FM 16: Topical Session: Dislocations in Functional Materials II (joint session MM/FM)

Time: Wednesday 15:45–17:15 Location: SCH/A251

Topical Talk FM 16.1 Wed 15:45 SCH/A251

Dislocations in perovskite oxides: similarities and differences — •Pierre Hirel — Univ. Lille, CNRS, INRAE, Centrale Lille, UMR 8207 - UMET - Unité Matériaux et Transformations, F-59000 Lille, France

The experimental discovery of room-temperature ductility in strontium titanate $SrTiO_3$ in 2001, has revealed the surprising mobility of dislocations in $\langle 110 \rangle \{110\}$ slip systems. Atomic-scale simulations have contributed to resolving the core structure of these dislocations, and their role in the ductile-brittle transition. Since then, similar ductile behaviour was found in related perovskite oxides $KNbO_3$ and $KTaO_3$. However, other perovskites like $BaTiO_3$ or $CaSiO_3$ remain essentially brittle at room temperature, despite having the same crystal lattice and similar chemical compositions as ductile perovskites.

FM 16.2 Wed 16:15 SCH/A251

Probing the Known Unknown of the Dislocation Dynamics in Oxides and Semiconductors — •Liming Xiong — NC State University, Raleigh, NC, USA

Dislocation dynamics in oxides and semiconductors are widely aware, but its exact nature and impact on the properties and functionality of these materials are not fully understood yet. One reason is that the well-established knowledge for dislocation dynamics in metals often can't fully explain or even fail when used for oxides and semiconductors. To fill this knowledge gap, here we will present a concurrent atomistic-continuum computational tool for probing the dislocation dynamics in oxides and semiconductors. This tool has a unique feature to accommodate the motion/multiplication of μm-long dislocations together with the atomic-scale core structure evolution along the dislocation within all within one single model. Taking dislocation-seeded SrTiO3 and ZnS as sample materials, we will: (i) map the core structure/stress along a dislocation line to its local charge states and motion mechanism; (ii) measure the dislocation mobility and its dependence on stress, temperature, dopant concentration, charge states, electrical field, light illumination, and dislocation line lengths ranging from nanometers to micrometers; (iii) predict how local internal stress builds up when a mesoscale dislocation slip interacts with an atomically structured grain boundaries, and how such a high local stress may initiate a crack in turn. A consolidation of such simulation data into constitutive rules needed by higher-scale models for interpreting experimental observations will be also discussed.

FM 16.3 Wed 16:30 SCH/A251

Electric Field Effects on Dislocation Motion in SrTiO3 via Mesoscale Indentation — •Alexander Frisch[1], Daniel Isaia[2], Oliver Preuss[2], and Xufei Fang[1] — [1]Institute for Applied Materials, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Department of Materials and Earth Sciences, Technical University of Darmstadt, Darmstadt, Germany

Dislocations in perovskite oxides have the potential of tuning functional properties of electroceramics, however their behavior and stability under externally applied electric fields remain elusive. Therefore, we investigated the effect of high densities of dislocations onto the dielectric breakdown behavior of SrTiO3, a model perovskite material. Lower dielectric breakdown strengths were found in the high-dislocation-density samples, engineered through the Brinell scratching method. Further, the effect of a 2 kV/mm electric field on the introduction and mobility of dislocations in SrTiO3 was investigated. While no changes to the dislocation plastic zone size, depth, or dislocation distribution were observed, the results suggest the stability of pre-engineered dislocation structures in perovskite oxides under applied electric fields. These results will be interpreted in the context of the dislocation charge state, associated electric field forces, and defect-modified electrical/thermal conductivity.

FM 16.4 Wed 16:45 SCH/A251

Generating a "ferroelectric metal" by preferential reduction of dislocations in $BaTiO_3$ — •Christian Rodenbücher[1], Gustav Bihlmayer[2], Carsten Korte[1], and Kristof Szot[3] — [1]Forschungszentrum Jülich GmbH, Institute of Energy Technologies (IET-4), 52425 Jülich, Germany — [2]Forschungszentrum Jülich GmbH, Peter Grünberg Institut (PGI-1), 52425 Jülich, Germany — [3]University of Silesia, Institute of Physics, 41-500 Chorzów, Poland

Redox processes in transition metal oxides are of high relevance for sensors, information technology, superconductivity, and energy conversion. Perovskites with mixed ionic-electronic conductivity, such as $BaTiO_3$, are of particular interest because oxygen nonstoichiometry controls electronic charge carriers and thus conductivity. Surprisingly, thermal reduction in vacuum can induce metallic behaviour with conductivities far exceeding predictions from point-defect chemistry. To clarify the origin of this metallic state, we investigate the electronic transport, electronic structure, and chemical composition of $BaTiO_3$ single crystals during annealing and cooling under ultrahigh vacuum. Surface-sensitive techniques such as XPS and LC-AFM allow us to correlate electronic structure changes with the insulator-to-metal transition. We find that surface-layer dislocations act as preferential reduction sites, forming conducting filaments that yield macroscopic metallic behaviour despite minimal overall oxygen loss. Metallic behaviour persists into the ferroelectric phase. Nanoscale mapping shows that metallic filaments and piezoelectrically active regions coexist thus explaining how a "ferroelectric metal" can exist.

FM 16.5 Wed 17:00 SCH/A251

Dislocation dynamics in Ni-based superalloys: atomistic simulations and uncertainty quantification — •Geraldine Anis, Thomas Hudson, and Peter Brommer — University of Warwick, Coventry CV4 7AL, UK

Ni-based superalloys exhibit extraordinary strength at high temperatures. This strengthening effect is largely attributed to precipitation strengthening, where dislocations are hindered by precipitates present in their microstructure. In our work, we model dislocation trajectories obtained from Molecular Dynamics (MD) simulations of Ni-Ni_3Al. A reduced model was developed to describe dislocation-interface interactions within this system, which captures important features of the MD dislocation trajectories. The developed model was tested on a representative system and was shown to capture a range of qualitatively different dislocation behaviour. The model parameter distributions were then determined using Differential Evolution Monte Carlo (DE-MC) sampling and a Gaussian process surrogate model. The present approach offers a means of identifying atomistic-scale parameters, which can be used to inform larger length scale simulations of dislocations. Determining parameter distributions using DE-MC means that parameter uncertainties can be propagated through a hierarchy of multiscale models. We illustrate how such uncertainty propagation can be achieved by considering a dislocation mobility law with quantified uncertainties in pure Ni. This work is part of a wider study aiming to model the deformation behaviour of Ni-based superalloys with a focus on quantifying and propagating uncertainties.