MM 30: Interfaces

Structure and Properties

Time: Wednesday 10:15–11:30 Location: H 0107

MM 30.1 Wed 10:15 H 0107

Tailoring the thickness of intermetallic interfacial nanolayers by temperature control of FSW in Al-Cu lap joints — •Roland Marstatt[1], Markus Krutzlinger[2], Johannes Luderschmid[1], Michael F. Zäh[2], and Ferdinand Haider[1] — [1]Chair for Experimental Physics 1, University of Augsburg, D-86159 Augsburg — [2]Institute for Machine Tools and Industrial Management (iwb), Technical University of Munich, D-85748 Garching

The Friction Stir Welding (FSW) process is suitable to join dissimilar materials. The solidus temperature is not exceeded during FSW. Hence, joints between dissimilar metals can be produced with minimal intermetallic phase formation. The intermetallic phases can cause embrittlement and also lower the electrical and thermal conductivity across the interface. However, nano-scale intermetallic layers between joining partners have been reported in literature repeatedly, and these play a key role in material bonding. The layer thickness is related to welding temperature via an Arrhenius law. However, the correlation of the process parameters and the interface structure is still a subject of ongoing research. In this study, the potential of temperature control during FSW in order to improve the joint quality has been analyzed. The influence on and control over intermetallic layer thickness was investigated by welding dissimilar lap joints of aluminium and copper at different temperatures. The temperature was controlled by varying the rotational speed using a PI-controller. The results expand the existing knowledge and prove the applicability of temperature control during FSW of dissimilar metals. Supported by the DFG as part of SPP1640.

MM 30.2 Wed 10:30 H 0107

Direct observation of novel structures and transitions in [111] tilt grain boundaries — •Thorsten Meiners[1], Timofey Frolov[2], Christian H. Liebscher[1], and Gerhard Dehm[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf — [2]Lawrence Livermore National Laboratory

It is well known that grain boundaries (GBs) have a significant influence on the materials macroscopic mechanical properties. Recently, thermodynamic models and atomistic calculations have predicted the possibility of GB phase transitions, which can alter the GB properties. In our study, we investigate the structure of symmetric and asymmetric [111] tilt GBs in copper by aberration-corrected scanning transmission electron microscopy (STEM) and molecular dynamics simulations (MD). The structural units of two symmetric Σ 19b tilt boundaries (46.83° [111]/{253} and 46.83° [111]/{178}) agree well with that obtained by the molecular static simulations. The symmetric 46.83° [111]/{178}) GB shows a regular pattern consisting of two structural units. In case of a asymmetric 46.83° [111]/{1-10}{9-2-7} tilt boundary we observe the same structural units, but now irregularly interrupted by a defect. These different structural units are also in agreement with MD simulations. At a special location, a sharp transition of the structural units with a stronger disorder at the asymmetric GB is observed. The coexistence of both structural motives provides first experimental evidence for the coexistence of two different GB phases. The differences in atomic ordering of the irregular structural units and transitions between structural motives will be discussed in detail.

MM 30.3 Wed 10:45 H 0107

A simple descriptor for energetics at fcc-bcc metal interfaces — •Linda Angela Zotti[1,2], Stefano Sanvito[2], and David D O' Regan[2] — [1]Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, 28049 Madrid, Spain — [2]School of Physics, AMBER and CRANN Institute, Trinity College, Dublin 2, Ireland

We developed a new and user-friendly method to calculate interface energies which avoids problems deriving from numerical differences between bulk and slab calculations (such as the number of k points along the direction perpendicular to the interface). We applied it to 36 bcc-fcc metal systems in the (100) orientation and found a clear dependence of the interface energy on the difference between the work functions of the two metals on the one hand, and the total number of d electrons on the other. Mechanical deformation was observed more in the fcc crystal than in the bcc counterpart. For each bcc metal, the interface energy was found to follow the position of its d- band, whereas the same was not observed for the fcc.

MM 30.4 Wed 11:00 H 0107

structural prediction of low-energy interface reconstructions of Σ 5 grain boundaries — •lin sun — Institut für Festkörpertheorie und Optik, Friedrich-Schiller-Universität Jena, Germany

We performed *ab initio* global structural predictions with the minima hopping method of interface reconstructions in three different silicon grain boundaries, Σ5(012), Σ5(031) and Σ5(521). We calculated interface energies and electronic density of states. Compared with locally optimized structures, our new structures have lower total energies and significantly smaller interface energies. We observed some recurrent geometrical features of the lowest energy interfaces: Si atoms prefer to form spiral structures rather than simiple rings. Concerning the electronic properties, defect energy levels in the band gap of locally-optimized interfaces can disappear after interface reconstruction. Our investigation suggests that global structural prediction is extremly important to predict the effect on transport and optical properties of grain boundaries in semiconductors.

MM 30.5 Wed 11:15 H 0107

Ab-initio based study of topological segregation of C impurities at Si grain boundaries — •Masud Alam, Liverios Lymperakis, Christain Liebscher, and Jörg Neugebauer — Max-Planck Institute for Iron Research,Max-Planck Str.1 , 40237 Duesseldorf, Germany

Interfaces significantly influence the properties of multi-crystalline Si. More specifically, they introduce states in the fundamental band gap thereby allowing preferential impurities segregation and/or the formation of stable or metastable equilibrium interface phases. In the present work we investigate the segregation of C impurities at flat and faceted Si Grain Boundaries (GBs). In a first step we employ density functional theory (DFT) calculations to parametrize Si, C and Si-C modified embedded atom method (MEAM) interatomic potentials. Careful benchmarks show that the potentials provide an accurate description of the atomic geometry and energetics of intrinsic Si GBs (Wulff diagram) as well as of the C segregation at the aforementioned interfaces. Based on the new potential, we identify the preferential carbon segregation at faceted GBs. Using this insight we are able to interpret recent experimental findings on the topological segregation of impurities at facet junctions. More specifically, the presence of the energetically favorable non symmetric Σ3 112 GB results in strong anisotropy of the strain field and hence in strong selectivity of C impurities at the GB junctions.