MM 32: Topical Session: Advanced Nanomechanics – Accelerating Materials Physics from the Bottom I

Time: Thursday 10:15–12:45 Location: SCH/A251

Topical Talk MM 32.1 Thu 10:15 SCH/A251

High-Throughput Nanomechanics and Data-Driven Workflows for Mapping Composition-Microstructure-Property Landscapes — •Ruth Schwaiger — Forschungszentrum Juelich, Institute of Energy Materials and Devices, IMD-1: Structure and Function of Materials, Juelich, Germany

Combinatorial and high-throughput (CHT) methods are enabling nanoscale mechanical studies that span broad compositional and microstructural spaces with unprecedented efficiency. This talk presents an integrated perspective on how automated nanoindentation, combinatorial thin-film libraries, and machine-learning analysis jointly accelerate the discovery of composition-microstructure-property relationships.

Combinatorial thin-film libraries provide dense, continuous coverage across multicomponent compositions, enabling systematic mapping of phase formation, defect structures, and mechanical response. For example, CHT workflows applied to Ni-Al coatings captured structural transitions and hardness trends across the phase diagram, enabling development of a mechanistic hardness model that integrates grain-size, solid-solution, and phase-fraction strengthening. To extract intrinsic material properties from such heterogeneous datasets, data-driven analysis methods, ranging from physics-informed regression to unsupervised clustering, allow the identification of mechanically distinct regions, quantification of data sufficiency, and robust separation of compositional, microstructural, and defect-driven effects.

MM 32.2 Thu 10:45 SCH/A251

Reliability of Interatomic Potentials for Surface- and Size-Dependent Mechanical Behavior — •Sriram Anand, Jan Janssen, Jörg Neugebauer, and Erik Bitzek — Computational Materials Design, Max-Planck-Institute for Sustainable Materials, Düsseldorf

Material properties at the nanoscale differ markedly from the bulk, largely due to the increased surface-to-volume ratio. Surface stresses in particular are thought to modify the elastic response and contribute to the anomalous mechanical behavior of nanoobjects. These effects are typically investigated using atomistic simulations; however, the interatomic potentials used in such studies are generally not fitted to surface stresses. As a consequence, both the quantitative values (e.g., Young's modulus) and, to a lesser extent, the deformation mechanism of nanoobjects obtained from simulations may deviate from physical reality.

Here, we present a systematic study of surface stresses, nonlinear elasticity, and stacking-fault energies in FCC metals as predicted by a broad set of classical and machine-learning interatomic potentials. Using first-principles data as reference, we compile a benchmark database of these key quantities and demonstrate - through tensile deformation of nanowires - how the choice of potential can markedly influence simulated mechanical properties and deformation behavior. Our benchmark of surface stresses, higher-order elastic constants, and fault energies provides a robust foundation for the accurate design of reliable next-generation nanoelectromechanical devices.

Topical Talk MM 32.3 Thu 11:00 SCH/A251

Expanding nanoindentation capabilities: Data-driven and novel experimental approaches — •Michael Wurmshuber[1], Matthias Glosemeyer[1], Pouya Hassanzadeh Sarhangi[1], Verena Maier-Kiener[2], Heinz Werner Höppel[1], and Matthias Göken[1] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany — [2]Montanuniversität Leoben, Leoben, Austria

As material discovery and manufacturing accelerate through artificial intelligence and additive manufacturing, high-throughput materials characterization is essential to ensure fast-paced material development. Here, nanoindentation with its capability to measure small material volumes and individual microstructural constituents in a quick manner, has the edge over classical slow-paced mechanical testing. Since Oliver and Pharr's groundbreaking work, nanoindentation has developed to extract not only hardness and modulus but numerous other mechanical properties through specialized indentation protocols. This talk presents two approaches to further extend the information space we receive from nanoindentation. First, we introduce a novel spherical indentation technique enabling local mapping of inelastic backstrain via loading-unloading-reloading experiments, allowing for the mapping of underlying geometrically necessary dislocation networks. Second, we demonstrate how artificial neural networks and ensemble methods can accelerate flow curve characterization from standard Berkovich nanoindentation. Together, these advances demonstrate how data-driven and experimental innovations can significantly expand the information accessible from nanoindentation measurements.

15 min. break

Topical Talk MM 32.4 Thu 11:45 SCH/A251

Additive Manufacturing and Nanomechancics - where is the Link? — •Ralph Spolenak — Laboratory for Nanometallurgy, Department of Materials, ETH Zurich, Switzerland

While size effects in mechanical properties of metals created by whisker growth and thin films had been known since the 1950s, the introduction of micro- and nanoscale subtractive manufacturing (also known as focused ion beam milling) became a game changer as it allowed to study size effects practically independent of the material and its microstructure. The contribution will focus on additive micro- and nanoscale manufacturing with voxel sizes down to 30 nm and how both the manufacturing process (with regards to microstructure control and chemistry) as well as the dimension influences mechanical properties. Comparison will be made to sputter deposited materials including self-organized microstructure, such as nanoporosity by dealloying or local pore formation by Kirkendall voiding, as well as nanostructured reactive multilayers. Finally, the potential combination of subtractive and additive processes will be discussed.

MM 32.5 Thu 12:15 SCH/A251

Mechanical Behaviour of Nafion Membranes — •Mateja Jovanović[1,2,3], Matthias Baldofski[2], Nicolas Bernhard[2], Marcin Rybicki[2,4], Miljan Dašić[3], and Igor Stanković[3,5] — [1]Institute of Technical Sciences of the SASA, K. Mihailova 35/IV, 11000 Belgrade, Serbia — [2]Freudenberg Technology Innovation SE&Co. KG, Hoehnerweg 2-4, 69469 Weinheim, Germany — [3]Institute of Physics, University of Belgrade, Pregrevica 118, 11080 Zemun, Serbia — [4]Freudenberg e-Power Systems GmbH, Bayerwaldstrasse 3, 81737 München, Germany — [5]Departamento de Ingeneria Mecanica, Universidad Tecnica Federico Santa Maria, Av. Espana 1680, Valparaiso, Chile

Proton Exchange Membrane Fuel Cells (PEMFCs) utilise polymer membranes like Nafion, valued for their proton conductivity and mechanical integrity. In this work, we examine the stress-strain response of Nafion membranes, focusing on how hydration, crystallinity, and temperature modulate mechanical behavior, using molecular dynamics simulations. Here, we demonstrate that membrane hydration level and structural ordering fundamentally influence mechanical properties under applied stress. Water distribution and polymer chain dynamics are closely connected to the stress-strain response, suggesting that structural organization at the nanoscale is crucial in governing overall mechanical performance across different conditions. By integrating clustering algorithms, structural descriptors, and stress-strain analyses, this study provides a comprehensive view of how membrane architecture and environmental factors govern mechanical performance.

MM 32.6 Thu 12:30 SCH/A251

The Fracture toughness of thin films — •Mathias Göken[1], Benoit Merle[2], and Jun Lou[3] — [1]Department of Materials Science & Engineering I, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany — [2]Materials Science and Engineering, Universität Kassel, Germany — [3]Department of Materials Science and NanoEngineering, Rice University, Houston, Texas, USA

The mechanical properties of thin films play a pivotal role for applications either as freestanding films or as coatings. So far, the understanding of the fracture toughness of very thin films and especially of their thickness dependence is limited. Bulge testing is a very reliable technique for characterizing the mechanical properties of thin films, where a freestanding film is subjected to a controlled pressure from underneath and the deflection of the film is recorded. Bulge tests

have shown that the fracture toughness of ductile and soft Au drops down to extremely low values of only 2 MPam1/2 if the film thickness is reduced to 100 nm. On the other hand, single layer graphene has shown a fracture toughness of around 4 MPam1/2. In this paper the thickness dependence of the fracture toughness is discussed based on an old and simple basic fracture mechanics concept derived by Bluhm and Knott in the 1960th. It is shown, that based on this model it is easy to predict the fracture toughness of thin films and their thickness dependence. The results agree surprisingly well with the experimental data on graphene and Au thin films.