MM 41: Interfaces II

Time: Thursday 11:45–13:00 Location: IFW D

MM 41.1 Thu 11:45 IFW D

Elastic and plastic properties of special grain boundaries in aluminium — •Rebecca Janisch, Naveed Ahmed, and Alexander Hartmaier — Interdisciplinary Centre of Advanced Materials Simulation (ICAMS), Ruhr-University Bochum, 44780 Bochum, Germany

To investigate the role of grain boundaries during deformation and fracture of polycrystalline materials, we perform an ab-initio density functional study of a series of special grain boundaries in aluminium. The goal is to find relationships between the characteristic mechanical properties of interfaces - such as the work of separation, and the grain boundary sliding resistance - and the grain boundary degrees of freedom. We perform "ab-initio tensile tests"at bulk and bicrystal supercells to determine the effective interface elastic constant, the work of separation, as well as the critical stress and displacement for cleavage. The results will be discussed with respect to the grain boundary character (tilt/twist) and misorientation angle. Information on grain boundary sliding can be gained by studying the γ-surface of the interface, Δ E(τ), with τ being a rigid shift parallel to the grain boundary. The morphology of the γ-surface depends on the periodicity of the interface, and thus again on the grain boundary degrees of freedom, and the nature of the chemical bonds. Several γ-surfaces will be compared and the different influences discussed.

MM 41.2 Thu 12:00 IFW D

Ab-initio calculation of stacking-fault energies in Al-based alloys. — Pim Schravendijk[1], •Thomas Gnielka[2], Christian Elsässer[1], and Peter Gumbsch[1,2] — [1]Fraunhofer IWM, Wöhlerstr. 11, 79108 Freiburg — [2]IZBS, Universität Karlsruhe (TH), Kaiserstr. 12, 76131 Karlsruhe

The energetic stability of planar defects as a function of segregated alloying elements in diluted aluminium alloys is studied via ab initio density functional theory (DFT) calculations with the local density approximation (LDA). Several simple and transition metals are chosen as alloying elements and introduced as a substitutional point defects in low concentration (less than 10 at.-%) in the bulk crystal and at planar defects of face-centered cubic aluminum.

Formation energies of planar defects with point defects are determined as a function of the alloying elements' species and concentration. This requires DFT total-energy calculations, for atomistic supercells of the planar defects and point defects, as well as for single crystals of experimentally known intermetallic phases of the alloying elements with the aluminium host metal.

The procedure is applied to extrinsic and intrinsic stacking faults as well as to twin boundaries, and it provides a practical and straightforward estimation for interface and segregation energies in alloys.

MM 41.3 Thu 12:15 IFW D

Ginzburg-Landau theory of grain boundary premelting — •Robert Spatschek[1,2] and Alain Karma[2] — [1]ICAMS, Ruhr-Universität Bochum — [2]Northeastern University Boston

Grain boundary premelting is a phenomenon that emerges from repulsive forces between two differently oriented grains in a polycrystal. Typically, different types of forces contribute to the interaction, but it turns out that in metallic systems often "structural forces" play the dominant role. They are the consequence of lattice incompatibiliies due to a misorientation or grain shifts, and provoke elastic deformations and the formation of dislocations.

Starting from the classical density functional theory or a phase field crystal model we develop amplitude equations to shed light on the forces between solid-melt interfaces on an analytical and numerical level. We find in particular that these forces are significantly shorter ranged than previously anticipated and predict a grain boundary premelting transition for bcc iron.

MM 41.4 Thu 12:30 IFW D

Surface Tension andWetting in Solder Connections — •André Wedi and Guido Schmitz — Institut für Materialphysik,Westf.Wilhelms-Universität,Wilhelm- Klemm-Str. 10, 48149 Münster, Germany

Wetting is an important pre-requisite of a reliable solder connection. However, it is only an indirect measure for the important specific energy of the reactive interface between solder and base metallization. In order to quantify this energy, we measured wetting angles of solder drops as well as interface tensions between different SnPb solders and organic flux at a reflow temperature of 250°C. For the latter, we used the Lecomte-De-Noüy ring method applying suitable geometric corrections. From the two independent data sets, the important energy of the reactive interface is evaluated based on Young's equation. Remarkably, although both, the tension between solder and flux and the wetting angle, reveal significant dependence on solder composition, the specific energy of the reactive interface remains almost constant in the range of 0 to 40 at% Pb. This indicates that the properties of the reactive interface are essentially controlled by the Cu_6Sn_5 intermetallic reaction product. Since this phase grows during reflow, the wetting angle should develop in time, but in our in-situ measurements of this angle no time dependence is seen. In the talk the consequences of this contradiction to existing models of reactive wetting are discussed.

MM 41.5 Thu 12:45 IFW D

Interface width of immiscible layered elements — •Patrick Stender, Guido Schmitz, Constantin Ene, and Henning Galinski — Institute of Material Physics, WWU Münster

Based on the thermodynamics of inhomogeneous systems, it is expected that the chemical transition at an interface between two immiscible components cannot be atomically sharp. Recently, we could demonstrate by atom probe tomography that interfaces of metallic multilayers are indeed of finite chemical width and that this width depends systematically on temperature in thermal equilibrium. Thus, the observed effect becomes especially important for multilayer periodicities in the nanometer range. In the case of GMR devices, it can be made responsible for thermal degradation.

In our work, the temperature dependence of the chemical width of layer interfaces of the binary systems Ag/Cu and Fe/Cr and the ternary system Cu/Ni81Fe19 is studied by atom probe tomography. Metallic triple and multilayers were deposited using ion beam sputter deposition technique. For all samples, an isochronal annealing was performed. Owing to the outstanding resolution of the atom probe tomography, a significant broadening of the interface is demonstrated on the depth scale between 1 and 2 nm.

Because all three systems are immiscible from a thermodynamic point of view and the derived activation energies are way too small to allow an interpretation by conventional interdiffusion, Cahn-Hilliard theory is used to explain the observed temperature dependence.