

MM 3: Transport - Atoms and Ions I

Time: Monday 10:15–11:30

Location: IFW A

MM 3.1 Mon 10:15 IFW A

Influence of magnetic transformation on bulk diffusion of Mn in iron — ●VLADISLAV KULITCKII¹, OMKAR HEGDE², TILMANN HICKEL², CHU-CHUN FU³, SERGIY DIVINSKI¹, and GERHARD WILDE¹ — ¹Institut für Materialphysik, Universität Münster, Germany — ²Max Planck Institute for Iron Research GmbH, Düsseldorf, Germany — ³Atomic Energy and Alternative Energies Commission, Gif-sur-Yvette, France

Comparing to a linear dependence in the paramagnetic state, the Arrhenius plot of self-diffusion in alpha-iron shows a downward curvature below the Curie temperature. The magnetic transformation-induced kink of diffusion in alpha-iron was also observed for such solutes as Co, Cr, or Ni. Here we are reporting the impact of the magnetic transition on bulk diffusion of Mn. Tracer diffusion was measured by a microtome (higher temperatures) and sputtering (low temperatures) sectioning methods using the radioactive isotope ⁵⁴Mn. The experiments are performed in a wide temperature range from 773 K to 1173 K. In obvious contrast to self-diffusion, a marginal if any impact of the magnetic transition on Mn bulk diffusion is found. The Mn bulk diffusion coefficient in alpha-Fe follows an Arrhenius dependence with the pre-factor of 0.0287 m²/s and the activation enthalpy of 282.8 kJ/mol. The experimental results are compared with the DFT-based theoretical predictions.

MM 3.2 Mon 10:30 IFW A

A DFT study of the electric field dependence of atomic migration barriers in hard magnetic L1₀ intermetallic phases — ●OSKAR TILL¹ and CHRISTIAN ELSÄSSER^{1,2} — ¹Freiburger Materialforschungszentrum FMF, Stefan-Meier-Straße 21, 79104 Freiburg — ²Fraunhofer IWM, Wöhlerstraße 11, 79108, Freiburg

We examine the effect of an external electric field on migration barriers of atoms near surfaces in ferromagnetic binary L1₀ intermetallics. Using DFT surface-slab models for various surface configurations we study hops of atoms in the vicinity of the crystal surface. We are especially interested in the transition from the disordered A1 phase to the ordered L1₀ phase of FeNi, a promising candidate for a rare-earth-free high performance hard magnetic material. The aims are an assessment in how far electromigration effects can be effective in processing hard magnetic materials, as well as a better understanding of electromigration in intermetallic phases. Hence we extend the scope to the L1₀ phases of FePt, MnAl and MnGa. These four alloys cover a wide range of thermal ordering time scales and related experimental feasibilities. The investigations are part of a joint project 'Processing magnetic materials enhanced by electric fields or currents' in the DFG SPP 1959 'Fields Matter'.

MM 3.3 Mon 10:45 IFW A

Combination of ⁷Li-Field-Cycling and T_{1ρ}-NMR experiments to investigate metallic lithium and lithium solid-state ion conductors. — ●PHILIPP SEIPEL, EDDA WINTER, and MICHAEL VOGEL — AG Vogel, Institut für Physik kondensierter Materie, TU Darmstadt

Nuclear Magnetic Resonance offers a broad range of possibilities for determining correlation times of lithium ionic motion in Li-Ion conductors in the range of 10⁰ s to 10⁻¹⁰ s. One method for determining the dynamics is to measure the spin-lattice relaxation T₁, which is sensitive to dynamics on the time scale of the inverse Larmor-frequency ω. For superconducting spectrometers, this is usually in the range of τ ≈ 10⁻⁹ s. In order to investigate slow processes, it is beneficial to measure T₁(ω) at low magnetic fields (ω ≈ kHz) whereas ⁷Li-Field-Cycling NMR is a powerful method to do so [1,2]. In these experiments, it is necessary to switch between low and high magnetic fields during the

measurement to enhance the signal intensity, whereby the measurable T₁ values are limited to ≥ 1 ms by a switching time. T_{1ρ} measurement is a nice method to extend the range of field cycling, because it is possible to measure T_{1ρ} values down to 10⁻⁴ s. However sample heating can cause limitations. Using metallic lithium as a model system, this study shows that both methods compliment each other nicely and with certain limitations, can also be used to determine activation energies for Li-ionic jumps in solid-state ionic conductors.

(1) M Haaks et al., PBR, 2017, DOI:10.1103/PhysRevB.96.104301
(2) J. Gabriel et al., SSNMR, 2015, DOI:10.1016/j.ssnmr.2015.06.004

MM 3.4 Mon 11:00 IFW A

Atomistic modeling of grain boundaries and their effects on oxygen vacancies in SrTiO₃ — ●CONG TAO^{1,2}, DANIEL MUTTER¹, DANIEL F. URBAN¹, and CHRISTIAN ELSÄSSER^{1,3} — ¹Fraunhofer IWM, Wöhlerstraße 11, 79108 Freiburg, Germany — ²IAM-CMS, Karlsruhe Institute of Technology, Straße am Forum 7, 76131 Karlsruhe, Germany — ³Freiburger Materialforschungszentrum FMF, Stefan-Meier-Str. 21, 79104 Freiburg, Germany

Point defects, especially oxygen vacancies, are involved in the accelerated grain growth behavior observed in strontium titanate (STO) perovskites in applied electric fields. The underlying mechanisms for the redistribution of oxygen vacancies along and across grain boundaries (GB) are not yet fully understood. In order to advance the understanding at the atomic scale, we employ classical atomistic simulations to investigate structures and properties of both the symmetric and asymmetric tilt GBs in SrTiO₃. To locate the energetically favored sites for oxygen vacancies, their formation energies are calculated and analyzed with respect to local electrostatic potentials in atomistic supercell models. The simulation results indicate that oxygen vacancies preferentially form in the vicinity of the GBs. In addition to formation energies, the paths for oxygen vacancies migrating from all possible sites to their nearest neighbor sites are identified and systematically analyzed. The landscapes of oxygen vacancy formation energies and migration barriers are critically discussed with respect to experimental observations, in order to elucidate the specific role of GBs in trapping oxygen vacancies in SrTiO₃ from both theoretical and practical viewpoints.

MM 3.5 Mon 11:15 IFW A

Mutual dependence of oxygen and vacancy diffusion in dilute iron alloys and the influence of substitutional atoms — ●XIAOSHUANG WANG, JÜRGEN FASSBENDER, and MATTHIAS POSSELT — Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

By combination of density functional theory (DFT) and an efficient method based on Atomistic Kinetic Monte Carlo (AKMC) the mutual influence of oxygen (O) and vacancy (v) diffusion in α-Fe and the effects of substitutional atoms (Ti, Y) are studied. Both oxygen and vacancy are mobile while the substitutional atoms are assumed to be immobile. Using DFT, binding energies between oxygen and vacancy at different neighbour distances and migration barriers for oxygen in the environment of a vacancy and for vacancy in the environment of an oxygen atom are determined. The most attractive state for oxygen and vacancy was found at the 1st neighbour distance. The O-v pair at the 6th neighbour distance is unstable and therefore it is impossible to reach via oxygen/vacancy jump. The newly-found simultaneous jumps of both O and v compensate the lack of state 6. By using the data obtained by DFT as inputs, the diffusion coefficient of oxygen and of vacancy are determined for given concentration of vacancy and oxygen atoms by an AKMC-based efficient method. Additionally, oxygen and vacancy diffusion were calculated in the first stage of thermal processing of ODS steel where O, Y, and Ti is purposely introduced.