

## MM 9 Interfaces

Time: Monday 14:45–16:15

Room: IFW D

MM 9.1 Mon 14:45 IFW D

**Ab-initio based multiscale calculations of low-angle grain boundaries in Aluminum.** — ●LIVERIOS LYMPERAKIS and JÖRG NEUGEBAUER — Max-Planck-Institut für Eisenforschung, Max-Planck-Str. 1, Düsseldorf

It is commonly accepted that grain boundaries have a central role in grain growth and recrystallization, and have significant contribution to the physical and mechanical properties of materials. A major challenge in describing extended defects such as low-angle grain boundaries is the large range of different length scales: The boundary consists of an array of dislocations where the core structure of each dislocation is rather localized, while the strain field is long range. In a previous study we have developed an ab-initio based multiscale approach that combines elements of density functional theory (DFT), empirical potentials, and continuum elasticity theory[1]. In the present study we have extended the formalism to an infinite array of ordered dislocations as realized in a low angle grain boundary. Based on this approach we have derived a diagram which predicts the energetically most stable boundary as function of the misorientation angle, the relevant displacement between the two grains, and the boundary-boundary separation distance. Based on this diagram we address the issue of grain boundary stability and we discuss recent experimental results.

[1] Phys. Rev. Lett. 93, 196401 (2004).

MM 9.2 Mon 15:00 IFW D

**Structure and reactivity at the Ti-Si boundary** — ●SIBYLLE GEMMING<sup>1,2</sup>, ANDREY ENYASHIN<sup>1,2</sup>, and MICHAEL SCHREIBER<sup>2</sup> — <sup>1</sup>Physikalische Chemie und Elektrochemie, Technische Universität, D-01062 Dresden. — <sup>2</sup>Institut für Physik, Technische Universität, D-09107 Chemnitz.

The density-functional band-structure investigation of several supercell models for the Ti(0001)|Si(111) interface reveals that an atomically flat interface is quite unstable due to the large lattice mismatch between the two constituents. The most realistic supercell model with a remaining strain of 1% yields a very low interface energy of only 0.28 J/m<sup>2</sup> with respect to fracture into the two unrelaxed surfaces. This adhesion is mainly due to an interfacial electron transfer from Ti to Si. Other possible model structures with higher local strains are even non-bonding, which indicates the pronounced influence of the elastic interactions. Density-functional molecular dynamics at an elevated temperature of 600 K, however, shows, that a silicide interlayer is formed at the interface, which significantly strengthens the interface and doubles the interface energy. Further investigations on the interfaces between Ti or Si and the reaction product TiSi<sub>2</sub> confirm, that the silicide layer at the interface is beneficial for the mechanical stability of the contact.

MM 9.3 Mon 15:15 IFW D

**Modelling and Characterisation of Interface Reactions between Diamond and Active Brazing Alloys** — ●CHUNLEI LIU<sup>1,2</sup>, ULRICH E. KLOTZ<sup>1</sup>, PETER J. UGGOWITZER<sup>2</sup>, and JÖRG F. LÖFFLER<sup>2</sup> — <sup>1</sup>Empa, Materials Science and Technology, Laboratory of Joining and Interface Technology, CH-8600 Dübendorf, Switzerland — <sup>2</sup>Laboratory of Metal Physics and Technology, Department of Materials, ETH-Zürich, CH-8093 Zürich, Switzerland

Diamond brazing has been deemed an effective route to the manufacture of high-performance diamond abrasive tools, and knowledge of the microstructure evolution of the interfacial area and the filler metal during the brazing process is of prime interest to enhance performance and to overcome existing problems. To reveal the microstructure evolution during the brazing process, we used a combination of thermodynamic modelling and sophisticated experimental techniques. A consistent thermodynamic database of the Cu-base filler metals was developed using the CALPHAD (Calculation of Phase Diagram) approach. The thermodynamic calculation and the experimental results show good agreement. Several alloy compositions and brazing temperatures were then selected according to the thermodynamic calculation for brazing trials. The interfacial structures were examined using FIB (Focused Ion Beam) and TEM (Transmission Electron Microscopy). The morphology of the reaction layers and nano-sized carbides grown at the interface between diamond and the alloy matrix were also studied to illustrate the reaction mechanism. These results are finally used for kinetic simulations, with

the aim of achieving better properties in brazed diamond tools.

MM 9.4 Mon 15:30 IFW D

**Examination of Grain Rotation Kinetics by Orientational Imaging Microscopy (OIM)** — ●M. ZIEHMER<sup>1</sup>, A. TSCHÖPE<sup>1</sup>, C. KRILL<sup>2</sup>, and R. BIRNINGER<sup>1</sup> — <sup>1</sup>Technische Physik, Universität des Saarlandes, 66041 Saarbrücken — <sup>2</sup>Elektrotechnik, Universität Ulm, 89081 Ulm

The specific grain boundary energy  $\gamma$  depends on the misorientation  $\theta$  of the adjacent grains. As a consequence, a torque which is proportional to the derivative of  $\gamma$  with respect to  $\theta$  is acting on the grains. Sufficient thermal energy provided, this torque results in a rotation of the grains into local energy minimum configurations.

There are several open questions concerning the functional form of  $\gamma$  with respect to  $\theta$  and the influence of grain boundary spatial extent on the rotation rate and the rotation mechanisms, which could all be enlightened by examining the rotation kinetics of individual grains.

We report on measurements of grain rotations in terms of the established method of spheres sintered onto a flat substrate. Both substrate and spheres are made of single crystalline copper. We take advantage of the progress in experimental techniques and use OIM for the measurement of the relative orientation of sphere and substrate. This method enables to study the rotations of single spheres over several orders of magnitude in grain boundary extent.

MM 9.5 Mon 15:45 IFW D

**Paradoxical grain-growth kinetics observed in Al under compression** — ●KEJING YANG and CARL KRILL — Materials Division, Albert-Einstein-Allee 47, University of Ulm, D-89081 Ulm, Germany

The mobility of grain boundaries in metals depends on stress in an intuitively reasonable manner: namely, compression slows the rate of boundary migration relative to that in the uncompressed state. Volkert and Lingk's discovery of *enhanced* boundary mobility in compressed Al films therefore came as a great surprise [1]. These authors attributed the faster grain growth in compressed regions to planarization of the film surface, which would be expected to reduce the pinning forces associated with grain-boundary grooving. We have tested this hypothesis in microcrystalline Al foils prepared by melt spinning. Since our samples are much thicker than the initial average grain size, a clear distinction can be drawn between surface and volume-related effects. Characterization by EBSD confirms the mobility enhancement induced by compression, but cross-sectional analysis suggests that the greatest increase in growth rate occurs in the center of the sample rather than at the surface! We discuss possible explanations for this observation in terms of mechanisms for boundary migration.

[1] C. A. Volkert and C. Lingk, *Appl. Phys. Lett.* **73** (1998) 3677.

MM 9.6 Mon 16:00 IFW D

**MD simulations about ordering and dynamics in Zr-crystal  $Ni_xZr_{1-x}$ -melt interfaces** — ●M. GUERDANE and H. TEICHLER — Institut f. Materialphysik d. Univ. Göttingen, 37077 Göttingen

The contribution reports results from molecular dynamics (MD) simulations about local order and dynamics in binary  $Ni_xZr_{1-x}$  melts in contact with Zr crystalline solid. The crystalline interface induces a local order in the way that the trigonal-prismatic structure elements (tp-elements), inherent to the  $Ni_xZr_{1-x}$ -melt, are attached to the crystalline wall in an ordered way. (110)-crystal interfaces show a marked roughness compared with (100)-interfaces, which can be attributed to a better adaptation of the tp-elements to the (100)- than to the (110)-surface. Atoms in the liquid surface layer have a lower energy than those in the crystal and in the interior of the melt. The ordered arrangement of the tp-elements in the liquid layer near the interface influences the atomic dynamics and seems to dominate the crystallization kinetics in the crystal/liquid couples. (Funded by the DFG, SPP 1120)