing a self-reporting Ti detection film.

The side charging cell offers enhanced testing stability, as hydrogen bubble formation does not influence the measurement. The innovative design enables its integration into other experimental setups and allows versatile sample geometries. Furthermore, it enables tests at varying distances from the hydrogen initiation point, make it a superior choice for evaluating diffusion phenomena.

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Physically recurrent neural networks for micromechanical analyses of composite materials undergoing plasticity and distributed damage

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Abstract

Multiscale modeling based on computational homogenization is a powerful approach to link microstructural features to structural performance, however its widespread adoption is prevented by the high computational costs. To address this problem, this presentation will describe an extension of a recent surrogate modeling approach, the Physically Recurrent Neural Network (PRNN), to include both plasticity and the effect of debonding at the fiber-matrix. The core idea of the PRNN is to implement the exact material models of the constituents into one of the layers of the network. To maximize the predictive accuracy and extrapolation capabilities of the network, various configurations of bulk and cohesive points are explored, along with different training dataset types and sizes.

*Speaker

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Deep Learning Mechanical Properties Classification of Metal-Ceramic Composites Using Nanoindentation Curves

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Abstract

Metal-ceramic composites display a distinctive microstructure wherein the metallic matrix and ceramic particles are interpenetrated and partially interconnected. This microstructure enables the combination of the hardness and wear resistance of the ceramic phase with the toughness and ductility of the metallic matrix. As a consequence, these materials are highly effective in certain applications that require resilience under extreme mechanical and thermal conditions. These composites present a significant challenge, as their mechanical behaviour is dominated by intricate interactions between the phases, particularly in proximity to interfaces or regions containing subsurface features. High-speed nanoindentation represents an effective tool for probing interactions at the nanoscale and for creating detailed hardness and elastic modulus maps. However, the mechanical phase identification remains challenging due to averaging in interphase regions and the influence of subsurface features on property measurements, which complicate interpretation and correlation.

To address these challenges, in this work, the morphology of the nanoindentation curves of each constituent phase of the composite material is incorporated to train a deep learning model to obtain a good micromechanical classification of the material. Before training the model, the nanoindentation curves were carefully analyzed to understand their shape and behavior depending on the location of the indentation on the material's surface. This included examining areas influenced by subsurface features, which were revealed through cross-sectional cuts made using Focused Ion Beam (FIB) techniques.

Properly labeled curves are transformed into images using the Gramian Angular Field (GAF), which is a representation for encoding time series as images. A ResNet neural network, was trained to analyze these images and facilitate phase classification. The resulting comprehensive classification distinguishes each distinct phase without interference from others, phases influenced by neighboring regions, ideal interphase where both phases contribute equally, and data representing failures or defects.

*Speaker

Understanding microstructure-property correlation of pearlitic steel by nanoindentation and machine learning-based modeling

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Abstract

Understanding and predicting the structure–property relationship is a cornerstone of materials science, particularly for designing advanced materials with tailored properties. The mechanical behaviors of pearlitic steel, widely used in demanding applications, are often dominated by the lamellae spacing, the colony shape and grain size, while several aspects concerning its microstructure-related properties have not yet been studied in detail.
In this study, a novel data-driven framework is proposed to predict local hardness in 100Cr6 steel based on the integration of advanced imaging techniques, nanoindentation measurements, and machine learning-based modeling. The workflow begins with the acquisition of high-resolution scanning electron microscopy images and electron backscatter diffraction data to capture the morphology of the microstructural phases. Convolutional Neural Networks (CNNs) are employed for automated image segmentation, enabling precise identification and quantification of microstructural features such as lamellae spacing and colony morphology. These segmented features are then integrated with corresponding nanoindentation hardness data to train a predictive machine learning model.
The results demonstrate that the morphology of ferrite and cementite phases significantly influences the localized hardness values. The developed model provides a fast prediction of the hardness, validated by detailed experimental measurements, and reveals new insights into the relationship between pearlite microstructure and mechanical properties.

*Speaker

Application of high-throughput materials science methods for rapid screening and optimization of ultra-strong light-weight alloys for automotive

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Abstract

Aluminium and its alloys are recognized for their advantageous properties, including high specific strength, low density, corrosion resistance, and excellent recyclability. These characteristics make them indispensable in industries such as aerospace, automotive, and military. In this study, we conducted high-throughput screening of an Al-Mg-Zr material library. Thin-film material libraries were fabricated using PVD, via magnetron sputtering, enabling a investigation of compositional and structural variations. The alloys were characterized using EDS for chemical composition analysis, XRD for structural evaluation, and nanoindentation to determine mechanical properties. By integrating these techniques, we analyzed the effects of synthesis parameters and chemical compositions on microstructure and their subsequent impact on mechanical performance. We observed that increasing zirconium content in the alloy was associated with a enhancement in mechanical strength. Notably, alloys with a yield strength reaching up to 1730 MPa were identified, significantly surpassing the 200-600 MPa range typical of conventional aluminium-based alloys. This exceptional strength may be linked to the formation of nanocrystalline grains and an extremely supersaturated solid solution, which are known to enhance mechanical properties through microstructural refinement and solid solution strengthening. These findings highlight the potential of Al-Mg-Zr alloys as high-strength materials, suggesting that higher zirconium content may affect the structure, therefore contribute to improved mechanical strength. These observations provide initial insights into the mechanisms that could underlie their enhanced properties. By identifying how variations in chemical compositions appear to influence the formation of grains and supersaturated solid solutions – potentially enhancing mechanical strength – this work contributes to the fundamental understanding of Al-Mg-Zr systems and supports their potential application as lightweight, high-strength materials. The findings of this study underscore the need for further investigation into the optimization and scalability of these alloys, presenting promising avenues for innovation in materials science and engineering.

*Speaker

Lab-on-a-chip nanomechanical study of annealing and stress-induced grain growth effects on plasticity and time-dependent deformation in sputtered Pt thin films.

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Abstract

Polycrystalline thin platinum films with thicknesses ranging from tens to hundreds of nanometers are used in MEMS devices owing to the desirable chemical, electrical, and mechanical properties of Pt for gas sensing, catalysis, electrodes, resistive heating, and structural/processing purposes where the film is subjected to high temperatures which inevitably affects the microstructure and in turn influences the performance of the coatings. In this work, we explore the effects of mechanical stress and elevated temperatures on the microstructure in the form of grain growth and subsequently the time-dependent mechanical behavior (creep) of Pt thin films utilizing state-of-the-art nanomechanical testing and characterization methods. Sputter deposited and freestanding dogbone patterned (lithography and XeF2 under etched) Pt films on Si wafer, with a thickness of 250 nm are uniaxially deformed under tension by UCLouvain Lab-on-Chip testing platform that employs internal stress (_˜1 GPa) of attached Si3N4 film for actuation. Multiple structures with varied stain levels remain under tension. The stress-strain curve and its evolution over time (constant stress creep test) are obtained. Examining and tracking the as-deposited specimens reveal a shift in strain and stress at both high and minuscule strains starting immediately after the release of the freestanding structure over a long time (_˜ a year). Stress-induced grain growth, rotation, and diffusion of the grain boundaries are the primary candidate mechanisms to explain these findings. Further investigation through scanning transmission electron microscopy and localized strain map via digital image correlation shines a light on the synergistic or competitive effect of these mechanisms. Annealing-induced grain growth prior to the application of the uniaxial tension reveals the effect of grain size and microstructure on the time-dependent behavior of Pt thin films. The results of this work would complement many advanced modeling studies that investigate grain boundary diffusion and creep (Coble creep).

*Speaker

MEMS Platforms for Automated and High-Throughput Micromechanical Testing of Silicon Nanowires

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Abstract

Silicon nanowires (SiNWs) are key to nanoelectronics, optoelectronics, and sensors due to their unique electrical, mechanical, and optical properties. The broad potential applications of NWs have driven the need for advanced mechanical testing methods. Traditional testing techniques, including MEMS-based platforms, face challenges in (i) manipulating and aligning nanoscale samples and (ii) imposing a specific stress state, both contributing to inconsistencies, i.e., a large scatter in reported mechanical properties. Co-fabricating the sample with the MEMS platform addresses the first challenge by ensuring precise alignment. The second challenge, however, requires a more versatile method that can impose the desired stress state while accounting for its impact on failure mechanisms. i) *Uniaxial testing*, though straightforward for mechanical property extraction, applies uniform stress across the cross-section, increasing the risk of brittle failure from pre-existing or fabrication-induced defects. ii) *Transverse loading*, while altering stress distribution, still introduces a uniform axial stress component that can contribute to failure. iii) In contrast, *pure bending* eliminates axial stress, localizing the highest stresses within a confined region, offering a more reliable approach for exploring deformation behavior. Each method has its strengths and limitations. Hence, a combination of all loading configurations ensuring consistent initial conditions and surface states is essential to provide a better understanding of SiNW mechanics. This study introduces a set of MEMS-based testing platforms, which are monolithically integrated with SiNWs. Twelve MEMS stages (four for each loading configuration) were fabricated on the same chip, with each stage containing one SiNW sample. A commercial micromechanical

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testing equipment (FemtoTools) with a micromanipulator tip is used to apply load in an automated fashion. The proposed fabrication and automated characterization approach reduces potential errors during the process and minimizes testing time. This technique is also applicable to other 1D nanomaterials, such as metal oxide NWs, for high-throughput mechanical characterization.

High strain rate nanoindentation up to 10,000/s and associated deformation mechanisms

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Abstract

The use of nanoindentation-based techniques to study high strain rate deformation behavior of materials is of immense scientific interest because it enables investigating the strain rate dependence of individual grains and small-scale structures. While nanoindentation impact tests, capable of reaching high strain rates, have been used for over two decades, they suffer from lack of indentation profile control and rapidly varying strain rate during impact. This makes extraction of reliable mechanical properties, for e.g. hardness, and determination of the representative strain rate, rather difficult. It is only recently that advances in nanoindentation instrumentation have enabled reaching constant strain rates > 100 s-1 in both micropillar compression and indentation. In this talk, I will present our recent progress in performing controlled, constant strain rate nanoindentation tests up to 10ˆ4 /s for reliable extraction of mechanical properties (hardness, modulus) and deformation activation parameters (strain rate sensitivity exponents, activation volumes). Typically, high speeds and fast unloading rates excite the resonance of the nanoindenter, which makes it difficult to extract hardness and modulus from the unloading curves using Oliver-Pharr method. Novel experimental protocols and calibration procedures were developed to circumvent this issue and to enable Oliver-Pharr method property measurements. Changes in indentation contact areas with increasing strain rates were studied systematically. Selected case studies of high strain rate nanoindentation testing on single and nanocrystalline metals will be presented to gain an overall understanding of the high strain rate deformation mechanisms in indentation. Indentation at high strain rates results in vastly different deformation substructure compared to quasi-static nanoindentation tests and micropillar compression, which will be discussed.

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Hardness values as a function of the degree of deformation for tungsten and doped tungsten fine wire

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Abstract

Due to the ever-growing demand for highly specialized products, the material requirements are constantly increasing. This demands the development of new alloys, as well as a better understanding of the influence of production conditions on the resultant materials characteristics. This contribution investigates the structure and property relationship, in particular the hardness as a function of the degree of deformation, for tungsten and potassium doped tungsten fine wire. The diameters of the fine wire range from 150 to 25 μm. To evaluate the hardness values, nanoindentation experiments are realized for all diameters. To also evaluate the influence of annealing at low temperatures, aiming for potential hardening by annealing effects, alike wire diameters for each alloy are chosen. Then the wires are annealed at a variety of temperatures below recrystallization, and subsequently tested again. For the nanoindentation experiments, the fine wires were embedded and measured locally with a displacement-controlled *in situ* nanoindenter inside a scanning electron microscope at room temperature. The received hardness values are correlated to the degree of deformation and assessed for changes according to the respective annealing temperatures.

*Speaker

HIGH TEMPERATURE SCANNING INDENTATION: LATEST RESULTS ON AMORPHOUS SELENIUM

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Abstract

The High-Temperature Scanning Indentation (HTSI) is a quasi-continuous nanoindentation measurement technique. Thanks to its fast indentation cycle and the possibility of applying it during heating treatments, it is possible to track material properties and the changes with temperature (1). Thus, HTSI can detect one or many critical phenomena like static recovery, recrystallization, glass transition, and brittle-to-ductile transitions. When applied to various materials such as pure cold-rolled copper, aluminum, and thin film metallic glass, HTSI has proven to be robust and effective in linking measurable properties to the microstructural evolution of materials (2,3).

This presentation will explore and open a discussion about our latest results on amorphous selenium. HTSI was used to measure, in-situ, Young's modulus, hardness, and creep properties during multiple heating cycles. We will showcase the trend of those properties in temperature and discuss them. A special focus would be to highlight the fundamental behaviors and transformations observed, mainly in the glass transition range. Moreover, we would like to report the observation of the photocrystallization phenomenon, under certain conditions. An intriguing behavior that expands our understanding of this material under thermal and optical stimuli.

(1) G. Tiphéne, P. Baral, S. Comby-Dassonneville, G. Guillonneau, G. Kermouche, J.-M. Bergheau, W. Oliver, J.-L. Loubet, High-Temperature Scanning Indentation: A new method to investigate in situ metallurgical evolution along temperature ramps, J. Mater. Res. (2021). https://doi.org/10.1557/s43578-021-00107-7.

(2) G. Tiphéne, G. Kermouche, P. Baral, C. Maurice, G. Guillonneau, J.-M. Bergheau, W.C. Oliver, J.-L. Loubet, Quantification of softening kinetics in cold-rolled pure aluminum and copper using High-Temperature Scanning Indentation, Mater. Des. 233 (2023) 112171. https://doi.org/10.1016/j.matdes.2023.112171.

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(3) S. Comby-Dassonneville, G. Tiphéne, A. Borroto, G. Guillonneau, L. Roiban, G. Kermouche, J.-F. Pierson, J.-L. Loubet, P. Steyer, Real-time high-temperature scanning indentation: Probing physical changes in thin-film metallic glasses, Appl. Mater. Today 24 (2021). https://doi.org/10.1016/j.apmt.2021.101126.

Small scale deformation of cemented carbides at high temperature

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Abstract

Cemented carbides represent one of the most successful applications of multiphase composites in structural engineering, owing to the distinct properties of their two primary constituents: hard ceramic particles embedded within a metallic binder. These hard metals exhibit an exceptional balance of strength and toughness, coupled with remarkable resistance to wear and abrasion. Consequently, they are widely utilized in cutting tools for manufacturing and in structural and wear-resistant components across various industrial sectors. Given their frequent exposure to elevated temperatures, understanding their high-temperature behavior is critical.

Enhancing the performance of cemented carbides in such environments requires a fundamental understanding of their deformation mechanisms at the nanoscale. This study integrates nanoindentation and advanced microscopy techniques to perform in-situ mechanical property measurements at temperatures up to 600∘C. The primary objective is to characterize the deformation mechanisms and micromechanical response of cemented carbides at both room and high temperatures, ultimately informing material optimization for extreme conditions.

To achieve this, micropillar compression tests were conducted, offering a highly controlled method for analyzing deformation mechanisms in cemented carbides. This technique minimizes constraining effects by employing a uniaxial loading mode and a reduced interaction volume, enabling precise assessment of plastic deformation fields. Focused Ion Beam (FIB) milling was employed not only for micropillar fabrication but also for post-deformation characterization through tomography. The integration of FIB milling with post-deformation analysis facilitates the detailed examination of localized deformation, crack initiation, and phase interactions. These insights are essential for advancing the mechanical and thermal performance of cemented carbides, ensuring their reliability in high-temperature applications.

*Speaker

Irradiation Hardening in Advanced Reduced Activation Ferritic-Martensitic Steels for Future Fusion Applications

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Abstract

Reduced activation ferritic-martensitic (RAFM) steels are a recent class of radiation-resistant steels designed to be used as the structural components of power-producing fusion reactors. In this work an advanced RAFM steel has been developed with superior radiation resistance with respect to the EUROFER-97 upon which it was based.

Self-ion irradiation campaigns up to 100 dpa at 350C show an increase in hardness of only 20%. The work hardening response, as determined from spherical nanoindentation, is unchanged between the as-received state and irradiation to 100 dpa, implying that the alloy should retain modest ductility under these conditions. Proton irradiations at 250C, 350C, and 400C demonstrate that the low temperature hardening embrittlement threshold is largely unaffected, increasing by only _˜50C with respect to EUROFER-97.
A refinement of alloy chemistry and a subsequent modification of the thermomechanical treatments to favour MX precipitates is therefore a very promising strategy for the further development of fusion steels.

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The Effect of Oxidation on the Compressive Strength of Ni Nanoparticles: a Nano-Mechanics Perspective

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Abstract

Faceted single-crystalline nickel (Ni) nanoparticles exhibit an ultrahigh compressive strength (up to 34GPa) unprecedented for metallic materials. This was attributed to three key factors. namely the high elastic shear modulus of Ni, smoothly curved nanoparticle edges, and the presence of a thin surface NiO layer (1). The objective of the present work was to tailor Ni-NiO core-shell nanoparticles with varied oxide layer thicknesses to optimize their strength. In this study, Ni–NiO core–shell structures with different thicknesses of the NiO shell were prepared by solid-state dewetting of thin Ni films deposited on sapphire substrate followed by high-temperature oxidation. The obtained Ni-NiO core-shell nanoparticles were systematically characterized using AFM, SEM, XRD, in-situ microcompression tests, and cross-sectional TEM. The results reveal a significant correlation between particle size and compressive strength across different oxidation levels. Notably, despite the uniform appearance of the top facets, increased oxidation leads to a gradual decrease of compressive strength. This phenomenon is attributed to a facet-dependent oxidation process and the Kirkendall effect, which induce the formation of Ni vacancies and their clusters at facet corners or within the Ni core, thereby compromising the overall strength of the nanoparticles.

Reference:
(1) Sharma, A., Hickman, J., Gazit, N. et al. Nickel nanoparticles set a new record of strength. *Nat Commun* 9, 4102 (2018). https://doi.org/10.1038/s41467-018-06575-6

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Small-Scale Plasticity in ZnO: Combined Experimental and Computational Insights

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Abstract

Zinc oxide (ZnO) is a compound semiconductor widely recognized for its electronic, optical, and piezoelectric properties, which enable diverse applications from optoelectronics to energy harvesting. Like other II-VI semiconductors, ZnO exhibits intriguing interactions between its electronic and structural properties, particularly regarding dislocation behavior (electroplasticity, photoplasticity, dislocation currents, *etc.*). While the structure of grown-in defects in ZnO has been extensively studied (1-3), the formation mechanisms of extended defects under external load remain poorly understood (4). In particular, questions persist about the relative activities of the different slip systems and their role in strain accommodation – knowledge crucial for manipulating dislocation populations and thereby controlling ZnO's properties.

This work investigates elementary deformation mechanisms in ZnO, focusing on prismatic and pyramidal slip systems through combined experimental and numerical approaches. We performed compression tests on FIB-machined micropillars with various crystallographic orientations using a displacement-controlled nanoindenter with a flat punch. This methodology enables precise control over loading conditions while allowing systematic study of orientation-dependent deformation behavior. The deformed specimens were characterized using both conventional and high-resolution transmission electron microscopy (TEM) to identify active slip systems and analyze dislocation microstructures. In parallel, atomistic simulations of generalized stacking fault (GSF) energies were conducted and a model was proposed to better interpret experimental observations.

References:

1. Nakamura et al., Crystals 8, 127 (2018)

2. Iwanaga et al., Phys. Status Solidi A 38, K119 (1976)

3. Li et al., Acta Mater. 175, 457 (2019)
4. Sung et al., Appl. Phys. Lett. 102, 241904 (2013)

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Toward High Strain Rate Spherical Nanoindentation Testing

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Abstract

Knowledge about the local mechanical behavior at high deformation rates is crucial to increase the safety of components that involve impact loadings such as bird impacts in the aviation industry, automobile crashes and many others.
In the past few years, the scope of nanoindentation has increasingly expanded toward high strain rates. However, the new developments are restricted to hardness measurements with Berkovich indenter tips and cannot capture the full stress-strain behavior of a material at high strain rates. While high-speed micropillar compression is a possible alternative, its widespread use is hindered by convoluted sample preparation and limited throughput. This calls for further development of spherical nanoindentation, which has already demonstrated its capability in capturing yield curves of various types of materials at conventional strain rates, and only requires plain, flat samples (1,2).

This talk will focus on both the technical implementation of high constant strain rate spherical nanoindentation and the development of custom methods to analyze the high-speed data. It will showcase a displacement-controlled instrument, which was designed around piezoelectric transducers and fast signal processing electronics allowing sampling rates of up to 1 MHz. Experimental measurements at strain rates of up to 10000 /s will be demonstrated, along with a discussion of the current bottlenecks in using spherical tips for high constant strain rate indentation.

Acknowledgement

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References

(1) Feldner, P., Merle, B. & Göken, M. Determination of the strain-rate sensitivity of ultrafine-grained materials by spherical nanoindentation. *J. Mater. Res.* **32**, 1466–1473 (2017).
(2) Leitner, A., Maier-Kiener, V. & Kiener, D. Essential refinements of spherical nanoindentation protocols for the reliable determination of mechanical flow curves. *Materials & Design* **146**, 69-80 (2018).

*Speaker

Second strain-gradient elasticity for centro-symmetric cubic materials

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Abstract

Second strain-gradient elasticity has been initially introduced by Mindlin (1) in order to describe surface effects such as surface relaxation. The constitutive law is however only written for the isotropic (O(3)-invariant) case. This results from the complexity of the constitutive law, which involves 18 parameters in the isotropic case, and this excludes crystalline materials, for which the description must hold at few inter-atomic distances. However, this limitation is particularly detrimental from the experimental point of view, since the crystal could serve as a marker in order to track the displacement field in the vicinity of the surface. We applied a tensor decomposition method (2) allowing to build tensors basis for centro-symmetric cubic materials (OxZ2-invariant) up to the 8th order in a three-dimensional space. These decompositions allow to express the second-strain gradient constitutive law , which involves 49 parameters and two cohesion moduli. These parameters thus control the anisotropic surface relaxation.

This is exploited to express the displacement field at various crystal surfaces as a closed-form. These relaxation fields are compared to those obtained by low-energy electron diffraction (LEED). This paves the way to the re-interpretation, in a continuum mechanics framework, of surface phenomena.

(1) R.D. Mindlin, Int. J. Solids Structures, 1 :417–438, 1965.
(2) Auffray, N., Abdoul-Anziz, H., & Desmorat, B. (2021). Explicit harmonic structure of bidimensional linear strain-gradient elasticity. European Journal of Mechanics-A/Solids, 87, 104202.

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Mechanical Characterization of Hazelnut Shell Powder-Reinforced Epoxy Composites for Sustainable Applications

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Abstract

This study investigates the mechanical properties of epoxy-based polymer matrix composites reinforced with hazelnut shell powder, focusing on tensile tests. Hazelnut shell powder, an abundant agricultural by-product, is used as a reinforcing material to enhance the mechanical performance of composites while promoting sustainability through waste reduction utilisation. In this study, hazelnut shells sourced from Giresun city, a region renowned for its high-quality hazelnuts, were mechanically ground, sieved to achieve particle sizes below 200 microns, and dried before their incorporation into the epoxy matrix at weight ratios of 10%, 20%, and 30%. The homogenised mixture was poured into moulds created by a 3D printer employing Fused Deposition Modelling. This additive manufacturing technique uses Polylactic Acid (PLA) filament for precise and standardised sample preparation. Tensile tests were performed using a universal testing machine to determine the ultimate tensile strength, elongation and modulus of elasticity. The results indicated that the incorporation of hazelnut shell powder influenced the mechanical properties of the composites, with varying effects depending on the filler content. These findings underscore the potential of hazelnut shell powder as a bio-based filler for epoxy composites and provide a sustainable alternative to synthetic reinforcements. The study advances the development of epoxy composites.

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Nitrogen-Doped PVD MoS Coatings: Enhanced Wear Resistance and Tribological Performance in Rolling-Sliding Contact

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Abstract

Friction causes energy loss and wear in mechanical parts, which can lead to high costs worldwide. To reduce these financial losses, lubricants are commonly used, with liquid lubricants being the most popular because they are easy to handle. However, there are situations where they may not be suitable, particularly in extreme conditions such as vacuum environments. In these cases, transition metal dichalcogenides (MoS2 or WS2) dry lubricants are used as an alternative. Molybdenum disulfide (MoS2) is often preferred, as it provides low friction and is stable across a wide range of temperatures and pressures.
In WS2, nitrogen doping was shown to significantly improve the mechanical properties and tribological performance of the coatings (1). This study investigates whether this processing can be extended to the more desirable MoS2 coatings. In detail, it explores the effects of nitrogen incorporation in PVD MoS2 coatings, which were deposited using reactive magnetron sputtering with varied gas flow rates. The coatings were systematically analyzed for surface morphology, roughness, thickness, density, chemical composition, and mechanical properties. To assess the impact of nitrogen doping on wear resistance and tribological behavior, these evaluations were conducted both before and after rolling-sliding tests. The findings reveal that nitrogen doping enhances wear resistance while preserving the friction coefficient under high loads.

(1) T. W. Scharf, A. Rajendran, R. Banerjee, F. Sequeda, *Thin Solid Films* **2009**, *517*, 5666.

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Investigation of the Potential of PTFE Coatings for Journal Bearings

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Abstract

The growing need for sustainable and lead-free alternatives to traditional white metal coatings has led to the exploration of PTFE (Polytetrafluoroethylene) coatings for journal bearings. PTFE coatings offer desirable properties such as low friction, high wear resistance, and chemical stability, making them a promising choice for industrial applications. While white metal coatings are widely used for journal bearings, their lead content presents significant environmental and health concerns, motivating the search for safer alternatives.
This study focuses on evaluating PTFE coatings applied to S355 steel journal bearings using epoxy spraying equipment. Different PTFE formulations, including pure PTFE, PTFE-MoS blends, and PTFE-glass fiber composites, were examined for their adhesion strength, microhardness, and microstructure. The adhesion strength was measured using an Elcometer adhesion tester, while microhardness testing provided insights into the coatings' resistance to localized deformation under load. Microstructure analysis was conducted to assess the coatings' integrity and bonding quality with the base material.
The findings of this research aim to demonstrate the suitability of PTFE coatings as a lead-free, sustainable alternative to traditional coatings in journal bearings. Key performance factors such as adhesion, microhardness, and material durability were evaluated to determine the effectiveness of PTFE coatings in high-performance applications. By focusing on environmentally-friendly materials, this study contributes to the development of more sustainable engineering practices in machinery components.

*Speaker

High-strength and non-brittle crystalline-amorphous PVD-ALD nanolaminates of amorphous alumina and AlCoCrFeNi high-entropy alloy

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Abstract

Over the past few decades, there has been extensive research interest in reducing characteristic length-scales in materials in order to achieve high strengths without compromising ductility. One popular strategy has been the refinement of grain size through "nanolaminate" architectures: alternating layers of two different materials with sub-micrometre thicknesses. For most material pairings deposited by physical vapour deposition (PVD), the alternating layers disrupt columnar grain growth, retaining sub-micrometre in-plane grain size through the thickness of sample. In parallel, a new approach to metallurgy emerged: the idea that near-equiatomic mixes of five or more elements should be stabilised in a single phase by their high entropy of mixing, rather than decomposing into intermetallic phases. This field of "high-entropy alloys" (HEAs) has produced some of the strongest metals ever reported, without compromising on ductility or toughness. We have combined these two strategies to create nanolaminate films using the AlCoCrFeNi HEA: both metal-metal fcc/bcc multilayers (exploiting the dependence of phase on Al content in this alloy); as well as metal-ceramic nanolaminates with 2 nm atomic layer deposition (ALD) amorphous alumina interlayers. Microstructural analysis confirms that the ALD layers effectively disrupt out-of-plane grain growth and retain small in-plane grain size. Micropillar compression experiments show that this system is exceptionally strong for a metal, and still plastic in its deformation. Through post-deformation TEM imaging, we show that the amorphous alumina interlayers deform in a ductile manner co-operatively with the metal layers, remaining continuous even under significant local strains. We discuss possible mechanisms capable of explaining the co-operative non-local deformation of the amorphous layer, and how these layers contribute to the nanolaminate's high strength.

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Nanoindentation study of NiTi shape memory alloys

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Abstract

The shape memory alloys (SMA) are characterized by a large reversible deformation (up to tens of percent), which significantly exceeds the elastic deformation of conventional metals. The shape memory effect is based on the phase transformation (martensite-austenite) which reverses the imposed deformation. The most prominent representative of shape memory metals is the nickel-titanium alloy NiTi (Nitinol). Its applications can be found in medicine, robotics, aerospace engineering, and many other fields of technology. This work focuses on the response of NiTi alloys to nanoindentation loading. Materials were prepared by two methods (rolling, spark plasma sintering) and underwent different heat treatments resulting in different transformation temperatures. During the deformation at the laboratory temperature, the materials exhibited either classical shape memory effect or pseudoelasticity. The test with Berkovich and spherical indenters were performed to evaluate the reversible deformation capability and resistance to functional fatigue (i.e. damage induced by cyclic repetition of the shape memory effect) of the alloys in different initial states.

*Speaker

Orienting grains for nanomechanical testing without EBSD

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Abstract

Electron backscatter diffraction (EBSD) is the standard technique for grain orientation determination in site-specific nanomechanical testing. However, it is not the only method available in a scanning electron microscope (SEM). For large-grained materials (on the order of a few microns), electron channeling patterns (ECPs) provide an alternative approach. This work demonstrates a method that combines ECPs with dynamic template matching to determine grain orientation. ECPs are acquired using a backscattered electron (BSE) detector while translating the sample stage. A dynamical simulation is then performed to generate an ECP master pattern, which serves as a reference for template matching. By comparing experimental ECPs to the simulated master pattern, we extract crystallographic information to guide the precise fabrication of micropillars for nanomechanical testing. This technique enables orientation selection even when EBSD is not available. We discuss its integration into existing FIB-based workflows.

*Speaker

Machine Learning in Thermoset Polymer Creep Modeling

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Abstract

The application of artificial intelligence (AI) in polymer modeling is a rapidly growing area that bridges material science and computational techniques. Researchers are leveraging AI to predict polymer properties, simulate molecular behavior, and optimize polymer synthesis processes, which were traditionally complex and time-consuming.
Thermoset polymers are widely used in various industries, including automotive, aerospace, and electronics, due to their excellent mechanical properties, thermal stability, and resistance to chemicals. However, these materials are prone to creep, a time-dependent deformation that occurs under sustained load, especially at elevated temperatures. Predicting the creep behavior of thermoset polymers is crucial for the design and reliability of components subjected to long-term loading conditions. Traditional methods for predicting creep behavior rely on empirical models and extensive experimental testing, which are time-consuming, costly, and sometimes inaccurate for complex material systems.
With the advent of machine learning (ML) techniques, there is an opportunity to develop predictive models that can accurately forecast the creep behavior of thermoset polymers based on material composition, processing parameters, and environmental conditions. This work aims to leverage ML to predict the creep behavior of thermoset polymers, thereby reducing the need for exhaustive experimental testing and enabling more efficient material design. For that purpose, the long-term creep behavior of epoxy is revealed by using the results of short-term creep tests with the help of ML. The ML methods are the regression model and multilayer perceptron (MLP) neural network. The ability to more accurately predict and optimize creep behavior will lead to improvements in product reliability and extended material life.

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Understanding nanoindentation statistical dispersion in ceramic - metal cemented carbides by numerical simulation and FIB tomography

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Abstract

WC-Co composites have a dual-phase structure with a hard carbide phase (WC) and a metallic binder (Co), leading to significant hardness variability in high-speed nanoindentation. This study combines simulated nanoindentations, based on 3D reconstructions from FIB tomography, with experimental data to correlate hardness with microstructural characteristics.
The analysis focuses on the percentage of binder near the contact point and its influence on indentation response. Simulations fully characterize the subsurface microstructure, unlike experimental data, where only the surface binder percentage is observable. A preliminary study determines the affected depth using a thin-layer model, analyzing hardness evolution as surface material thickness decreases. Real microstructural meshes are then generated, and the percentage of 3D and 2D binder is obtained.
Experimental tests include an indentation map and SEM imaging to determine the 2D binder percentage. A FIB tomography of the nanoindentations further aids in the 3D study. Results show that simulations produce accurate force-displacement curves and hardness maps comparable to experimental data. A clear correlation exists between volumetric binder percentage and hardness, but surface binder percentage shows greater data dispersion, indicating it cannot directly predict mechanical properties. This study shows the importance to use statistical analysis and numerical simulations to correctly extract mechanical properties of different phases in high speed nanoindentations maps.

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Defect-driven microstructural evolution and mechanical characterization of CoCrNi, Fex(CoCrNi)100-x and CoCrNi/Fe nanolaminate complex compositional alloy thin films

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Abstract

Complex compositional alloy thin films (CCA-TFs) are studied for their ability to combine mutually exclusive properties llike strength, ductility. CoCrNi TFs films exhibit high hardness (_˜9 GPa) and yield strength (_˜3.4 GPa) due to their columnar structure with planar defects (1, 2). The addition of Fe stabilizes FCC phase, reducing grain size _˜20 nm and increasing hardness _˜10 GPa (3). However, the relationship between CCA composition, microstructure, mechanical behavior remains unclear, and a thin film nanoengineering approach to boost mutually exclusive mechanical properties by controlling chemical heterogeneity and phase structure is still an open field.
This study focuses on CoCrNi, Fex(CoCrNi)100-x CCA-TFs synthesized by magnetron sputtering, varying Fe from 13 to 29 at.%. CoCrNi CCA-TF displayed a columnar structure with dual FCC-HCP phase, high density of stacking faults and twinning, resulting in H = 9.7 GPa, E = 204.4 GPa. Adding Fe stabilized the FCC phase with fewer defects, reducing H and E to 7.6 GPa and 185 GPa, respectively, owing to a higher stacking fault energy (32.5 mJ m–2) (4).

Based on these findings, CoCrNi/Fe (FCC/BCC) nanolaminates were fabricated with bilayer periods () of 70, 35, and 20 nm. These nanolaminates showed high adhesion and improved H. Micropillar compression tests revealed yield strengths of 2.8 GPa and plasticity of _˜40% when was reduced to 20 nm. This results from interface engineering, which blocks dislocations and crack propagation.

Overall, this study shed light on the understanding of composition-microstructure-mechanical

*Speaker

property relationship in CoCrNi and Fex(CoCrNi)100-x CCA-TFs. CoCrNi/Fe nanolaminates reported tailored and enhanced mechanical behaviour, with potential applications in hard coatings and microelectronics.

(1) Yuanying Y, et al., J. Mater. Res. Technol, 21, 2022 (2) Yvonne (Yi-Ting) Lin, et al., Surf. Coat. Technol., 424, 2021 (3) Nagy, P et al., Surf. Coat. Technol., 386, 2020 (4) Y. Wang et al., Acta Mater, 154, 2018

Selecting Protein Crystal Structure for Optimal Scoring of Protein-Ligand Interactions

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Abstract

Non-Covalent Interactions between target protein (P) and ligands (L) determine the P-L binding affinity. Appropriate approach for modeling P-L binding is based on Semi-empirical Quantum-Mechanical (SQM) methods. Promising solution for determining P-L binding affinity predictions is universal physics-based scoring function SQM2.20. Term predictions refers to the fact that results obtained via simulations are confronted with reliable experimental results. Performance of SQM2.20 has been rigorously verified over a benchmark dataset named PL-REX (Protein–Ligand Refined EXperiment) consisting of high-resolution crystal structures and reliable experimentally determined P-L binding affinities (PL-REX comprises 10 diverse protein targets, with 164 QM-optimized P-L complexes).

We have examined the variability of SQM2.20 scoring using a single receptor, in case of each protein target of PL-REX. System preparation for scoring includes annealing of hydrogen atoms in protein. Hydrogen annealing is affected by the value of random seed, which is set as input parameter. Out of 100 considered cases (10 protein targets x 10 different random seeds), 94 cases belong to the interval with absolute difference in squared Pearson coefficient R^2 from the value averaged per protein target of 0.05. Such result allowed us to establish the difference in R^2 values of $2 \cdot 0.05 = 0.1$ as a significant change in scoring results.

Each of protein targets of PL-REX comprises different protein crystal geometries. The same applies to protein crystal geometries of two additional CDK2 systems, which were considered. We have investigated the impact of protein crystal structure on SQM2.20 scoring result over PL-REX dataset and two additional CDK2 systems in the next two cases: within ligand series, and when using protein crystals with different ligands (here CDK2 protein target was used as an example). Our general conclusion is that the sensitivity of scoring on crystal's geometry is low, which is advantageous for applications.

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Investigation of the Mechanical Behavior of Graphene-Reinforced Magnesium via Experimental and Finite Element Method

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Abstract

Magnesium matrix composites are highly regarded for their exceptional strength, low weight, and ease of machining, making them well-suited for applications in aerospace, automotive, and biomedical fields. While ceramic reinforcements have been extensively explored, the remarkable properties of graphene have recently gained significant interest. This research investigates how shaping pressure (150-600 MPa), sintering temperature (490 ∘C to 610 ∘C), sintering duration (30-180 minutes), and graphene content (0.15-0.75 wt.%) influence the mechanical and wear characteristics of magnesium composites. The optimized composite, incorporating 0.15 wt.% graphene and sintered at 520 ∘C for 60 minutes, exhibited outstanding properties, including a density exceeding 96%, a hardness of 44.34 HV, a compressive strength of 300 MPa, and a wear rate of 8.52 × 10 mm^3/Nm. Increasing graphene content beyond this level led to diminished properties due to agglomeration. At lower concentrations, graphene enhances mechanical properties, whereas at higher amounts, it functions as a lubricant, promoting particle sliding. Finite element method (FEM) simulations demonstrate that 0.15 wt.% graphene improves stress distribution and stiffness by creating localized stress concentrations and serving as load-bearing sites. These results emphasize graphene's ability to improve magnesium composites, provided that processing parameters are carefully controlled to prevent agglomeration. The study highlights the importance of balancing graphene content to optimize mechanical performance while preserving structural integrity.

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Investigation of the Mechanical Behavior of Graphene-Reinforced Magnesium via Experimental and Finite Element Method

Emine Özlem Dengiz*†[1,2], Cengiz Görkem Dengiz*[2], and Mevlüt Gürbüz[3]

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Abstract

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Quantitative Analysis of Nanoscale Mechanical Behavior in Hybrid Materials Through Nanoindentation and FEM Simulations

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Abstract

This study examines the nanoscale mechanical behavior of hybrid materials composed of alternating crystalline and amorphous phases, focusing on the role of nanostructural geometry in determining mechanical performance. Nanoindentation experiments were conducted on hybrid material samples with layer thicknesses ranging from 20 nm to 100 nm. The mechanical properties, including hardness and elastic modulus, were measured using a Berkovich indenter under maximum loads of 2 mN, with load-displacement curves analyzed to capture deformation mechanisms.
The experimental results showed that materials with 50 nm layer thickness exhibited the highest hardness (6.8 GPa) and elastic modulus (130 GPa), attributed to optimized stress distribution at the interfaces. In contrast, samples with 100 nm layers demonstrated reduced hardness (4.5 GPa) and elastic modulus (105 GPa), indicating a diminished influence of nanoscale confinement.

Finite element method (FEM) simulations were performed to validate the experimental findings. Simulations modeled the stress-strain behavior at the nanoscale, incorporating experimentally measured properties and phase distributions. The FEM results closely matched the experimental data, with deviations below 3%. Stress concentration maps revealed that smaller layer thicknesses minimized localized plastic deformation, enhancing overall mechanical strength.
This integrated approach highlights the critical influence of nanoscale geometrical features on the mechanical behavior of hybrid materials. The findings provide valuable insights for designing advanced materials with tailored properties and support the MecaNano Action's mission to advance multiscale understanding of mechanical behavior in nanostructured materials.

*Speaker

Nanoindentation and Defect Dynamics in Irradiated Fcc NiFe Alloys: Insights from Experiments and Atomistic Modeling

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Abstract

We present the effects of irradiation-induced defects on the nanomechanical response of NiFe alloys through a combination of experimentally guided nanoindentation and atomistic simulations. Defects in the irradiated materials were characterized using TEM images, providing essential input for MD simulations of overlapping collision cascades to prepare irradiated samples at various doses (2). The simulations revealed mechanisms of defect formation and evolution, including the emergence of an A15 Frank-Kasper phase within the {111} plane in pure Ni, Ni.Fe., and Ni.Fe. at fluences up to 2×10^{1} ions/cm^2, serving as a precursor to Frank loop nucleation (1). In Ni.Fe., compact 3D precipitates heavily decorated with Fe atoms were observed. However, these precipitates remained too small to evolve into Frank loops, even at elevated fluences. Nanoindentation experiments and simulations demonstrated a notable increase in hardness in irradiated alloys compared to their pristine counterparts (4,5). From the atomistic modeling, we provide detailed analyses of the irradiated samples revealed surface morphologies, dislocation densities, and strain mappings to discuss the mechanisms of dislocation pinning during mechanical loading due to irradiation-induced defects. These defects were found to obstruct dislocation motion, contributing to the enhanced hardness of the material.
(1) E. Wyszkowska et al. Nanoscale 15, 4870 (2023).
(2) A. Ustrzycka et al. Int. J. Plasticity 182, 104118 (2024)
(3) L. Kurpaska et al. Materials & Design 217, 110639 (2022).
(4) F. Dominguez-Gutierrez et al. J. Appl. Phys. 135, 185101 (2024)

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Suppressing shear band instability for strong and ductile crystal/glass nanolaminates

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Abstract

Crystal/glass nanolaminates (NLs) present mutually exclusive mechanical properties by combining the strength of the glass phase with the ductility of the crystalline phase. For instance, optimizing the layers thickness of Cu/CuZr NLs suppresses shear band instability and promotes co-deformation, achieving a strength of 2.5 GPa and 40% plasticity in compression (1,2). However, the role of deformation mechanisms and interface interactions in suppressing shear band instability remains incompletely understood. Additionally, BCC/glass NLs remain largely unexplored despite their proven potential to present high strength and ductility (3).
Here, we synthesized 2 μm-thick Fe/Zr40Cu60 (crystal/glass) NLs by magnetron co-sputtering. We varied the Zr40Cu60 thickness (10-90 nm), keeping the Fe at 10 nm, to investigate the size-dependent deformation-mode transition. In a second approach, we varied the bilayer period between 20-80 nm at equal volume fractions, tuning the interface density. This study aims to establish architectural and interface engineering strategies to suppress shear band instability.

The hardness of the Fe/Zr40Cu60 NLs exceeds individual layer values, reaching 9.6 GPa for the 10/10 nm NLs due to the sharp interfaces blocking the shear band. Micropillar compression tests reveal that thicker Zr40Cu60 layers (90 nm) lead to localized shear bands, whereas thinner layers show delayed shear band instability. Combining interface and architecture effects, 20/20 nm exhibits an exceptional 45% compressive plasticity and yield strength of 1.96 GPa due to effective shear band instability suppression.

Overall, our findings provide insights into the nanoengineering of crystal/glass NLs interfaces and architectures to enhance their mechanical properties effectively.
(1) J. Y. Kim *et al.*, Adv Funct Mater, vol. 21, no. 23, Dec. 2011. (2) W. Guo *et al.*, Acta Mater, vol. 80, 2014. (3) F. Qin *et al.*, Mater. Sci. Eng. A, vol. 891, 2024.

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Analysis of the physical properties of CdxZn1-xS-based nanocomposites synthesized through sonochemical and SILAR methods

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Abstract

The work detailed here examines the developmentof CdxZn1-xS-based nanocomposites produced by sonochemical methods and the Successive Ionic Layer Adsorption and Reaction (SILAR) technique. To evaluate their effecton the production of nanoparticle yield Cd0.4Zn0.6S nanoparticles, three different stabilizers-polyvinyl alcohol(PVA), 3-mercaptopropionic acid (3-MPA), and styrene-were used. In addition, nanocomposites with varying Cd: Zn ratios (x =0.2, 0.4, 1) were fabricated to study their structural, optical, and morphological properties. The SILAR method facilitated the synthesis of nanocomposites with x values of 0.1, 0.2, and 1, while temperature-dependent synthesis of Cd0.2Zn0.8S was pursued at 25∘C, 45∘C, and 65∘C.XRD analysis indicated that SILAR samples using PVA as a substrate showed prominent PVA peaks. In contrast, sonochemical samples had less intense stabilizer-related peaks and more pronounced CdxZn1-xS diffraction peaks, suggesting improved crystallinity due to fewer defects and crystallization induced by ultrasonic waves. Both techniques successfully produced ternary CdxZn1-xS compounds in the hexagonal phase. However, for x = 1, SILAR yielded hexagonal CdS, while the sonochemical method resulted in cubic CdS, which can be attributed to the energy supplied by ultrasonic waves.SEM images illustrated that sonochemical nanocomposites contained both small and large crystallites, while SILAR samples either adhered to the polymer surface or formed fragments. The bandgap energy (Eg) values were lower for sonochemical samples (2.80 eV and 2.25 eV) compared to SILAR samples (3.05 eV and 3.45 eV), reflecting blue and red shifts, respectively, associated with interactions involving defects and the morphology of the nanoparticles. The band gap energy depends on particle size, quantum confinement, and surrounding environment, with SILAR producing 5.42 nm particles and sonochemical yielding 3.06 nm for CdS nanoparticles. FTIR spectra indicated shifts in the absorbance of functional groups, implying variations in metal-sulfide bonding and particle size depending on the synthesis method.

*Speaker

Interfaces as dislocation density fields for bridging length scales in nanomechanics

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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, defects as diverse as dislocations and high-angle grain boundaries, as well as interactions among them, in both cubic and hexagonal crystals. Assessments of this approach with cubic (Cu, Al) and hexagonal (Mg, Ti) materials is also presented. The prediction by means of machine learning approaches of interfaces characteristics as represented by dislocation density fields is also explored. In the light of our results, the implication of such a discrete-to-continuum crossover for bridging scales in nanomechanics is discussed.

*Speaker

Review of Auxetic properties of textile structures

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Abstract

The research field of auxetics, materials or structures exhibiting a negative Poisson's ratio, has received attention because of the unusually advantageous material properties that can be achieved with it, such as high indentation resistance and high shear resistance. In the past decades, the theoretical understanding of different factors that can lead to an auxetic behaviour has advanced greatly. This review aims to describes the auxetic structures that have currently been identified and designed in textile structure

This review describes the most common basic structures analysed in the literature in textile structures. A number of alter native auxetic arrangements have been proposed in the literature. Still, most of these structures exploit the same principles and mechanisms. Finally, the concepts described in this review can directly be expanded to 3D auxetic configurations. These are achieved in different ways, with the most common being compressed foams, where the cellular bubble takes the shape of an auxetic kinematic configuration similar to the re-entrant hexagonal structure . More complex configurations, based on three-dimensional well-defined unit cells, include different 3D versions of textile structures is reported.

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Comparative Analysis of the Gao-Nix Model and Multifractal Scaling Law Model for Indentation Size Effect

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Abstract

In this study, we performed a comprehensive investigation into the differences between the Gao-Nix (GN) model and the Multifractal Scaling Law model through the analysis of experimental hardness data. By comparing these two models, we derived a characteristic length for the GN model and a critical characteristic length for the Multifractal Scaling Law model. The experimental data facilitated a detailed comparison, revealing the underlying similarities and differences between the two models.
Both models employ similar formulas but diverge in the method used to calculate the characteristic lengths h* and L*. The GN model utilizes a direct calculation approach, while the Multifractal Scaling Law model incorporates a more complex scaling mechanism to determine the critical characteristic length. Despite these differences, both models exhibited satisfactory fitting with the experimental data, demonstrating their robustness in capturing the hardness behavior of materials.

To further refine the GN model and improve its applicability, we propose a modified Gao-Nix formula: (H/H0)2=1+(h⋆/h)2(H/H_0)ˆ2 = $\sqrt{}${1+(ℏˆ ∗ /ℎ)̂2}.$Thismodificationincorporatesvariationsinthecriticalcharacteristi$

*Speaker

Temperature and strain rate dependent indentation size effect at shallow indentation depths

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Abstract

Indentation size effect (ISE), i.e., size-dependent increase in hardness, occurs in plastically deformable materials when the size of the indent approaches the critical length scale. In metals, in which the plastic deformation is mediated by the slip dislocation movement, this critical length scale is associated with the (average) dislocation spacing. The ISE makes it difficult to compare the results obtained at different (in particular small) loads that are needed for characterization of e.g. small particles or thin layers.
In metals, the ISE can be described by the Nix-Gao model based on the concept of geometrically necessary dislocations required by the indenter induced permanent shape change. This model almost perfectly predicts the ISE for indentations at the micrometer scale but overestimates the hardness for very shallow indentation depths pointing out some of its limitations. The deviation of measured hardness from values predicted by Nix-Gao model is affected by several factors (as e.g. the indenter geometry), which complicates the analysis and comparison between the results published by different authors. However, the most important factor appears to be lattice friction stress (1).

This contribution focuses on the effect of temperature on ISE at shallow indentation depths in (100) oriented silicon iron single crystal which is a model material for bcc (iron-based) metals and alloys. The variation of material parameters describing the effective plastic zone is shown and related to the change of the prevailing slip mechanism with the temperature and strain rate.

(1) Haušild Petr. On the breakdown of the Nix-Gao model for indentation size effect. Philosophical Magazine, 2021, 101, p.420-434.

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Integrating Machine Learning and Data Mining Techniques with Surface Texture Analysis to Explore Wetting and Optical Properties of CuAg Alloys

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Abstract

Copper-Silver (CuAg) alloys, due to their unique properties including high electrical and thermal conductivity and excellent corrosion resistance, have a diverse range of applications in industries such as electrical engineering, chemical processing, and aerospace (1). We investigated the effect of surface texture on the wetting and optical properties of these alloys. The CuAg alloys were synthesized on textured Si substrates in the form of Material Libraries consisting of alloy thick layers with a concentration gradient 0-100 at. % by PVD method (1). Chemical composition, thickness, and phase content of the samples were examined by XRF and XRD measurements. The surface texture and local optical properties were measured by Colorimetric Microscopy (C-Microscopy) approach (2), which delivers information on colorimetry and morphology at microscale. We observed correlation between alloy layer thickness and surface optical properties (reflectance R, colorimetric variables). By measuring the alloy surface wetting properties via water contact angle (CA) measurements, we found that CA is strongly influenced by the alloy layer thickness. We also noted that different surface texture parameters, as measured from color-calibrated images by C-Microscopy, influence CA and optical properties. Finally, we employed a Machine Learning-based regression model to predict water CA based on measured surface texture parameters and optical parameters. We successfully achieved an accuracy of the model for water contact angle prediction in the range of around 5 degrees. Our studies contribute to understanding of alloys under various surface conditions.

(1) K. Wieczerzak et al., Adv. Sci. 10, 2302997 (2023)
(2) B.R. Jany, Micron 176, 103557 (2024)

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Modification of the matrix-reinforcement interface in Ni-SiC composites

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Abstract

Mechanical properties of composites depend on matrix, reinforcement as well as their interface performance. For a given material system, one can tailor the properties in manufacturing process.
Spark Plasma Sintering (SPS) is a method to obtain bulk Ni-SiC samples, where their microstructure can be controlled by time, pressure and temperature of process. Those parameters also influence interfacial behaviour (1).
On the other hand, co-electrodeposition (CED) is used for Ni-SiC coatings. In this case microstructure is changed with current mode and its density, temperature or stirring. However, the standard SEM observations show that interface is rather unaffected by those parameters (2).
In this work, we compare matrix-reinforcement interface in Ni-SiC composites prepared by SPS or CED. Additionally, we use a protective layer on SiC particles used for CED to modify the interface in this process.
The experimental part consists of SEM, EDS, XRD characterization as well as mechanical testing with nanoindentation and micro-beam bending.
Results show a significantly different interface depending on process, as well as its different mechanical behavior.

(1) S. Nosewicz et al. *The influence of spark plasma sintering on multiscale mechanical properties of nickel-based composite materials,* Materials Science and Engineering: A, 891, 146001, 2024
(2) P. Jenczyk et al. *Application of SiC particles coated with a protective Ni layer for production of Ni/SiC co-electrodeposited composite coatings with enhanced tribological properties.* Ceram. Int. 45, 23540–23547, 2019

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Investigation of Mechanical and Physical Properties of Polyphenylene sulfide (PPS) Matrix Composite Reinforced with GNP and MWCNT

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Abstract

Advancing technology and modern engineering applications demand increasingly higher performance from materials. Composite materials are thus widely utilized in numerous industries due to their exceptional mechanical properties, lightweight nature, and customizable structures. Among high-performance thermoplastics, polyphenylene sulfide (PPS) is particularly notable for its high-temperature resistance, chemical stability, and ease of processing, making it a key material in aerospace, automotive, and electronics sectors. Enhancing PPS's properties through reinforcement with graphene nanoplatelets (GNPs) and multi-walled carbon nanotubes (MWCNTs) has shown significant potential for meeting demanding requirements, including improved thermal conductivity. In this study, PPS-based composites were fabricated by incorporating varying weight fractions of GNPs and MWCNTs via melt mixing, followed by injection molding. The mechanical, thermal, and structural properties of these composites were systematically evaluated. A remarkable 49.2% increase in tensile strength was observed with 5 wt% MWCNT reinforcement. Both additives also contributed to a hardness improvement of approximately 50%. Scanning electron microscopy (SEM) analysis confirmed the homogeneous dispersion of the reinforcing materials, which effectively hindered crack propagation. Additionally, the nano-additives enhanced the crystallization process, as evidenced by an increase in crystallization temperature (Tc) due to nucleation effects. Notably, a 10 wt% MWCNT reinforcement achieved the highest thermal conductivity improvement, yielding a 1375% increase compared to pure PPS. These findings underline the promising potential of GNP and MWCNT reinforcements to enhance PPS composites, offering tailored solutions for high-performance applications across diverse industries.

*Speaker

Investigation of the Potential of PTFE Coatings for Journal Bearings

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Abstract

The growing need for sustainable and lead-free alternatives to traditional white metal coatings has led to the exploration of PTFE (Polytetrafluoroethylene) coatings for journal bearings. PTFE coatings offer desirable properties such as low friction, high wear resistance, and chemical stability, making them a promising choice for industrial applications. While white metal coatings are widely used for journal bearings, their lead content presents significant environmental and health concerns, motivating the search for safer alternatives.
This study focuses on evaluating PTFE coatings applied to S355 steel journal bearings using epoxy spraying equipment. Different PTFE formulations, including pure PTFE, PTFE-MoS blends, and PTFE-glass fiber composites, were examined for their adhesion strength, microhardness, and microstructure. The adhesion strength was measured using an Elcometer adhesion tester, while microhardness testing provided insights into the coatings' resistance to localized deformation under load. Microstructure analysis was conducted to assess the coatings' integrity and bonding quality with the base material.
The findings of this research aim to demonstrate the suitability of PTFE coatings as a lead-free, sustainable alternative to traditional coatings in journal bearings. Key performance factors such as adhesion, microhardness, and material durability were evaluated to determine the effectiveness of PTFE coatings in high-performance applications. By focusing on environmentally-friendly materials, this study contributes to the development of more sustainable engineering practices in machinery components.

*Speaker

A comparative study on the nanotribological properties of amorphous and polycrystalline forms of MoS2 using Nano-Indenter and AFM.

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Abstract

This study compares the wear and friction behavior of polycrystalline and amorphous MoS2 thin films using nanoindentation and atomic force microscopy. Samples were prepared by magnetron sputtering. Scratches by indenter were generated on films of different thicknesses (2.4 μm for polycrystalline, 1.1 μm for amorphous) under normal loads from 0.1 to 2 mN and scratch speeds from 5 to 500 μm/s. The amorphous film consistently showed superior wear resistance: its scratch grooves were roughly half as deep and wide as those on the polycrystalline sample under identical test conditions. Both materials exhibited a wear volume that increased with normal load, in accordance with the Archard law, while scratch speed showed only a minimal effect. Furthermore, we have used AFM to characterize the lateral (friction) force *FL* acting on a sharp silicon tip sliding on amorphous and polycrystalline MoS2 in their pristine conditions or after scratching them with the Berkovich indenter. The friction measurements were conducted with a scan speed of 5 μm/s and a normal force up to 70 nN. Frictional measurements revealed a linear increase with a regular load but with a marked drop in the coefficient of friction in scratched regions, which became smoother after testing. In the wear track formed on the amorphous material, the RMS roughness was indeed found to decrease by a factor of 5 (from 54 nm to 11 nm). On the polycrystalline material, it appears that the RMS value was reduced by a factor of 2 (from 24 nm to 12 nm). A comparison of independent nanoindentation tests also allows us to conclude that the polycrystalline form is more friable than the amorphous one and, therefore, less suited as a solid coating in ambient conditions.

*Speaker

Effect of Chitosan Particle Size on the Mechanical Performance and UV Degradation of Low-Density Polyethylene–Chitosan Composites

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Abstract

This study investigates the effect of chitosan particle size on the UV degradation and mechanical properties of Low-Density Polyethylene–Chitosan (LDPE/CH) and LDPE–Nanochitosan (LDPE/CHNP) composites. The composites were fabricated using solvent casting and peroxide-initiated melt compounding methods, incorporating chitosan nanoparticles of varying sizes. Mechanical analysis revealed that tensile strength and elastic modulus increased with decreasing chitosan particle size, with the LDPE/CHNP composite containing 15% nanochitosan (≤100 nm) achieving a maximum elastic modulus of 23.10 MPa and tensile strength of 3.52 MPa.

UV degradation studies were conducted by placing the samples in a UV-light chamber with a total radiant exposure of 2.50 × 10 J/m^2 for 18 weeks. Degradation was evaluated using weight loss measurements, FTIR analysis for chemical bond changes, SEM for morphological alterations, and tensile testing for mechanical degradation. Results indicated that nanochitosan-loaded composites exhibited higher degradation efficiency, with the 20% CHNP sample showing 50% weight loss and a degradation rate of 0.12 g/d after 21 days. Morphological analysis confirmed superior dispersion of nanochitosan, leading to enhanced mechanical stability and biodegradability. The addition of palm oil as a plasticizer improved hydrophilicity and further accelerated degradation. However, these findings highlight that adding nanochitosan to low-density polyethylene (LDPE) not only makes the material stronger but also helps it break down faster under UV light, making it a more eco-friendly alternative to traditional plastics.

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In-Situ TKD Tensile Testing Reveals Complex Nanoscale Deformation Twinning in Rhenium

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Abstract

Deformation twinning (DT) plays a central role in the plastic deformation of hexagonal close-packed (HCP) metals, due to their insufficient amount of slip systems. DT can enable plasticity along the c-axis when pyramidal slip is not possible. However, DT has also been associated with reduced ductility, high residual stresses, and the promotion of fracture. As a result, DT complicates the broader adoption of HCP metals in industry. While DT has been extensively studied, fundamental questions persist regarding twin nucleation, growth mechanisms, and the interaction of twins with surrounding microstructural features, such as grain boundaries and other twins. This study employs a novel in-situ transmission Kikuchi diffraction (TKD) methodology developed in-house at EMPA Thun, which is capable of sub-10 nm resolution orientation mapping during micro tensile testing (1). Applied to single-crystal Rhenium under c-axis tension, we reveal previously unobserved mechanisms relating to the commonly observed extension twin (ET), specifically the formation of secondary ETs within primary ETs. Together with interactions between intersecting primary twin variants, the secondary ETs lead to the formation an apparent nanograined microstructure. Based on the insights gained into the fundamental deformation mechanisms of Rhenium, implications for its accommodation of plastic strain are discussed. This includes the effect of secondary ETs on twin thickening mechanisms and fracture behavior, particularly considering the expected intense shear localization at the interfaces of matrix and secondary ET.

*Speaker

Scale-Bridging Nanoindentation to Probe Structural Heterogeneity in Amorphous Metals

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Abstract

Commonly amorphous metals are considered as being homogenous. In recent year the consensus has drastically shifted towards a structural heterogeneity with the aid of Synchrotron and TEM experiments. The given heterogeneity in the material could be probed with different micromechanical testing techniques e.g. Nanoindentation. This poster will show scale bridging nanoindentation on different amorphous metals regarding the onset of plasticity and surface heterogeneity of systematically designed sample sets.

*Speaker

Room-temperature recrystallization of Mo induced by nanoindentation

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Abstract

We performed nanoindentation on molybdenum (Mo) single-crystal (SC) and polycrystalline (PC) samples utilizing a spheroconical indenter. Load-displacement curves of SC samples exhibited characteristic pop-in (displacement burst) indicating an abrupt transition from elastic to plastic deformation at the maximum elastic shear stress of 12-16 GPa. On the contrary, much weaker pop-ins were observed in the PC sample (the corresponding maximum shear strength was below 0.5 GPa). The cross-sectional transmission electron microscopy of the indented area in SC samples revealed the formation of new near-surface grains when the loading was terminated manually immediately after the pop-in event. By contrast, no new grains could be observed in the PC sample, indicating that the pop-in and recrystallization are correlated. We propose that the dislocations nucleated during a singular pop-in event are driven by high elastic stress and promote lattice rotation and formation of the high-angle grain boundary (HAGB), whose existence was confirmed by the orientation maps below the imprints obtained with the precession electron diffraction. When the SC Mo sample was continuously indented to the loads significantly exceeding the first pop-in, no visible new grains were formed. Molecular dynamics simulations disclosed that the small near-surface grains are destroyed by further indentation, correlating with the experimental observation. Our results shed new light on the deformation mechanisms during the nanoindentation of defect-free Mo. Room-temperature recrystallization is unprecedented for Mo which usually recrystallizes at temperatures above 1000 ∘C.

*Speaker

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Metal-Ceramic Nanolaminate Design for Enhanced Thermal and Mechanical Properties

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Abstract

Metal-ceramic multilayer composites show improved strength, ductility, and toughness due to the synergistic effects of their distinct intrinsic properties and characteristics. In such composites, interface strengthening and microstructural control through grain size and layer refinement is critical in determining mechanical properties. In this study, we fabricate and test nanolaminates composed of metallic alloy layers with thicknesses ranging from 30 to 120 nm, alternating with thin amorphous Al2O3 interfaces measuring 2 to 5 nm. The metal and oxide are deposited using physical vapor deposition (PVD) and atomic layer deposition (ALD), respectively, within a hybrid deposition chamber, without breaking the vacuum.
The incorporation of these thin amorphous oxide interfaces between the metal layers serves several purposes: a) it disrupts the columnar growth of the metal alloy film, allowing for a smaller and more controlled grain size, b) it regulates diffusion, c) it inhibits the propagation of dislocations and twins, and d) it controls grain boundary migration and recrystallization during annealing.
As a model system, we fabricated Cu1-x – Alx multilayers and subjected them to various annealing and mechanical tests, including (HT)-nanoindentation, micropillar compression and in situ tensile testing combined with transmission Kikuchi diffraction (TKD). By adjusting the aluminum content, we can accurately control the stacking fault energy in the interlayer, thereby affecting the formation and size of nano-twins. We will also discuss the contributions of several small-scale mechanisms, such as Hall-Petch strengthening, solid solution effects, and interface strengthening.

*Speaker

Micro-mechanical evaluation of coatings produced by micro-arc oxidation of titanium

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Abstract

Micro-arc oxidation (MAO), also called plasma electrolytic oxidation (PEO), is a popular electrochemical method of surface modification of so-called "valve metals" like titanium, enhancing their properties like biocompatibility, osseointegration, antibacterial protection, etc. In this way, a new class of medical implants may be developed, providing unusual performance. Oxidation of titanium-based materials significantly increases their originally poor wear resistance due to the high hardness of the formed oxides. The disadvantage of MAO coatings is the inherent porosity associated with the action of micro-arcs and the evaporation of part of the material. Additionally, the produced coating is characterized by a multiphase and fine-grained microstructure. Therefore, analysis of mechanical properties such as hardness using conventional methods causes averaging of information from different microstructural elements. Accurate analysis of the hardness of individual microstructure features requires the use of micromechanical methods coupled with real time observations (in-situ testing).

Therefore, in this work, the hardness of the MAO coatings was analyzed with the use of FT-NMT04 FemtoTools indenter installed in SEM microscope equipped with FEG eletron gun on the metallographic sections of the samples (embedded in resin). For this purpose, the Berkovich indenter was used and an indentation depth was set at 100 nm. The MAO coatings were deposited on cylinders made of hydrostatically extruded titanium of commercial purity. The tribological properties of the samples were studied by performing scratch and wear tests. The microstructure and surface topography of the coatings were investigated with FEI Versa 3D scanning electron microscope.

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*Speaker

Prediction of Mechanical Properties using DIC analysis and Machine Learning

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Abstract

Digital image correlation (DIC) stands out as a powerful technique, providing a visual representation of strain maps during mechanical deformation while generating extensive data at every pixel, revealing surface strain components [1]. The true potential within this dataset is unveiled through materials informatics, seamlessly incorporating advanced statistical and machine learning methodologies. However, challenges arise when a comprehensive understanding is lacking, potentially leading to overfitting artifacts and unsuccessful machine learning training. To address this concern, the utilization of unsupervised machine learning techniques, exemplified by principal component analysis (PCA), proves to be insightful in navigating these complexities and can be used extracting valuable information from DIC strain data [2, 3].

In our study, we investigate inferring the mechanical properties of materials solely using local strain information produced by DIC with the use of our developed techniques based on unsupervised ML. As an example, we demonstrate the detection of the transition to the plastic deformation stage and prediction of plasticity localization using experimental DIC data from "creep" and "uniaxial tension" mechanical tests, as well as synthetic data from nano-indentation simulations.

* Speaker

Effect of Ag-doping concentration on the structural and optical properties of NiO nanoparticles

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Abstract

In the presented work, pure and Ag-doped NiO nanoparticles were synthesized by sonochemical method and subsequent calcination process at 400℃. For the synthesis NiSO47H2O and NaOH were used as initial reagents and polyvinylpyrrolidone was used stabilizing agent. In order to study the effect of doping concentration, AgxNi1-xO nanoparticles were synthesized with various dopant amount (x=0.02, 0.04, 0.06 and 0.1). The obtained nanostructures were investigated using X-ray diffraction, UV-visible spectroscopy, FTIR spectroscopy, transmission electron microscopy. Five broad diffraction peaks observed at 2 *theta*=37.40º, 43.36º, 62.98º, 75.42º and 79.58º corresponding to the (111), (200), (220), (311) and (222) planes in the diffractogram of the undoped sample indicates the formation of surface-centered cubic NiO. These results are in good agreement with JCPDS #47-1049. No peaks related to silver or silver (I) oxide (Ag2O) were observed in the diffractograms of doped samples. NiO nanoparticles doped with 2%, 4%, and 10% Ag crystallized with a preferred (200) orientation, while NiO nanoparticles doped with 6% Ag crystallized with a preferred (111) orientation. According to UV-vis. spectroscopy measurements, absorption peaks were observed at wavelengths of 279.6 nm, 281.8 nm, 275 nm, 282.6 nm, and 281.8 nm in the spectrum of undoped and 2%, 4%, 6%, 10% Ag doped NiO nanoparticles, respectively. The weak intensity peak observed at 601 cm-1 wavenumber in the IR spectrum of undoped NiO nanoparticles is assigned to the Ni-O vibrational frequency. This characteristic peak was observed at 599 cm-1 in the spectrum of NiO nanoparticles doped with 10% Ag and these results confirm the formation of NiO. Based on TEM measurements, undoped NiO nanoparticles have spherical morphology and the size is in the range of 3.24 nm-12.09 nm. No changes in morphology occurred after doping for Ag0.1Ni0.9O nanoparticles and the size is in the range of 3.04 nm-16.34 nm.

*Speaker

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Unsupervised Machine Learning for Nanoindentation Mapping Analysis and Microstructural Correlation

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Abstract

Nanoindentation mapping provides high-resolution mechanical property distributions across multiphase materials or materials with gradient properties. However, extracting meaningful patterns from such large datasets requires advanced data-driven techniques. This study leverages unsupervised machine learning (ML) approaches, particularly clustering algorithms, to analyze nanoindentation mappings and correlate them with microstructural maps obtained from techniques such as Electron Backscatter Diffraction (EBSD), confocal microscopy, Atomic Force Microscopy (AFM), and Optical Microscopy (OM). The clustering approach enables the identification of distinct mechanical zones, facilitating a deeper understanding of structure-property relationships.

To ensure optimal clustering performance, different methods (e.g., k-means, Gaussian mixture model, DBSCAN, hierarchical clustering) are classified and evaluated using criteria such as the silhouette score, Davies-Bouldin index, and Calinski-Harabasz index. This systematic evaluation helps refine data-driven segmentation of mechanical heterogeneities and improves the robustness of microstructure-property correlations. Then, to enhance efficiency and reproducibility, the entire dataflow is implemented and automated using the PyAnsys library, enabling seamless integration with a materials database developed within Granta MI. Beyond facilitating experimental data interpretation, this workflow supports material design and mesoscale simulations by providing reliable, data-driven input parameters for computational modeling.

Finally, ithis study, different specimens-including advanced steel, composite coatings, and additively manufactured (AM) polymers-are analyzed, and the results are presented, highlighting the effectiveness of the proposed methodology in characterizing complex material systems.

*Speaker

REGULATION OF RELEVANT GENE EXPRESSIONS IN CELLS AND BACTERIA BY DYNAMIC MECHANICAL CONDITIONING

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Abstract

Solid mechanical and fluid mechanical signals are ever-present in all living organisms across all pertinent time and size scales. The fate of cells as to their differentiation, growth, migration or apoptosis depends to a large extent on the mechanical information they sense, integrate and respond to.
How the cells sense and transmit forces from their environment to their nucleus is under intense investigation in recent years, but we are still far from having a clear picture of the associated events.

In this presentation we examine two different cell types: bovine capillary endothelial cells (EC) and *Staph. epidermidis* bacteria with respect to structural and gene expression changes that take place under controlled application of specific stresses. In the case of ECs a combination of mechanical stresses results in significantly different responses, while in bacteria fluid shear stresses have been the cue to examine their responses.
A concluding remark: dynamic mechanical test conditions are important in revealing epigenetic changes in cells and bacteria.

*Speaker

Hybrid Composite production for Defense Industry

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Abstract

The purpose of this study is to produce hybrid composites for use as armor materials in the defense industry. Titanium was used as the matrix material in the study. Titanium is a preferred material in the defense industry due to its wear resistance and hardness properties. Graphene, which has become a popular material in recent years in the manufacture of metal matrix composites due to its exceptional mechanical and solid lubricant properties, was preferred as the reinforcement material. Boron carbide (B4C) was preferred as another reinforcement material due to its high flexural strength, high modulus of elasticity, high hardness, wear resistance, high fracture toughness, compressive strength, chemical reaction resistance, and heat resistance. In the study, the hybrid composite was produced by powder metallurgy method. According to the study results, the mechanical properties (compressive strength, hardness) were increased by 30%. The wear rate was significantly reduced. It was observed that TiC and TiB whisker structures formed in the microstructure were effective on mechanical properties. Acknowledgement; This study was supported by TUBITAK with project code 124M749.

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Nanowear in molybdenum disulfide studied by molecular dynamics simulations

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Abstract

Molybdenum disulfide (MoS2) is a layered material that has been used as a solid lubricant for decades(1). The experimental verification of superlubricity in the early nineties for crystalline MoS2 coatings in ultrahigh vacuum conditions(2) sparked again the interest for molybdenum disulfide. Since then, a lot of effort has been devoted in order to understand (and possibly control) the complex phenomena taking place during sliding in such a system, *e.g.* the formation of crystalline layers from molecular precursors(3) or from amorphous material(4). On the contrary, the understanding of abrasive wear processes on such a material is still in an early stage.

In this study, we performed molecular dynamics (MD) simulations in order to shed light on the elementary steps in the wear process of MoS2 with atomistic detail. A rigid diamond tip has been used to indent a six-layer thick system, and then the tip has been dragged in order to scratch the material. The position and the force acting on the tip has been followed for more than 20 ns, together with the damage done on the substrate. Different MoS2 orientations and normal loads have been considered. The trajectory analysis revealed that the tip moved in a stick-slip fashion, somehow recalling the dynamics that take place during sliding. Such a behavior has also been observed in atomic force microscopy (AFM) experiments.

References

(1) T. Spalvins, J. S. Przybyszewski, *NASA Technical Note* D-4269 (1967).

(2) J. M. Martin *et al.*, *Phys. Rev. B*, **48**, 10583 (1993).

(3) S. Peeters *et al.*, *Appl. Surf. Sci.*, **606**, 154880 (2022).

(4) P. Nicolini *et al.*, *ACS Appl. Mater. Interfaces*, **10**, 8937 (2018).

*Speaker

Contact mechanics and tribological properties on polymers: An experimental approach.

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Abstract

Contact mechanics plays a role in tribology, especially for viscoelastic materials such as polymers. In this presentation, I will quickly remind the principle of the atomic force microscopy circular mode (AFM circular mode) and its advantages for probing tribological properties of polymers. This original AFM mode was applied for probing the adhesion force in a sliding nano-contact on rigid polymer materials such as, poly-methacrylate of methyl (PMMA) and polycarbonate. Our experimental results show that the adhesion force increases with the sliding velocity in an intermediate regime. The comparison between the shapes of the force curves before and after this regime sustain the assumption that this behavior may be rely on a transition between a JKR-like contact mechanics to a DMT-like contact mechanics. In addition, the preliminary results reporting the evolution of the friction coefficient with the sliding velocity support the idea that friction of viscoelastic materials such as polymers is governed by the adhesion in the contact.

*Speaker

Comparative analysis of plastic deformation in Zr-Cu-Ag metallic glasses: insights from micropillar and bulk sample compression tests

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Abstract

Metallic glasses are promising materials with broad applications duo to their outstanding properties. This study investigates the mechanical behaviour of Zr50Cu37Ag13 and Zr42Cu40Ag18 alloys through micropillar and bulk sample compression tests. Both alloys were synthesized using arc melting and tested at strain rates from 10-4 to 10-1 s-1. Micropillar tests revealed significant plastic deformation with serrated flow, showing yield strengths of 1468-1590 MPa for Zr50Cu37Ag13 and 1512-1758 MPa for Zr42Cu40Ag18. Bulk tests indicated limited plasticity, particularly in Zr42Cu40Ag18, which exhibited brittle fracture due to the Zr2Ag phase. Negative strain rate sensitivity (SRS) was observed in all micropillar tests and in Zr50Cu37Ag13 bulk samples, while Zr42Cu40Ag18 bulk samples exhibited positive SRS. Analysis of serrated flow in micropillars revealed significant stress drops ($\Delta\sigma$) that increased with decreasing strain rate, indicating active shear band formation and propagation. In contrast, bulk samples exhibited smaller stress drops, reflecting their different deformation mechanisms. Fracture morphologies revealed vein-like patterns in Zr50Cu37Ag13 bulk samples and mixed characteristics in Zr42Cu40Ag18samples, highlighting the influence of sample size and composition on plasticity and mechanical behaviour. This work was supported by the Polish National Agency For Academic Exchange (grant numbers PPN/IWA/2019/1/00061/U/00001).

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Structure of Ta/TaN nanolayered systems investigated by Transmission Electron Microscopy

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Abstract

One of the most important challenges of modern materials engineering is to improve the efficiency and durability of materials, which directly translates into reduced raw material consumption. In many applications, these goals are achieved by strengthening and functionalizing the surface, especially in the case of nanocoatings. The material for the study is Ta/TaN multilayer systems. Electron microscopy (HR STEM, electron diffraction, EDS, EELS) was used to characterize their structure. Geometric parameters (thickness of Ta and TaN component layers, ratio of thickness of metallic to ceramic layers) were determined and their chemical and phase composition was verified. Then, their mechanical properties were characterized using the nanoindentation technique. The last stage was a detailed examination of the indentations created during mechanical tests in order to better interpret the obtained results.

*Speaker

Optimal safety loads and design of polymer nanocomposites under static loading

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Abstract

In the present study, the optimal safety loads and geometry design (layer thicknesses and length) of polymer nanocomposites(PNC), have been found by the multi-parameter optimization procedures (MOPs). As an objective function in MOPs the theoretically developed analytical criterion for no delamination in PNC interfacial layer is used. It is based on the analytical solutions for the interfacial shear stress (ISS) in the layered PNC, subjected to static loading. Two multi-parameter optimization procedures are formulated and solved, first one by Genetic algorithm (Mathcad) and second one - deterministic (Mathematica). By simultaneously varying the 5 parameters (layer thicknesses, length and the magnitude of mechanical load) in preliminary fixed constrained intervals, the safety intervals of the parameters (without delamination) for 5 different PNC are obtained. The obtained results can be used for the fast testing of the existing and a new created electronic or sensor devices, at which similar PNC are part of, to assure their safety work.

Acknowledgements

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Improved thermal stability of Cu nanoparticle thin films via atomic layer deposition

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Abstract

Metallic nanoparticles (NPs) exhibit intriguing properties as a consequence of their spatial confinement and their high surface-to-volume ratio and find applications in functional surfaces. A topic rising in importance is the utilization of NPs as catalysts for energy conversion and storage. To facilitate more advanced use of NPs, a thorough understanding of their synthesis-structure-property relations is crucial. In this study, porous 300 nm thick Cu nanoparticle films (particle diameter 10 nm) are fabricated via Magnetron Sputtering Inert Gas Condensation (MS-IGC) and subsequently coated with an amorphous Al2O3 layer (0-20nm) via atomic layer deposition (ALD). Cross-sectional transmission electron microscopy analysis confirms conformal ALD coverage of the porous structures. Thermal stability of the nanoparticle films is studied with *in situ* heating X-ray diffraction experiments, tracking both the overall evolution of microstructure and stresses in the Cu as a function of annealing temperature (max. 810∘C) and oxide layer thickness. Nanoparticle films without ALD undergo complete densification, while particle mobility is significantly reduced with the protective ALD coating. These results are crucial for and in good agreement with their catalytic performance, peaking at an oxide layer thickness of 2-5 nm, with a minimal tradeoff between stability and catalytic activity/selectivity of Cu. Our findings should facilitate the deposition of NP-based films with higher efficiency and with tailored morphology, making this technique more attractive for e.g. the synthesis of thin film catalysts.

*Speaker

Phase Stability and Mechanical Properties of Cobalt Nanoparticles

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Abstract

Cobalt nanoparticles have attracted high interest due to their unique combination of functional and magnetic properties, making them highly relevant in fields such as energy storage, catalysis, and biomedicine. A unique feature of metallic cobalt is reversible phase transformation between hexagonal close-packed (HCP) and face-centered cubic (FCC) structures. This martensitic transformation occurs because the difference of Gibbs energies between the two phases is very small. The transformation temperature can be tuned by pressure and alloying elements. Most previous studies of metallic cobalt focused on bulk samples, leaving the understanding of cobalt nanoparticles incomplete. This study aimed at determining the mechanical properties of cobalt nanoparticles and correlating them with their phase transformation behavior. Defect-free Co nanoparticles were fabricated via solid-state dewetting of Co thin films deposited on sapphire substrates. Although at room temperature the HCP phase is thermodynamically more stable than its FCC counterpart, obtaining the HCP nanoparticles has proven difficult, as most employed synthesis methods favored the formation of FCC phase due to kinetic and size-related constraints. A combination of atomic force microscopy, scanning electron microscopy, and X-ray diffraction was employed to systematically investigate the equilibrium crystal shape of cobalt and to identify the phase composition of the nanoparticles. In-situ micro compression tests of the nanoparticles were performed using Hysitron PI85 picoindenter. Our results demonstrated that defect-free, FCC cobalt nanoparticles with equilibrium crystal shape were obtained after dewetting. This state of the nanoparticles was preserved after prolonged thermal treatments in the stability region of the HCP phase. The stress-strain curves obtained in micro compression tests indicated ultrahigh strength of the FCC nanoparticles in the range of tens of GPa. Finally, we correlated the ultrahigh strength of the FCC nanoparticles with their exceptional phase stability.

*Speaker

Advanced characterization of metal-oxide-metal interfaces produced by combined ALD/PVD deposition

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Abstract

Atomic Layer Deposition (ALD) and Physical Vapor Deposition (PVD) are widely recognized as critical deposition techniques for creating uniform, high-quality multilayer coatings on a diverse range of materials, including polymers and metals. Combined, these methods are uniquely suited to fabricate and study metal-oxide interfaces and nanolaminates with outstanding control over film thickness at the atomic scale. Using combined ALD/PVD deposition, a series of Al/Al2O3/Al interfaces have been fabricated, with oxide thickness ranging between 0-1 nm (0-0.5 TMA, 0.5 H2O-1 to 8 ALD cycles). In the as-deposited state, the interface between Al and alumina layers is still visible even if only one-half ALD cycle of H2O is performed. The thermal stability of the interfaces is a function of layer thickness and annealing temperature. Ongoing research will be presented, including Atom Probe Tomography (APT) and *in situ* X-ray Diffraction (XRD) annealing experiments, helping to further understand the nucleation behavior of ultrathin ALD films and thermal dissolution of the ultrathin oxide layers.

*Speaker
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Influence of temperature and impact energy on microstructural evolution and deformability of Inconel 925 nickel-based superalloy

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Abstract

Nickel-based superalloys are used in many industrial applications within the chemical, petrochemical, energy, and aerospace industries, operating under special conditions that require high mechanical strength and corrosion resistance at elevated temperatures. This study investigates the high-temperature deformation behaviour of Inconel 925 superalloy by analysing its deformability and microstructural evolution within the 1050 – 1200∘C temperature range. The microstructural evolution was examined using XRD (X-Ray Diffraction) and SEM-EBSD (Scanning Electron Microscopy - Electron Backscatter Diffraction) techniques, while deformability was assessed through the upsetting method using a gravity-drop hammer. Experimental data on the deformation resistance, specific mechanical work, and plasticity were collected and analysed as functions of deformation temperature and impact energy. Results indicate that increasing the deformation temperature enhances the plasticity, while an in-depth analysis of the plasticity's rate of increase as a function of impact energy revealed that higher impact energy leads to a more significant rise in plasticity. Additionally, it was observed that the deformation resistance decreases with increasing temperature across all impact energies. Similarly, specific mechanical work also exhibits a decreasing trend with rising deformation temperature, regardless of impact energy.
Keywords: deformability; microstructural evolution; deformation resistance; plasticity; nickel-based superalloys.

Acknowledgments

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HDPE reinforced with CDs with enhanced processing lifespan and improved recyclability traceability

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Abstract

Sustainable utilization of polymers depends on their efficient recycling and ability to retain their critical physical properties for further processing. High-density polyethylene (HDPE) represents 15–25 % of all plastic waste globally, and similar to other thermoplastics can be recycled for reuse (1). During the recycling process, the material is exposed to thermo-mechanical and thermo-oxidative conditions, which can result in chain scission and other reactions, such as branching and crosslinking (2). Therefore, it is imperative to develop new functional composites, that are recyclable, maintain adequate properties for reuse, and support plastic circular economy and sustainability. This work reports the development of advanced HDPE nanocomposites reinforced with carbon dots (CDs) to enhance processing longevity and enable recyclability traceability. For that purpose, several nanocomposites were prepared by thermal mixing using HDPE and different loading of CDs (0.1, 0.5 and 1.0 wt%). The composite containing 0.5 wt% CDs demonstrated a 17% increase in tensile strength after one recycling, with a maximum strain of 11%, significantly outperforming the neat HDPE. Additionally, incorporating 0.1 wt% CDs reduced the wear rate by up to 98%, highlighting substantial improvement in durability. To validate enhanced processability after recycling, 3D-printed specimens were fabricated using recycled materials. The composites doped with 0.1 wt% CDs exhibited excellent printability even after three consecutive recycling cycles. The optical characterization revealed a quenching of blue phosphorescence associated with the carbonyl groups of the polymer backbone. This phosphorescence was seen to be highly dependent on the CDs content, decreasing with increasing CDs content. Moreover, progressive luminescence changes were observed according to the number of recycling cycles, enabling quick and reliable traceability and sorting using a standard smartphone camera. This innovative technology represents an environmentally friendly and easily implementable solution for rapid, automated, and industrial recycling processes, offering significant potential for advancing the HDPE circular economy.

*Speaker

Analytical Modeling of Wear Mechanisms in Nanocontacts: Influence of Applied Load and Material Composition

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Abstract

This study investigates wear mechanisms in a nanocontact through experimental data and analytical modelling. Due to time constraints in simulating long-wear experiments, an analytical approach was adopted, revisiting Tysoe's model (Tribology Letters, 2017). Molecular dynamics revealed that applied load influences bond breakage and debris formation, while SEM images confirm no visible wear on the AFM probe. The analytical model on the other hand predicts continuous wear, but experiments show wear cessation in pure metals, unlike in composites or alloys. We propose refining the model to include the evolution at the nanoscale of two phases in a composite system subject to friction and wear. These findings provide insights into material-dependent wear behaviour, with further research planned on counter-body interactions.

*Speaker

Advanced tools for G200 nanoindenter: - motorized tilt correction stage to optimize flat punch measurement - motorized 8" wafer vacuum chuck allows full size wafer measurement

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Abstract

SURFACE has been building special components for nanoindenter systems for many years. As a former european distributor for Hysitron (1996-2005) and MTS nanoinstruments (2005-2008), we have always been able to fulfill customer requests that would not be available at the nanoindenter manufacturer. At this conference we will present two further solutions for the G200 nanoindenter.
Motorized tilt stage:

Flat punch indenters are commonly used as probes for nanoindentation due to the fact that the contact area is easy to define. Furthermore the contact area with the sample is usually much larger compared to conical or pyramidal geometries. The larger contact area extends the field of applications to softer materials like soft polymers or gels. The contact formation between the flat punch indenter tip and a flat sample surface is depending on the tilt angle between both normal directions. Above a certain depth or load the flat punch forms a "full contact" with the sample. Depending on the actual tilt angle and the sample thickness, this can be a limitation for the measurements quality. Strategies for evaluating the tilt mismatch and for tilt compensation are presented and discussed.

Motorized 8" wafer chuck:

This stage is fixing flat, wafer like substrates on a vacuum chuck. The actual substrate size can vary from some cm2 up to a full 8" wafer. The software allows the entire surface of the wafers to be measured in the G200, ensuring that there are no differences in the local frame stiffness. Only under this condition are the measurement results comparable and an area-related quality statement possible. Results of these stiffness mappings are presented.

*Speaker
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Use of non-equilibrium thermodynamics to derive a variable entanglement density constitutive model for entangled polymer melts

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Abstract

To understand the dynamical behavior of polymeric systems and enable industries to predict the behavior of new, advanced polymer-based materials via execution of numerical calculations of large-scale viscoelastic flows in complex geometries, constitutive models must be developed that can accurately describe the complex flow response of high molecular weight (MW) polymers, either in melts or in solutions. Said models must be simple, mathematically tractable, numerically stable, and not violate physical laws (such as thermodynamics). In such systems, chain uncrossability leads to developing topological interactions known as entanglements. When chains are forced to flow, they are deformed and oriented; thus, certain entanglements are lost but new entanglements can be created. Over the years, several research works have focused on deriving closed-form constitutive equations to elucidate the interrelation between applied flow and stress in entangled polymer melts or concentrated polymer solutions, the vast majority assumes that the average number of entanglements per chain remains constant (i.e., unaffected by flow). In this presentation, such a model will be presented which will explicitly account for a variable-entanglement density using non-equilibrium thermodynamics (NET). It proposes two evolution equations: one for the average number of entanglements per chain and one for the orientation of entanglement strands. By utilizing the same value for the convective constraint release (CCR) parameter for three molecular weights, the model can accurately explain the loss of entanglements caused by the applied flow, according to a direct comparison with results from non-equilibrium molecular dynamics simulations. The CCR relaxation time depends on the trace of the inverse of the orientation tensor instead of an explicit dependency on the velocity gradient. Finally, the stress tensor contains an additional contribution inspired by the Curtiss-Bird or tumbling snake model. Overall, the model proposed here builds upon the work of Ianniruberto-Marrucci when stretching is not considered.

*Speaker

Abusing the Sink-In Coefficient to Quantify Pile-Up in Nanoindentation

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Abstract

The phenomena of pile-up and sink-in in nanoindentation have a significant effect on the contact area between the indenter and the sample, causing it to deviate from the nominal cross-sectional area of the punch. The Oliver-Pharr method corrects for the effect of sink-in through the contact depth, which is calculated from the measured depth, load and stiffness. However, Oliver-Pharr cannot take into account any pile-up formation, leading to overestimated values of the hardness and Young's modulus.
While it has been recognized for long that these values cannot be trusted, there has yet been little interest in understanding the specifics of the error propagation throughout the Oliver-Pharr equations.

In this research, we investigated the pile-up formation across a wide range of mechanical properties, using microstructurally graded samples as high-throughput model materials. The magnitude of the pile-up is assessed from atomic force (AFM) micrographs of the residual indents and compared to the apparent sink-in coefficient, which is defined as the ratio between Oliver-Pharr contact depth and indentation depth (hc/h).

Surprisingly, our measurements evidence an inverse relationship between the Oliver-Pharr sink-in coefficient and the actual amount of pile-up. The poster will discuss this apparent paradox, as well as the outlooks for deriving a straightforward pile-up correction method.

Acknowledgement
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*Speaker

Colorimetry and Tribology of Ultrapure Copper Micromodification

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Abstract

Methods of coloring metals without the need of chemical processing have been extensively studied in recent years as they are considered as low-cost, environmentally-friendly and offer a wealth of applications in different fields of science and industry (1). We investigated a method of ultrapure copper controlled micromodification with the sandpaper with normal force 1.9 N and speed 6.5 cm/s. This resulted in the formation of particular microholes and microgrooves. We analysed the modified samples with the Colorimetric Microscopy (C-Microscopy) approach (2) to obtain colorimetric and surface morphology information at the microscale. We found relevant correlations between structural features induced by micromodification and sandpaper characteristics. We also investigated the effect of crystallographic grains direction and size, as determined by SEM EBSD, on the micromodification experiments. We see very strong effect of the copper grains direction and size on the copper wear rate by abrasion. To describe local optical properties of the modified copper samples we performed hyperspectral reflectance reconstruction at microscale by C-Microscopy from collected color calibrated (D65 illuminant) images. This allowed us to extract from the experiments 109 surface structures which have a similar reflectance R by clustering hyper-reflectances using Machine Learning technique K-Means. The analysis shows that one can obtain control over the local optical properties (i.e. reflectance R, color) by particular surface micromodification. Our studies show a pathway of using controlled micromodification techniques for copper local optical properties changes.
(1) B. Groussin et al., Adv. Opt. Mat. 12, 2302071, 2024
(2) B. R. Jany, Micron 176, 103557, 2024

*Speaker
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Unlocking Micromechanical Insights: Explainable Machine Learning and Feature Engineering applied to Nanoindentation Data

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[4]Materials Center Leoben Forschung GmbH – Austria
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Abstract

Nanoindentation has evolved into a method for performing rapid mechanical property characterisation, allowing for easy collection of vast amounts of data. To get insights, Elastic Modulus and Hardness maps are usually plotted to condense the data into a human-readable way. If the constituents making up the material are different enough in terms of Elastic Modulus and Hardness, their properties can easily be extracted from such maps. If not, the data have to be deconvoluted. For this reason, unsupervised machine learning methods such as the K-means algorithm are often used and have been shown to be performant. This even leads to the implementation of such algorithms as applications in standard nanoindenter software, allowing every experimentalist to access machine learning methods easily. Each clustered data point is usually only represented by its Elastic Modulus and Hardness. The question that this talk tries coin is why, despite enormous efforts to create meaningful micromechanical features utilised in solving the reverse-nanoindentation problem in the past, these features have not yet been used in clustering mechanical property data. The advantages of such features will be shown in the case of a curated High-Speed Steel Dataset consisting of 3300 individually human-labelled indents of four different High-Speed Steels. It will be demonstrated using unsupervised and supervised (explainable) machine learning that utilising features from all parts of the indentation curve can deconvolute maps that cannot effectively be clustered using the Elastic Modulus and Hardness while additionally gaining insights by explaining the model's prediction using methods based on cooperative game theory.

*Speaker
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2D spherical nanoindentation reveals nanoscale roughness of microscopic contacts

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Abstract

We have investigated diamond-silicon oxide contact lubrication by 2-dimensional (2D) materials with a 2D nanoindentation apparatus. These investigations have revealed that the friction and the shear modulus of the contact can be reduced by more than 3 times even if a single layer of graphene is added at _˜1 GPa maximum pressure. Furthermore, the vertical stiffness investigation of the contacts has shown a consistent number of layers dependency for the same normal load and depth (_˜3.5 nm) on the same silicon oxide substrate. The bare silicon oxide vertical stiffness was found by diamond spherocone (5 μm radius) as 38 kN/m; while 1 , 2 and 4 layer graphene on silicon oxide was found as 35.5, 33.5 and 31 kN/m, respectively. More interestingly, the vertical stiffness of the 1-, 2- and 4-layer graphene became equivalent to the initial bare silicon oxide stiffness while the bare silicon oxide increased to 57.5 kN/m (about _˜51% increase) after an oscillatory sliding period at 80 Hz. Inspection by atomic force microscopy (AFM) revealed that the graphene surfaces have about 20% less roughness under ambient conditions while the kurtosis (a measure of sharpness of the nano-asperities) is at least an order of magnitude lower when compared with the bare "ultra-flat" silicon-oxide. The post-shear surface inspections support the increased vertical stiffness on graphene as the silicon oxide surface imprint is visible on the AFM images. Therefore, we suggest that the lubrication effect is mainly due to the graphene sheet's asperity smoothing benefits with associated wear protection. The measurement of the vertical stiffness for single atomic layer on a substrate is not possible with a sharp tip, so the spherical nanoindentation has become a reliable tool for deep investigation of the bulk-interface mechanics in both normal and lateral directions.

*Speaker

Characterisation of Titanium Matrix Composites with Hybrid Reinforcements of AlO and Functionalised Graphene Nanoplatelets

Cantekin Kaykılarlı[1], Hasibe Aygül Yeprem[2], and Deniz Uzunsoy*†[3]

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[3]Deniz Uzunsoy, Bursa Technical University – Turkey

Abstract

Titanium matrix composites (TMCs) are utilised in the automotive, marine, military, and aerospace sectors. TMCs exhibit remarkable strength, high fatigue strength and biocompatibility, excellent chemical resistance, and high elastic modulus. The most commonly utilised reinforcement materials for TMCs include SiC, B4C, Al2O3, TiO, LaO, graphene, TiB, ZrO, and TiC. This study involved the production of TMCs-reinforced aluminium oxide (AlO) and functionalised graphene nanoplatelets (FGNP) via ultrasonic-assisted powder metallurgy and pressureless sintering. FGNP in varying amounts (0.1, 0.3, and 0.5 wt.%) and AlO (5 wt.%) were reinforced into the TMCs via mechanical alloying for five hours in a high-energy ball mill and using ethanol as a process control agent. GNP was functionalised using TritonX-100. The mechanically alloyed powders were pressed by a hydraulic press under uniaxial pressure of 450 MPa and sintered at 1200∘C for two hours in an argon flow. The characteristics of the Ti-5Al2O3-xFNGP composites were analysed using X-ray diffraction (XRD), optical microscopy (OM), scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDX), dimensional measurement, the Archimedes method, microhardness, and wear tests. The results indicated that adding FGNP enhanced relative density, hardness, and wear resistance.

*Speaker
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Microstructure-Property Relationships in Template-Assisted Electrodeposited Zinc Micropillars: A Comparative Study with FIB-Milled Specimens

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Abstract

Template-assisted electrodeposition represents an emerging microscale additive manufacturing technique for fabricating pure metal structures with high spatial resolution, with applications ranging from aerospace to biomedical fields. In this process, a non-conductive template is created on a conductive substrate, followed by metal electrodeposition into the template spaces; subsequent template removal yields free-standing metallic microcomponents. This approach combines expertise in 2D coating electrodeposition with the ability to create 3D structures, resulting in specimens with controlled chemical purity and tailored grain structure. In this study, we demonstrate a method combining two-photon lithography and electrodeposition to synthesize arrays of ultrafine-grained zinc micropillars, enabling direct fabrication of micromechanical test specimens.

To establish comprehensive microstructure-mechanical property relationships, we conducted a comparative analysis between these additively manufactured micropillars, and conventional Ga- and Xe-focused ion beam (FIB)-milled specimens prepared from zinc electrodeposited under identical conditions. Mechanical characterization was performed through compression tests at room temperature across different strain rates. Template-assisted electrodeposited (TAED) specimens exhibited consistently higher yield strengths compared to FIB-milled samples across all tested strain rates. Strain rate sensitivity and activation volume analysis revealed differences between TAED and FIB-milled specimens, suggesting differences in dominating deformation mechanisms. These differences were investigated through detailed microstructural characterization of sample cross-sections using Transmission Kikuchi Diffraction (TKD), enabling analysis of grain size, orientation, and boundary characteristics. The study aims to determine whether these mechanical property discrepancies originate from the electrodeposition process (template vs. 2D coating deposition and associated microstructural variations due to non-uniform current distribution) or from FIB-induced modifications during micropillars preparation.

The successful fabrication of these 3D microstructures showcases the potential of this methodology for creating complex architectures while maintaining control over material properties.

*Speaker
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This work reveals challenges in a mechanical characterization of micromechanical samples, providing crucial insights for the design of microarchitectured materials.

Systematic exploration of refractory high entropy alloys using high-throughput techniques and machine learning

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Abstract

The demand for alloys with exceptional high-temperature mechanical properties is crucial in industries such as aerospace and power generation. Refractory high entropy alloys (RHEAs) are promising candidates due to their high melting points and strength in extreme environments. This study focuses on exploring RHEAs within the Cr-Mo-Nb-Ta-V-W system. We synthesized a material library (MatLib) using physical vapor deposition on a silicon wafer, resulting in approximately 35,000 distinct alloys. The process was precisely calibrated to achieve equimolar composition and maximum configurational entropy at the center of the MatLib. Selected regions underwent chemical analysis using X-ray fluorescence and structural studies with X-ray diffraction, analyzed using Le Bail refinement to determine lattice parameters and crystallite size. High-throughput nanoindentation was employed to measure mechanical properties. The resulting data were used to train an artificial neural network to predict the properties of RHEAs beyond the tested compositional space.

*Speaker

Grain Boundary Segregation Landscape in Mg Alloys: From Solute Decoration to Clustering and Structural Transitions

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Abstract

Grain boundary (GB) segregation plays a crucial role in tailoring the mechanical properties of lightweight Mg alloys. Our recent studies map the landscape of solute segregation in Mg alloys, from solute decoration in infinitesimally dilute solid solution to clustering and structural transitions beyond the dilute limit. Using a correlative approach combining atom probe tomography, density functional theory calculations, and atomistic simulations, we reveal the concentration-dependent progression of solute segregation behavior at GBs. At low concentrations, solute atoms exhibit site-specific decoration, driven by local atomic environment variations, resulting in inhomogeneous GB segregation. As solute concentration increases, transition elements significantly enhance solute binding and clustering through synergistic effects. At even higher concentrations, solute-induced GB structural transitions emerge, leading to defect phase formation. Our findings provide atomistic insights into the mechanisms of GB segregation and contribute to the fundamental understanding of GB engineering for improved mechanical performance in Mg alloys.

*Speaker

Road to Failure: AFM Indentation of Polymers

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Abstract

Indentation methods range from the macro- to the nanoscale and with the decrease in scale more challenges arise. While researchers mostly understand micro- and nanoindentation methods, indenting with an atomic force microscope (AFM) is still relatively new with limited use in the chemistry or biology fields. However, AFM indentation has many uses in materials science and especially in polymer coatings. To illustrate the challenges of AFM indentation a case study on Epoxy-Silicon coatings with future aerospace applications will be shown. Compared to nanoindenters, AFM indentation has more crucial calibrations steps and specific data export routines for data analysis using contact mechanics models. AFM indentation has the advantage of utilizing mapping on an even smaller scale compared to modern nanoindenters and higher resolution surface imaging before and after. The AFM indentation results will be compared to Berkovich and Cube Corner indents made to similar depths and with similar loading-unloading functions. Differences in hardness and reduced elastic modulus between the measurement techniques as well as a proposed testing workflow will be presented.

*Speaker

Machine Learning-Driven High-Throughput Analysis of Damping Effects in Silicon-Based Cantilever Resonators with Metallic Coating

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Abstract

Micromechanical and nanomechanical resonators serve as essential components in a wide range of applications, including resonant sensing and energy harvesting. Resonance testing plays a fundamental role in characterizing the dynamic behavior of MEMS devices, providing insights into critical properties such as energy dissipation and structural integrity. Automated high-throughput resonance testing of silicon-based cantilever resonators with various metallic coatings offers valuable insights into the damping effects on resonance frequency and quality factor. A comprehensive study is conducted on a full wafer containing 580 devices, each hosting four cantilevers with varying dimensions, to evaluate damping mechanisms. These cantilevers are analyzed in both uncoated (reference) state and with metallic coatings of varying coverage percentages and materials, including aluminium, platinum, and molybdenum. Machine learning (ML) serves as an effective tool for interpreting complex patterns in large datasets, facilitating the identification of trends and dominant damping mechanisms that are otherwise difficult to discern. A ML framework is applied to analyze the extensive dataset, incorporating features such as cantilever dimensions, die location on the wafer, and coating parameters. Predictive models are developed to estimate changes in resonance frequency and quality factor while isolating the dominant damping mechanisms. Particular attention is given to the contributions of thermoelastic damping and surface effects, which have a significant impact on the dynamic performance of silicon cantilevers. This research highlights the importance of integrating automated high-throughput testing with ML to enhance the understanding of damping mechanisms in MEMS resonators. The results provide a foundation for the design of high-performance cantilever resonators tailored to specific applications, particularly those requiring the minimization of damping losses.

*Speaker

Materials Informatics in Academia: Challenges and Opportunities

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Abstract

Material informatics in academia presents several unique challenges. Firstly, the interdisciplinary nature of the field demands instructors to navigate through diverse subjects like materials science, data analysis, and computational techniques, requiring a breadth of expertise. Additionally, the rapid evolution of technology necessitates constant updating of course content to keep pace with emerging tools and methodologies. Limited access to specialized software and hardware can also hinder effective instruction. Moreover, bridging the gap between theoretical concepts and practical applications poses a challenge, as students and researchers must grasp both abstract theories and their real-world implications. Fostering collaboration between students and researchers with varying backgrounds, from engineering to computer science, requires innovative pedagogical approaches to ensure an inclusive learning environment. Overcoming these challenges requires continuous adaptation, collaboration across disciplines, and a commitment to staying at the forefront of technological advancements. Lastly, some examples of collaborative projects between Ansys and universities are given to illustrate how to overcome these challenges.

*Speaker