

MA 22: Focus Session: Magnetism in Materials Science: Thermodynamics, Kinetics and Defects III (joint session MM/MA)

Magnetism V

Time: Tuesday 11:45–13:00

Location: H 0106

Topical Talk MA 22.1 Tue 11:45 H 0106
Grain boundary migration and grain growth in non-ferromagnetic metals under the impact of a magnetic field — ●DMITRI A. MOLODOV — Institute of Physical Metallurgy and Metal Physics, RWTH Aachen University, 52056 Aachen, Germany

Grain boundary migration can be induced by a magnetic field, if the anisotropy of the magnetic susceptibility generates a gradient of the magnetic free energy density across the boundary. In contrast to curvature driven boundary motion, a magnetic driving force also acts on planar boundaries so that the motion of crystallographically fully defined boundaries can be investigated. The magnetically driven motion of planar symmetric and asymmetric tilt grain boundaries was studied in high purity bismuth and zinc bicrystals. Boundary migration was measured in-situ by means of a polarization microscopy probe and the corresponding migration activation parameters were obtained. The results revealed that grain boundary mobility essentially depends on the misorientation angle and the inclination of the boundary plane.

As it has been demonstrated in a series of experiments on polycrystalline zinc, titanium and zirconium, as well as by computer simulations, grain growth in magnetically anisotropic non-ferromagnetic materials can be substantially affected by a magnetic field. This manifested itself by significant changes in the development of the grain growth texture during magnetic annealing compared to annealing at zero field. The magnetically induced texture changes are caused by the generation of an additional magnetic driving force for grain growth/shrinkage.

MA 22.2 Tue 12:15 H 0106
Stability and magnetic properties of grain boundaries in the inverse Heusler phase Fe_2CoGa and in bcc Fe — ●DANIEL F. URBAN¹, WOLFGANG KÖRNER¹, GEORG KRUGEL¹, ANNA LEHNER¹, and CHRISTIAN ELSÄSSER^{1,2} — ¹Fraunhofer IWM, Freiburg, Germany — ²University of Freiburg, FMF, Germany

Grain boundaries (GBs) in the cubic inverse Heusler phase Fe_2CoGa are investigated by means of first principles calculations based on density functional theory. The results are compared to those of corresponding GBs in bcc Fe. Besides the energetic stability, the analysis focuses on the magnetic properties of the GBs. The inverse Heusler phase offers a variety of interesting low energy GBs. It is found that such GBs do not lead to a breakdown of the local magnetic moments at the interface, as observed for some of the GBs in bcc Fe. Instead there is partially even a substantial enhancement near the GB. Nevertheless, the integrated increase in total magnetic moment is very similar for GBs in both materials. The analysis of the ferromagnetic coupling indicates that the coupling across such low energy interfaces

is not reduced with respect to the single crystal of Fe_2CoGa , whereas in bcc Fe a weakening or even decoupling of two grains can occur.

MA 22.3 Tue 12:30 H 0106
Magnetic properties of the CrMnFeCoNi high-entropy alloy — OLDŘICH SCHNEEWEISS¹, ●MARTIN FRIÁK^{1,2}, MARIE DUDOVÁ¹, DAVID HOLEC³, MOJMÍR ŠOB^{2,1,4}, DOMINIK KRIEGNER⁵, VÁCLAV HOLÝ⁵, PŘEMYSL BERAN⁶, EASO-P. GEORGE⁷, JÖRG NEUGEBAUER⁸, and ANTONÍN DLOUHÝ¹ — ¹Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Republic — ²Central European Institute of Technology, CEITEC MU, Masaryk University, Brno, Czech Republic — ³Department of Physical Metallurgy and Materials Testing, Montanuniversität Leoben, Leoben, Austria — ⁴Department of Chemistry, Faculty of Science, Masaryk University, Brno, Czech Republic — ⁵Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic — ⁶Nuclear Physics Institute, Academy of Sciences of the Czech Republic, Řež, Husinec, Czech Republic — ⁷Institute for Materials, Ruhr University, Bochum, Germany — ⁸Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

The equiatomic CrMnFeCoNi high-entropy alloy undergoes a paramagnetic-to-spin-glass transition at 93 K and a ferromagnetic transition at 38 K while maintaining its fcc structure down to 3 K (Phys. Rev. B 96 (2017) 014437). We study the local atomic magnetic moments in this material by *ab initio* calculations. We find the Cr magnetic moments aligning antiferromagnetically with respect to a cumulative magnetic moment of their first coordination shell. The magnetic moments of Fe and Mn atoms remain high (between 1.5 and 2 μ_B), while the local moments of Ni atoms effectively vanish.

MA 22.4 Tue 12:45 H 0106
Effect of magnetic transition on grain boundary diffusion of Mn in α -iron — VLADISLAV KULITCKII, SERGIY DIVINSKI, and ●GERHARD WILDE — Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, Münster, Germany

Grain boundary diffusion of Mn in α -Fe has been studied in both, B- and C-types kinetic regimes in a wide temperature range of 473 to 1173 K. The concentration profiles were measured applying the radiotracer technique with serial sectioning by microtome and using the ⁵⁴Mn radioactive isotope. As a result, Mn segregation at general high-angle grain boundaries of α -Fe is estimated. The grain boundary diffusivities were found to exhibit a distinct non-linear Arrhenius temperature dependence that is discussed in terms of the impact of the magnetic transition on Mn grain boundary diffusion.