KFM 2: Focus: Dislocations in Ceramics: Mechanics, Structures and Functionality (joint session KFM/MA)

Contrasting the common (mis)belief that ceramics are brittle, a new horizon of dislocation engineering in ceramics is being revealed, where dislocations are used to harness the mechanical and electro-functional properties. This session will bring together researchers who are interested in dislocations in ceramics, covering experiments and simulations, to stimulate new ideas for dislocation-based mechanics, characterization, and functionality in ceramics.

Chair: Dr. Xufei Fang (TU Darmstadt), Dr. Till Frömling (TU Darmstadt)

Time: Monday 14:30–17:05 Location: POT 51

Invited Talk KFM 2.1 Mon 14:30 POT 51

Formation of conducting channels along of dislocations in $SrTiO_3$ — •Christian Rodenbücher[1], Kristof Szot[2], Gustav Bihlmayer[3], and Carsten Korte[1] — [1]Forschungszentrum Jülich GmbH, Institute of Energy and Climate Research (IEK-14) — [2]University of Silesia, Institute of Physics, 41-500 Chorzów, Poland — [3]Forschungszentrum Jülich GmbH, Peter Grünberg Institut (PGI-1), 52425 Jülich, Germany

$SrTiO_3$ has become one of the most extensively studied metal oxides due to its exceptional electronic properties, which hold promising potential for applications in energy conversion and electronics. A key feature of $SrTiO_3$ is that its electronic transport properties are closely related to oxygen nonstoichiometry, which can be manipulated via redox reactions. Our nanoscale investigations on crystals and ceramics employing imaging techniques such as local-conductivity atomic force microscopy (LC-AFM) reveal that the reduction process is highly complex and heterogeneous on the nanoscale. Along extended defects such as dislocations there are easy reduction sites where oxygen vacancies are preferentially generated. In this way, filaments with high conductivity evolve around the dislocations in the originally insulating matrix and act as nanoscale short circuits. Upon application of mechanical stress, these filaments can even be moved through the crystal together with the dislocations. These findings not only can explain failure mechanisms in solid oxide electrolytes, but also raise fundamental questions regarding the mechanisms of electronic transport and superconductivity in self-doped transition metal oxides.

KFM 2.2 Mon 15:00 POT 51

Dislocation engineering in oxides at room temperature: understanding the competition between plasticity and cracking — •Xufei Fang — Technical University of Darmstadt, Alarich-Weiss-Str. 2, 64287 Darmstadt, Germany

Dislocations in ceramic oxides are drawing increasing attention owing to their promising physical properties, such as dislocation-tuned electrical conductivity, thermal conductivity, and electro-mechanical properties. However, due to the brittleness of most oxides at room temperature, it remains a great challenge to engineer dislocations without forming cracks, which is a prerequisite for harnessing the functionalities. Here, we demonstrate dislocations can be effectively introduced into various ceramic oxides (SrTiO3, BaTiO3, KNbO3, TiO2) at room temperature by using nanoindentation pop-in stop tests. Interestingly, we find a size-dependent competition between purely dislocation-dominated plastic deformation under a critical tip radius and a concurrent appearance of cracks and dislocations when the tip radius is larger than a certain value. We further extend the deformation scale up to the millimeter regime and identify a reversal of the above size-dependent competition. We will address the underlying mechanisms by examining the dislocation nucleation, multiplication, and motion individually to shed new light on the dislocation mechanics in oxides, particularly at room temperature. Last but not least, the dislocation-tuned electrical and thermal conductivity will be briefly showcased using our developed methods for dislocation engineering.

KFM 2.3 Mon 15:20 POT 51

Tuning dislocations in ferroelectric oxides by cyclic Indentation: dislocation toughening, domain fragmentation and phase stabilisation — •Oliver Preuss, Fangping Zhuo, Enrico Bruder, Christian Minnert, Jürgen Rödel, and Xufei Fang — Department of Materials and Earth Sciences, Alarich-Weiss-Str. 2, 64287 Darmstadt, Technical University of Darmstadt

In light of the growing research interest in dislocation-tuned functionality in ceramics, promising proofs-of-concept have been most recently demonstrated enhanced ferroelectric properties, electrical conductivity, and superconductivity. Yet introducing dislocations into brittle ceramics remains a grand challenge, especially at room temperature. Here, we demonstrate a simple method using a large Brinell indenter to cyclically indent the sample surface to tune the dislocation densities over 4 orders of magnitude (from 10^{10} m^{-2} up to 10^{14} m^{-2}) in single-crystal $KNbO_3$. A large, crack-free plastic zone (200 μm in diameter) is achieved on the sample surface at room temperature. More interestingly, both damage tolerance and fracture toughness have been improved. The interactions between dislocations and other microstructure features are examined in detail by optical microscopy, electron channelling contrast imaging, piezoresponse force microscopy methods and μ-Raman spectroscopy to shed light on the impact of dislocations on the mechanical properties as well as microstructural evolution. Our findings open new questions that may raise interest for further studies in ductile ceramics such as dislocation-domain wall interaction, domain wall fragmentation and strain-induced phase stabilisation.

15 min. break

Invited Talk KFM 2.4 Mon 15:55 POT 51

Plastic properties of MgO : Insights from numerical modeling — •Philippe Carrez — Université de Lille, F-59000 Lille, France

Plastic properties of crystalline materials depend not only on the nature of the defects present in the crystal but also and more substantially on their mobilities and mutual interactions. This is typically the case for the creep properties of magnesium oxide (MgO), which has been the subject of numerous investigations over the years. Yet, the atomistic details of dislocation-point defects, dislocation-dislocation or dislocation-grain boundary interactions remain poorly described.

Nowadays, numerical modeling offers the possibility of modeling mechanical properties from the description of the elementary mechanisms of plasticity. As an example, we will discuss the interaction between 1/2<110>{110} dislocations and point defects in MgO. We will show how the edge dislocation core, within a region across the glide planes that expands over several Burgers vector, is a sink for vacancies, and thus enhances the pipe diffusion at moderate temperature. At higher temperature, point-defect absorption or emission along the dislocation lines allow the dislocation climb mechanism and can impact creep properties of MgO. We will thus show how atomic-scale simulations can elucidate the atomic configurations of the various jog configurations structure and give access to their formation energies.

KFM 2.5 Mon 16:25 POT 51

Dislocation-tuned Schottky barrier in oxide ceramics — •Mehrzad Soleimany[1,2], Till Frömling[1], Lukas Porz[1], Enrico Bruder[1], Marin Alexe[2], and Jürgen Rödel[1] — [1]Department of Materials and Earth Sciences, Technical University of Darmstadt, 64287 Darmstadt, Germany — [2]Department of Physics, University of Warwick, CV4 7AL Coventry, UK

For decades manipulation of interfaces and point defects in semiconductors have been the main focus of scientists for tuning the functional properties of materials. However, dislocations which are considered as one-dimensional defects, have not only been neglected but also tried to be avoided due to the assumption that they degrade desired properties of semiconductors. Nevertheless, it has recently been shown that this speculation can be challenged and dislocations can even be used to tune the thermal, electrical, and ferroelectric properties of materials, especially when they are introduced in high densities. In this work dislocation densities higher than $4\times$ 10^{13} m^{-2} were introduced in a large volume of the n-type and p-type $SrTiO_3$ by mechanical deformation and cyclic loading. That has been confirmed via sample thinning

and electron channeling contrast imaging. Utilizing electrochemical impedance spectroscopy and DC electrical measurements, we showed that based on doping, dislocations can reduce the Schottky barrier in the n-type $SrTiO_3$ by a factor of seven and can increase that by a factor of three in the p-type one.

KFM 2.6 Mon 16:45 POT 51

Tailoring ceramic functional properties of YSZ with dislocations — •Till Frömling, Qaisar Muhammad, and Jürgen Rödel — 1Division of Nonmetallic-Inorganic Materials, Department of Materials and Earth Sciences, Technical University of Darmstadt, Alarich-Weiss-Str. 2, Darmstadt 64287, Germany

The defect chemistry of zirconia is usually modified by doping with high levels of yttrium. This induces a very high oxygen vacancy concentration which is responsible for the excellent ionic conductivity. There is a high demand for even better oxygen conductors because this would benefit applications like solid oxide fuel cells and solid state electrolyzers. Nevertheless, a limit has been reached concerning the doping strategy. Therefore, we suggestion to use dislocations as one-dimensional defects. These have so far been mostly disregarded as defects for modification of functional properties but are finding increasing attention recently. However, ceramics are generally brittle and thus not easily plastically deformable. Besides the difficulty of introducing dislocations into ceramics, their exact influence on functional properties is still unclear. Our investigations of yttria-stabilized zirconia show that mechanically introduced dislocations can enhance ionic conductivity significantly. This illustrates the opportunity to tune ceramics beyond what can be achieved by chemical doping.