MM 10: Computational Materials Modelling III

Time: Monday 15:45–17:30 Location: IFW B

MM 10.1 Mon 15:45 IFW B

Atomistic simulations of dislocations in strontium titanate — •Pierre Hirel[1,2], Matous Mrovec[1,2], and Christian Elsässer[1,2] — [1]Institut für Zuverlässigkeit von Bauteilen und Systemen (IZBS), Karlsruher Institut für Technologie, Kaiserstr. 12, 76131 Karlsruhe (Germany) — [2]Fraunhofer-Institut für Werkstoffmechanik IWM, Wöhlerstr. 11, 79108 Freiburg (Germany)

Strontium titanate (STO) is a perovskite oxide whose large dielectric constant makes it an attractive material for modern microelectronic applications. In contrast to the ongoing interest in electrical properties of STO, its mechanical properties came to the attention of the scientific community only in 2000 after a surprising discovery of a ductile-to-brittle-to-ductile transition. It was found that STO can deform plastically at room temperature, but the properties of dislocations mediating the deformation remain up to now a matter of debate.

The present study investigates the properties of dislocations in STO by means of atomistic simulations. The investigations are based on a multi-scale approach that uses both quantum-mechanical first-principles calculations and classical atomistic simulations with a rigid-ion potential. We compute the core structures of both screw and edge dislocations and analyze possible dissociation types and their relation to macroscopic mechanical behavior. The glide of dislocations under applied stress is studied directly by molecular dynamics simulations as well as indirectly using the nudged elastic band method. Our simulation results are compared to high-resolution transmission electron microscopy observations.

MM 10.2 Mon 16:00 IFW B

Elasticity and Screw Dislocations in W-Re and W-Ta Alloys — •Hong Li[1,2], Lorenz Romaner[2], Claudia Ambrosch-Draxl[2], and Reinhard Pippan[1] — [1]Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Jahn Straße 12, 8700 Leoben, Austria — [2]Chair of Atomistic Modelling and Design of Materials, University of Leoben, Franz Josef Straße 18, 8700 Leoben, Austria

Using a first-principles approach, the elastic properties as well as the core structure of the 1/2<111> screw dislocation in W-Me (Me=Ta, Re) alloys are investigated from the atomistic point of view. For a range of Ta/Re concentrations the lattice parameter, bulk modulus, and elastic constants are calculated and compared with pure W to study the influence of solute atoms on the elastic properties. A periodic quadrupolar arrangement of the dislocation is employed to model the core structures. We show that W and W-Ta alloys at all concentrations exhibit a symmetric core structure. In contrast, W-Re alloys exhibit a gradual transition to asymmetric cores. Furthermore, the critical stress which has to be applied to move the dislocation at 0K (Peierls stress σ_p) is calculated to determine the mobility of dislocations. The reduction of σ_p and a change of slip plane explain the brittle to ductile transition in W upon Re alloying. However, for W-Ta alloys the reduction of σ_p is found only with high Ta concentrations. Finally, we investigate the correlation between the core symmetry and the γ-surfaces for both W-Me cases.

MM 10.3 Mon 16:15 IFW B

DFT study of impurities at grain boundaries in α-Fe — Elwira Wachowicz and •Adam Kiejna — Institute of Experimental Physics, University of Wrocław, Wrocław, Poland

The effects of several metalloid (B), metalloid-like (C, P) and non-metallic impurities (N, O and S) on structure, energetics and mechanical properties of Σ3 (111) and Σ5 (210) grain boundaries (GBs) in ferromagnetic α-Fe have been studied by density functional theory and the projector augmented wave method. Two different concentrations and positions of impurity atoms at the GB were considered. Most of the impurities enhance the relaxation of the interplanar spacing of the pure grains. Interstitial impurities at both GBs increase separation of the grains while substitutional ones in general either do not alter or decrease it. Segregation of impurity atoms at the GBs and their embrittling/strengthening effect is explored and discussed in terms of its chemical and mechanical components. At the Σ5 GB for all impurity atoms considered the positions in the boundary layer are energetically favored independently of interstitial or substitutional site, whereas the enrichment of the Σ3 GB is favored for the impurities of the interstitial sites as well as for a substitutional P and C. In most cases, impurity atoms both in interstitial and substitutional positions at GBs act as embrittlers. The magnetic moments on the impurities are very small and in most cases align antiparallel to the moments on the neighboring Fe atoms.

MM 10.4 Mon 16:30 IFW B

Simulation der Korngrenzenbeweglichkeit in Aluminium mittels Molekulardynamik — •Volker Mohles und Jian Zhou — Institut für Metallkunde und Metallphysik, RWTH Aachen University, Aachen

Die Beweglichkeit von Korngrenzen und speziell ihre Temperaturabhängigkeit sind von größter technischer Bedeutung für die Rekristallisatioskinetik in industriellen Wärmebehandlungen. Daher gibt es in der Literatur eine Reihe von Molekulardynamik-Simulationen, in denen Korngrenzen durch eine synthetische, kristallorientierungsabhängige Kraft im Bewegung versetzt werden, um so die Mobilitäten der Korngrenzen abzuleiten. Die Ergebnisse bisheriger solcher Simulationen stehen in Hinblick auf die Temperatur- und Winkelabhängigkeit der Mobilitäten jedoch in starkem Widerspruch zu entsprechenden gemessenen Werten. Im vorliegenden Beitrag wird gezeigt, dass diese Widersprüche aus zwei unabhängigen, gravierenden Ungenauigkeiten der bisherigen Simulations- und Auswertungstechnik resultieren. Es werden Verbesserungen der Methodik vorgestellt, mit denen diese Ungenauigkeiten unterbunden werden können. Am Beispiel simulierter und experimenteller Ergebnisse zu reinem Aluminium wird gezeigt, dass Molekulardynamiksimulationen mit korrigierter Methodik verlässliche Mobilitätswerte für Korngrenzen vorhersagen können.

MM 10.5 Mon 16:45 IFW B

Plasticity of Cu and Pd nanoparticles in nanoextrusion — •Antti Tolvanen[1,2] and Karsten Albe[1] — [1]Institute of Materials Science, Darmstadt University of Technology, Germany — [2]Department of Physics, University of Helsinki, Finland

Recent transmission electron microscopy experiments have shown how nanoparticles can be encapsulated inside carbon onions and electron irradiation induced contraction of these onions can be used to apply pressure of tens of GPa to the encapsulated particle [1]. If an orifice is opened to the carbon onion, this system can be used to study the extrusion of the encapsulated material through this orifice. Therefore studying the extrusion of metallic nanoparticles from such nanocontainers provides information on the plasticity of individual nanograins. In this study, the results of molecular dynamics simulation of the extrusion of Cu and Pd nanoparticles pressurised in spherical force field mimicking the behaviour of contracting carbon onion are presented. We compare the plastic behavior single-crystalline nanoparticles of Cu and Pd with multiply-twinned nanoparticles. The effects of the low and high stacking fault energies of Cu and Pd, correspondingly, and the effect of twins on the dislocation nucleation and propagation is reported for both metals.

[1] L. T. Sun et al, Phys. Rev. Lett. 101, 156101 (2008)

MM 10.6 Mon 17:00 IFW B

DFT calculation on Fe/ZrO_2-Interfaces — •Jürgen Kutzner and Jens Kortus — Technische Universität Bergakademie Freiberg

Interface structures of the Fe/ZrO_2-system are presented. We investigated several possible orientations and configurations by means of density functional theory. Special emphasis was put on mechanical stability, termination of the different interface-structures and magnetic effects. The energetic comparison gives a view on the order of occurrence. As an addition, some experimental data is presented.

MM 10.7 Mon 17:15 IFW B

Studying grain growth in $SrTiO_3$ by diffraction contrast tomography and simulation — •Melanie Syha[1], Wolfgang Rheinheimer[2], Michael Bäurer[2], Erik M. Lauridsen[3], Wolfgang Ludwig[4], and Daniel Weygand[1] — [1]Karlsruher Institut für Technologie, IZBS, — [2]Karlsruher Institut für Technologie, IKM ,Kaiserstr. 12, 76131 Karlsruhe, Germany — [3]Risø National Laboratory for Sustainable Energy, 4000 Roskilde, Denmark — [4]European Synchrotron Radiation Facility, 38043 Grenoble, France

A comparison of the three dimensional (3D) grain structure in $SrTiO_3$ measured by diffraction contrast tomography (DCT) experiments and

mesoscale grain growth simulations is presented. The objective of this study is to explain the recently observed growth anomaly in $SrTiO_3$. The simulations allow for a systematical parameter variation, while the DCT experiments yield fundamental insight on structure and crystallography in 3D. In conjunction, these methods give access to the details of the topological quantities in grain structures and form an appropriate tool to study the influence of interface parameter variations on the grain morphology. The applied simulation tool is a 3D vertex dynamics model capable of handling inclination and misorientation dependent interface properties in structures consisting of several thousand grains. Using existing experimental data on orientation dependent interface energies/mobilities, as well as DCT results on structure, grain/pore shape and crystallography as input, the model has been enabled to depict the microstructural evolution of $SrTiO_3$ during annealing. A detailed comparison with 3D annealing experiments is provided.