FM 13: Topical Session: Dislocations in Functional Materials I (joint session MM/FM)

Time: Wednesday 10:15–11:30 Location: SCH/A251

FM 13.1 Wed 10:15 SCH/A251

Mechanical seeding of dislocations for room-temperature plasticity in ceramics — •Wenjun Lu[1], Jiawen Zhang[1], and Xufei Fang[2] — [1]Department of Mechanical and Energy Engineering, Southern University of Science and Technology, Shenzhen, 518055, China — [2]Institute for Applied Materials, Karlsruhe Institute of Technology, Karlsruhe,76131, Germany

The pursuit of room-temperature ductile ceramics has long been hindered by their inherent brittleness. Here, we demonstrate a simple strategy to seed mobile dislocations at room temperature with densities up to 1014 m-2, enabling ceramics to sustain plastic compressive strains exceeding 30%. These dislocations multiply through cross-slip and motion, effectively suppressing brittle fracture without high-temperature processing. Using in situ nano-/micromechanical deformation and ex situ bulk tests, we bridge the length scales of plasticity and reveal a strong dependence of yield strength and flow behavior on dislocation density. Specifically, SrTiO3 micropillars transition from brittle fracture (dislocation-free) to plastic yield when mechanically seeded dislocations are present. Yield strength first decreases then rises with increasing dislocation density, reflecting complex structural evolution observed via transmission electron microscopy. These findings highlight dislocation engineering as a viable pathway toward ductile ceramics and open avenues for tuning their mechanical and functional properties through room-temperature dislocation plasticity.

Contribution: Wenjun Lu is the Speaker.

FM 13.2 Wed 10:30 SCH/A251

Impact of mechanically seeded dislocations on the mechanical properties of perovskite ceramics — •Jiawen Zhang[1], Xufei Fang[2], and Wenjun Lu[1] — [1]Southern University of Science and Technology, Shenzhen, China — [2]Karlsruhe Institute of Technology, Karlsruhe, Germany

The inherent brittleness of functional ceramics severely hinders their engineering application. The strong ionic and covalent bonds in ceramics make dislocation nucleation, motion, and multiplication difficult at room temperature. Recent research challenges the conventional perception of ceramics as inherently brittle materials, with dislocations emerging as a promising avenue for enhancing their mechanical properties. By using a Brinell ball indenter to perform surface scratching, crack-free plastic deformation zones with tunable dislocation density can be generated on the ceramic surface. The dislocation generation mechanism and dislocation-dominated plastic deformation mechanism were investigated by introducing dislocations into perovskite SrTiO3 and KTaO3. Room temperature micropillar compression tests then revealed that as the mechanical seeded dislocation density increased,SrTiO3 exhibited a *brittle* to *ductile* transition as the dislocation density increased from ~1010 m-2 to ~1014 m-2. However, the (001) KTaO3 single crystal exhibits a *brittle* to *ductile* then to *brittle* transition as the dislocation density increased from ~1010 m-2 to ~1015 m-2. Additionally, the yield strength displayed a complex trend, initially decreasing and then increasing in these two perovskite oxide ceramics.

FM 13.3 Wed 10:45 SCH/A251

Dislocation interaction with a tilt low angle grain boundary in bi-crystal SrTiO3 — •Kuan Ding[1,2], Atsutomo Nakamura[3], Patrick Cordier[4,5], and Xufei Fang[3,6] — [1]Department of Materials and Earth Sciences, Technical University of Darmstadt, 64287 Darmstadt, Germany — [2]Max Planck Institute for Sustainable Materials, Max-Planck-Straße 1, 40237 Düsseldorf, Germany — [3]Department of Mechanical Science and Bioengineering, Osaka University, 1-3 Machikaneyama-chou, Toyonaka, Osaka, 560-8531, Japan — [4]Unité Matériaux et Transformations, Université de Lille, 59655 Villeneuve d'Ascq Cedex, France — [5]Institut universitaire de France (IUF), 75005 Paris, France — [6]Institute for Applied Materials, Karlsruhe Institute of Technology, Kaiserstr. 12, 76131 Karlsruhe, Germany

For applications of ceramics with dislocation-tuned mechanical and functional properties, it is pertinent to achieve dislocation engineering in polycrystalline ceramics. However, grain boundaries (GBs) are effective barriers for dislocation glide at room temperature. It is critical to understand the fundamental processes for dislocation-GB interaction. We investigated a bi-crystal SrTiO3 with a 4° tilt GB. Brinell indentation was used to generate a plastic zone at the mesoscale without cracking, allowing for direct assessment of GB-dislocation interaction. Together with dislocation etch pits imaging and transmission electron microscopy analysis, we observe dislocation pileup, storage, and transmission across the LAGB. Our observations reveal new insights into dislocation-GB interaction at room temperature at mesoscale.

FM 13.4 Wed 11:00 SCH/A251

Dislocation-Mediated Extraordinary Room-Temperature Plasticity in Inorganic Semiconductors — •Xiaocui Li[1] and Yang Lu[2] — [1]Department of Materials Science and Engineering, City University of Hong Kong, Kowloon, Hong Kong SAR, China — [2]Department of Mechanical Engineering, The University of Hong Kong, Pokfulam, Hong Kong SAR, China

Inorganic semiconductors, with their ionic or covalent bonds, are typically brittle at room temperature, restricting their use in flexible electronics. Our recent study reveals that all-inorganic perovskite (CsPbX3, X=Cl, Br, I) single-crystal micropillars can achieve extraordinary room-temperature plasticity with average plastic strain of ~64% (Nat. Mater. 2023, 22, 1175). They can be morphed into distinct geometries without cracks or cleavage. The deformation is mediated by partial dislocations on {011}<0-11> slip system, featuring four equivalent variants that address the lack of deformation pathways in ionic crystals. Sequential activation of variants prevents strain hardening and crack formation caused by dislocation reactions. First-principles calculations attribute this plasticity to low slip barriers enabling sustained deformability and strong Pb-X bonds preserving crystal integrity. Leveraging this deformability, we developed shape-customizable optoelectronic devices that maintain stable functional properties and bandgap energies post-deformation. This discovery overturns the notion of brittleness in inorganic semiconductors, and provides a foundation for advanced applications in flexible electronics and deformable sensors.

FM 13.5 Wed 11:15 SCH/A251

Dislocations as Key Enablers on the Road to Functional and Resilient Oxide Ceramics — •Oliver Preuss[1], Enrico Bruder[2], Zhangtao Li[3], Yinan Cui[3], Jinxue Ding[1], Philippe Carrez[4], and Xufei Fang[1] — [1]Institute for Applied Materials, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Division Physical Metallurgy, Department of Materials and Earth Sciences, Technical University of Darmstadt, Darmstadt, Germany — [3]Department of Engineering Mechanics, Tsinghua University, PR China — [4]Materials and Transformations Unit, Université Lille, Lille, France

Designing oxide ceramics that unite high mechanical resilience with strong functional performance is challenging. We show that introducing ultra-high dislocation densities ($\approx 10^{15}$ m^{-2}) into materials such as MgO and SrTiO$_3$ provides a direct route to enhance both damage tolerance and functional properties. Cyclic Brinell ball scratching at room temperature generates near-surface, dislocation-rich zones of arbitrary size and shape. These regions markedly alter fracture behaviour, arresting propagating cracks and suppressing crack initiation, as demonstrated by Vickers indentation and quasi-in situ DCDC tests. Crystal-plasticity phase-field simulations reproduce the observed toughening mechanism. The dislocation networks also improve transport properties, increasing electrical conductivity while reducing thermal conductivity by nearly half: an advantageous combination for thermoelectric performance. This work establishes a practical strategy for dislocation engineering to achieve oxide ceramics with combined mechanical robustness and enhanced functionality.