MM 49: Interfaces I: Structure and Segregation

Time: Thursday 10:15–11:45 Location: H 0107

MM 49.1 Thu 10:15 H 0107

First-principles and tight-binding studies of symmetrical tilt grain boundaries in bcc-Fe — •Jingliang Wang, Georg K. H. Madsen, and Ralf Drautz — ICAMS, Ruhr-Universitätsstr. 150, D- 44801 Bochum, Germany

Using density functional theory (DFT), we studied the stability of a series of low-Σ symmetrical tilt grain boundaries (STGBs) in bcc-Fe. A systematic strategy was applied to seek the most stable configuration. All STGBs studied in this work possess a similar GB energy except for the more stable Σ3(112)-GB. We present the correlations between the GB energies and local atomic structures. Based on the results from DFT calculations, we modified the recently-developed othogonal tight-binding (TB) model for iron and we show that the modified TB model is able to predict the correct GB structure and give GB energies in good agreement with DFT. We validated the model for twist GBs and apply it to study the stability of realistic models of GBs in martenstic steels.

MM 49.2 Thu 10:30 H 0107

On the origin of anisotropic lithiation of Si — •Ashkan Moradabadi[1], Jochen Rohrer[2], Karsten Albe[2], and Payam Kaghazchi[1] — [1]Physikalische und Theoretische Chemie, Freie Universität Berlin, Takustrasse 3, 14195 Berlin, Germany — [2]Institut für Materialwissenschaft, Fachgebiet Materialmodellierung, Technische Universität Darmstadt, Jovanka-Bontschits-Str. 2, 64287 Darmstadt, Germany

Si nanowires (SiNW) are promising candidates for next-generation lithium-ion battery anodes. Lithiation of SiNW anodes proceeds by the movement of interfaces between lithiated amorphous Li_xSi and pristine crystalline Si in a core-shell structure. Experimental studies show that first-cycles of lithiation of SiNWs lead to an anisotropic expansion of SiNWs. In this work, we present density functional theory calculations on Li incorporation in SiNWs using surface and interface geometries. We find that in opposition to the results based on (commonly-used) surface models, the anisotropic expansion of SiNWs does not originate from orientation-dependent barriers for Li diffusion across the Li_xSi/Si interfaces. Due to the disorder nature of interfaces these barriers are distributed isotropically. Instead, here we find that the anisotropic swelling is a consequence of orientation-dependent interface energies and the fact that high-energy interfaces are more mobile than low-energy interfaces.

MM 49.3 Thu 10:45 H 0107

Why calculated energies of grain boundary segregation are unreliable when segregant solubility is low — Pavel Lejček[1], •Mojmír Šob[2,3,4], Václav Paidar[1], and Václav Vitek[5] — [1]Institute of Physics, Academy of Sciences of the Czech Republic, Prague, Czech Republic — [2]Central European Institute of Technology, CEITEC MU, Masaryk University, Brno, Czech Republic — [3]Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Republic — [4]Department of Chemistry, Faculty of Science, Masaryk University, Brno, Czech Republic — [5]Department of Materials Science and Engineering, University of Pennsylvania, Philadelphia, PA, USA

We demonstrate that density functional theory based calculations of segregation energies at interfaces are often unreliable when the bulk solid solubility of the segregant is lower than that corresponding to one solute atom per computational repeat cell. In this case, the calculated energy of a solute in the bulk cannot be used when evaluating segregation energies. We document this problem by analyzing the measured and calculated grain boundary segregation energies in nickel and bcc iron available in the literature. On the other hand, even when using repeat cells that are not sufficient for reliable evaluation of the segregation energy, the change in the grain boundary cohesion (strengthening/embrittling energy) may be obtained with a reasonable accuracy.

MM 49.4 Thu 11:00 H 0107

Tensile strength of Ni grain-boundary with segregated sp-impurities — •Miroslav Černý[1,2,3], Petr Šesták[1,2], Petr Řehák[1,2,3], Monika Všianská[1,3], and Mojmír Šob[1,3,4] — [1]Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Republic — [2]Faculty of Mechanical Engineering, Brno University of Technology, Brno, Czech Republic — [3]Central European Institute of Technology, Brno, Czech Republic — [4]Faculty of Science, Masaryk University, Brno, Czech Republic

Grain boundaries (GB) represent extended planar defects with a crucial effect on macroscopic strength of polycrystalline materials. In this first principles study, we calculate the ideal tensile strength of Σ5(210) tilt GB in nickel crystal under uniaxial loading applied perpendicularly to the GB plane. A repeat cell containing 64 atoms is subjected to three different modes of simulated deformation comprising rigid grain shift, uniaxial deformation with optimized atomic coordinates and fully optimized uniaxial loading (ionic positions in the supercell as well as the cell shape are optimized at each step of deformation). Results for these models are compared and tensile strength of clean GB is compared with that of GB with segregated impurities (S and Al) and with the results of previous studies. Differences in computed values show not only the effect of the impurities on the ideal strength but also the importance of full lattice optimization during the simulation of tensile test.

MM 49.5 Thu 11:15 H 0107

Theoretical strength of Σ5 (210) GB in FCC cobalt with segregated interstitial and substitutional sp-impurities — •Petr Šesták[1,2], Miroslav Černý[1,2,3], Petr Řehák[1,2,3], Monika Všianská[1,3], and Mojmír Šob[1,3,4] — [1]) Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Republic — [2]Faculty of Mechanical Engineering, Brno University of Technology, Brno, Czech Republic — [3]Central European Institute of Technology, Brno, Czech Republic — [4]Faculty of Science, Masaryk University, Brno, Czech Republic

Grain boundaries (GBs) determine many mechanical properties of polycrystalline materials, in particular their strength. Moreover, the impurities contained in the material tend usually to segregate at the GBs and thus they can have a strong negative or positive influence on its mechanical characteristics. In this first-principles study we simulate the uniaxial tensile test of FCC cobalt containing the Σ5 (210) tilt GB with segregated sp-impurities. The uniaxial deformation was performed along an axis perpendicular to the GB. The impurities Al, Ga, In, Sn, Sb and Te were considered in substitutional positions at the GB and Si, P, S, Ge, As and Se in interstitial positions. The strength of segregated GBs was compared with the strength of the clean GB. The uniaxial deformation was realized using two different approaches. In the first one the repeat cell was continually optimized during the entire deformation path and in the second one the deformation corresponded to a rigid separation of grains along a defined plane without any cell optimization.

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