MM 63: Functional Materials: Performance, Reliability and Degradation

Time: Thursday 15:30–16:45 Location: C 230

MM 63.1 Thu 15:30 C 230

Combining DFTB and Structure Mapping for the Prediction of Transition Paths in the Deactivation of ZnO@Cu Catalysts — •Artem Samtsevych, Chiara Panosetti, Karsten Reuter, and Christoph Scheurer — Fritz-Haber-Institut der MPG, Berlin

Solid-solid transformations are common in the aging of functional materials like catalysts. Understanding these transformations at the atomistic level is thus crucial for a resilient design. In practice, this requires identifying minimum energy pathways between basins on a complex free energy surface. While chain-of-state methods help obtain corresponding pathways, they are generally challenged by the exponential growth of the number of possible transition pathways with system size and the computational cost of the underlying first-principles, typically density-functional theory (DFT), energy evaluations.

Here we address both challenges by employing geometry- and topology-based mapping techniques for the efficient generation of suitable initial transition pathways and a machine learning-based optimization of density-functional tight binding (DFTB). The former techniques map the atomic structures and unit cells or the graphs of interatomic bonds of the connected basins. The latter optimization of the DFTB repulsive potential [1] establishes this technique as a computationally efficient surrogate for the DFT energetics. We illustrate the combined general workflow by studying the aging process in ZnO@Cu catalysts, which involves the transformation of the ZnO overlayer from a graphitic-like to wurtzitic structure.

[1] C. Panosetti *et al.*, J. Chem. Theory Comput. **16**, 21818 (2020).

MM 63.2 Thu 15:45 C 230

Structural and chemical behavior of cBN at high pressure and temperature — •Lars Olschewski[1], Gabriel Brune[1], Tountzer Dereli[2], Monika Kipp[2], Dirk Biermann[2], and Jörg Debus[1] — [1]Department of Physics, TU Dortmund — [2]Institute of Machining Technology, TU Dortmund

Solids need to withstand high temperatures and heavy forces while they are used in extreme thermo-mechanical environments, like high-speed precision-grinding applications. Cubic boron nitride (cBN) is commonly exploited as abrasive material, because it is structurally stable and resistant to oxidation typically until temperatures of 1300°C.

For applying strong normal and tangential forces (tens of N) and high temperatures, the mechanically most stable (sp^3-hybridized) cBN may change into its hexagonal form or its crystal structure may transform into an amorphous mixture of stressed and anisotropic sp^2- and sp^3-hybridized bonds. In that context, studying the anisotropies in the tensile, compressive and shear strain as well as surficial chemical reaction products is highly interesting.

This structural and chemical behavior is investigated by confocal Raman scattering and tip-enhanced Raman spectroscopy. They allow for sensitively characterizing topographic features at the nanoscale combined with data on, *e.g.*, the chemical composition.

MM 63.3 Thu 16:00 C 230

Optimizing In_3SbTe_2 crystallization towards phase change memory application — •Yiming Zhou and Matthias Wuttig — I. Institute of Physics (IA), RWTH Aachen University, Sommerfeldstraße 14, 52074, Aachen, Germany

Traditional phase change materials like $Ge_2Sb_2Te_5$ are characterized by their low crystallization temperatures, resulting in insufficient data retention. In contrast, In_3SbTe_2, an indium-based chalcogenide, exhibits remarkable characteristics including notably high crystallization temperatures and resistance contrasts. However, its multi-stage crystallization process has raised challenges to switching reliability and device endurance. To address this problem, an investigation into the crystallization behavior of In_3SbTe_2 through controlled annealing processes has been conducted.

The large density changes during the crystallization process and the as-deposited crystallite contribute to the adhesion problem. This gives rise to the strain relaxation-induced crystallization behavior. With the Te adhesion layer, the operational stability range for In_3SbTe_2 crystallization can be significantly expanded. Moreover, manipulating the thickness of the Te adhesive layer can tune the preferred orientation for In_3SbTe_2 crystallization.

This refined crystallization study has culminated in the fabrication of confined and nano-bridge phase change memory devices. Notably, a marked enhancement in yield has been observed for both device architectures, representing substantial progress toward practical implementation.

MM 63.4 Thu 16:15 C 230

Thermomechanical properties of diamond abrasive grains — •Gabriel Brune[1], Tountzer Dereli[2], Lars Olschewski[1], Monika Kipp[2], Dirk Biermann[2], and Jörg Debus[1] — [1]Department of Physics, TU Dortmund — [2]Institute of Machining Technology, TU Dortmund

Abrasive grains are subjected to high thermomechanical stress during high-speed precision grinding. While cubic boron nitride is often used for its high hardness and thermal resistance, diamond - with its superior hardness - provides better grinding results. However, when machining steel at temperatures of about 600°C, graphitization of the diamond surface is a major issue lowering the structural and chemical stability.

These structural and chemical changes including the influence of O_2 and interfaces between sp^2 and sp^3 hybridized areas within the carbon network are in the focus of our studies. Accordingly, a series of diamond abrasive grains exposed to differently high thermomechanical loads was analyzed. Spatially resolved Raman spectroscopy of the diamond surface reveals the structural properties of the grains. Based on shifts of the diamond Raman peak at 1332 cm^{-1}, tensile and compressive strain up to 200 MPa is determined. In particular, the observation of the D peak (around 1350 cm^{-1}) and G peak (around 1550 cm^{-1}) indicates the local formation of amorphous carbon clusters. From the peak shapes it is possible to estimate local maximum surface temperatures (= 660°C) [APL Mater. 11, 031106 (2023)] that occured during the grinding process.

MM 63.5 Thu 16:30 C 230

Influence of flash lamp annealing on the martensitic microstructure of epitaxial Ni-Mn-Ga films — Yuru Ge[1,2], Satyakam Kar[3,2,1], Fabian Ganss[1], Thomas Schumann[1], René Hübner[1], Lars Rebole[1], and •Sebastian Fähler[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, 01328 Dresden — [2]TU Dresden, Faculty of Mechanical Science and Engineering, 01062 Dresden — [3]Leibniz IFW Dresden, Institute for Metallic Materials, 01069 Dresden

The application of shape memory materials are based on a reversible martensitic transformation, which changes structure and microstructure. All applications like high stroke actuation, sensing, ferroic cooling, and energy harvesting, benefit from a high cycle frequency, as this allows for high power density. For this, thin films are of particular interest as their high surface-to-volume ratio enables fast heating and cooling. However, up to now the influence of fast heating and cooling on the martensitic microstructure is unknown. Here we examine the influence of flash lamp annealing on epitaxial Ni-Mn-Ga films. Single-crystalline films are suitable as a model system since they allow for an undisturbed, well-ordered hierarchical martensitic microstructure after slow cooling. We examine all levels of this twin-within-twins microstructure by a combination of XRD, SEM and TEM before and after flash lamp annealing with a duration of 3 ms at different energy densities. We observe substantial changes at all levels of twinning, which we attribute to the finite time available to form a hierarchical microstructure and the thermal stress between film and substrate.