MM 35: Structural Materials II

Time: Wednesday 11:45–12:45 Location: H52

MM 35.1 Wed 11:45 H52

First-principles study of carbon segregation in bcc iron symmetrical tilt grain boundaries — •Jingliang Wang, Georg K. H. Madsen, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, Universitätsstr. 150, D-44801, Bochum, Germany

Using density functional theory (DFT), we studied the C segregation behavior to three low-Σ symmetrical tilt grain boundaries (STGBs) in bcc-Fe. For each GB, we examined potential segregation sites and demonstrated that the most stable segregation sites always possess the greatest coordination number and maximum nearest Fe-C neighbor distance. Thereby a geometric criterion for predicting the segregation sites for more general GBs is suggested. We rationalized the geometric criterion by splitting the solution energy into chemical and mechanical contribution. The chemical contribution is shown to be related to the coordination number, whereas the mechanical contribution is related to the Fe-C bond length. The effect of C on the GB energies depends on the GB structure. The open GBs are stabilized by C segregation and the GB energy continuously decreases by increasing the C concentration while the compact GB shows an opposite trend.

MM 35.2 Wed 12:00 H52

Origin of the off-stoichiometry of Fe-Mn-Al-C kappa carbides: An ab-initio explanation of atom probe tomography data — •Poulumi Dey[1], Roman Nazarov[2], Biswanath Dutta[1], Mengji Yao[1], Michael Herbig[1], Martin Friák[3], Tilmann Hickel[1], Dierk Raabe[1], and Jörg Neugebauer[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, D-40237 Düsseldorf, Germany — [2]Livermore National Laboratory, Livermore, CA 94550, USA — [3]Institute of Physics of Materials, v.v.i., Academy of Sciences of the Czech Republic, CZ-61662 Brno, Czech Republic

Quaternary Fe-Mn-Al-C alloys have exceptional mechanical properties such as high strength and ductility. In a certain composition range these alloys show a microstructure that comprises of an austenitic Fe-based matrix along with regularly arranged nano-sized kappa carbides which strongly strengthens the material. The nominal composition of kappa carbide is (Fe,Mn)3AlC, but our atom probe tomography measurements have indicated reduced C and Al contents in these carbides. Using density functional theory calculations, we succeeded to explain the experimentally observed off-stoichiometry with respect to C as a consequence of minimizing the elastic strains emerging in coherent microstructures. The off-stoichiometric concentration of Al can also be explained to a certain extent by a strain minimization caused by Mn antisite defects on the Al sub-lattice in kappa carbide. However, this effect becomes only significant if C vacancies are present in the vicinity of the antisite. We therefore demonstrated that the phenomena of depleted interstitial C and substitutional Al are coupled.

MM 35.3 Wed 12:15 H52

Structure of the high entropy alloy Al_xCrFeCoNi: fcc versus bcc — •Masako Ogura[1], Tetsuya Fukushima[2], Rudolf Zeller[1], and Peter H. Dederichs[1] — [1]Peter Grünberg Institute and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, Jülich, Germany — [2]Graduate School of Engineering Science, Osaka University, Toyonaka, Japan

High entropy alloys (HEAs) are disordered multi-component systems with equal or near-equal atomic ratios. They have simple solid solution structures, e.g., bcc and fcc structures, stabilized by the high disorder entropy effect. The structure of HEAs with Al such as Al_xCrFeCoNi and Al_xCrFeCoNiCu changes from fcc to bcc with increasing the Al concentration. In this study, we investigate the effect of Al on the structure of the HEA Al_xCrFeCoNi on the basis of first-principles electronic structure calculations. The calculations are performed with the KKR Green's function method in the framework of the density functional theory using GGA. The disordered alloys are simulated by the coherent potential approximation or supercell calculations with several hundred atoms. We discuss the change from fcc to bcc structures and the importance and stability of partially disordered B2 and $L1_2$ structures.

MM 35.4 Wed 12:30 H52

First-principles investigations on intermetallic ϵ-Al_5Fe_2 phase — •Lilit Amirkhanyan and Jens Kortus — TU Bergakademie Freiberg, Institute for Theoretical Physics, Germany

The iron-aluminum system is of commercial and technical interest, as it has low density, high thermal conductivity, high strength and formability. The ϵ-Al_5Fe_2 structure is a high-temperature phase in the Al-Fe binary system, which is stable between 1368 K - 1504 K [1].

We investigated the ϵ-Al_5Fe_2 intermetallic phase, using density functional theory (PAW pseudopotential) calculations in order to understand the Al and Fe preferred sites. Our study focused of four different possible crystallographic site changes between Al-Fe positions. For each case we optimized the structure, minimizing the ground-state energy, the atomic forces and the stresses. This structure was then used to calculate the bulk module. The elastic properties contain information on the stability of the investigated structures. Further, we investigated the magnetism in the phase.

References

1. Vogel, SvenC. and Stein, Frank, P.Martin. Applied Physics A **99(3)**, [607-611], 2010