MM 35: Transport in Materials: Diffusion, Charge or Heat Conduction

Diffusion

Time: Friday 10:15–11:45 Location: H22

MM 35.1 Fri 10:15 H22

Influence of second phase precipitation on bulk diffusion of Ni in the CoFeMnNiV high-entropy alloy — •Aditya Burla[1], Mohan Muralikrishna Garlapati[1], Aditya Srinivasan Tirunilai[2], Guillaume Laplanche[2], Gerhard Wilde[1], and Sergiy V Divinski[1] — [1]Institut für Materialphysik, Universität Münster, 48149 Münster, Germany — [2]Institut für Werkstoffe, Ruhr-Universität Bochum, 44780 Bochum, Germany

High-entropy alloys (HEAs), or multi-principal element alloys represent a new class of metallic materials that offer tremendous opportunities for advancing materials science due to their vast compositional space and exceptional properties. While tracer diffusion and sigma phase precipitation kinetics in the Co-Cr-Fe-Mn-Ni system have been widely studied, the interaction between the two has received limited attention. The present work focuses on an equiatomic CoFeMnNiV HEA, in which Vanadium is known to have a strong tendency to stabilize the sigma phase. Therefore, this element promotes its precipitation in the CoFeMnNiV alloy, particularly at temperatures below ~1080°C, even after short anneal times of just 1 h in the fully recrystallized state. In this study, bulk diffusion of Ni is investigated using the radiotracer technique. A strong impact of sigma phase precipitation on the self-diffusion kinetics was discovered and analyzed. The obtained tracer diffusivities follow an Arrhenius-type relationship when estimated in the stable microstructures, whereas concurrent precipitation enhances the tracer diffusion rates.

MM 35.2 Fri 10:30 H22

Investigation of lateral hydrogen diffusion in polycrystalline molybdenum trioxide thin films — •Tim K. Hecker, Martin Becker, and Peter J. Klar — Institute of Experimental Physics I and Center for Materials Research, Justus Liebig University Giessen, Giessen, Germany

Molybdenum trioxide thin films were prepared by RF sputter deposition exploring a wide range of growth parameters. To characterise the thin films, electrochemical, Raman, and XRD experiments were conducted. In order to gain a deeper understanding of the diffusion of hydrogen in these thin films, the samples were microstructured with a PMMA film in a way that restricts the contact surface with the electrolyte to a narrow stripe-like gap. This enables the lateral diffusion of hydrogen beneath the PMMA film to be studied using a transmission experiment, making use of the electrochromic properties of molybdenum trioxide. This increases the accessible spatial and temporal scale by several orders of magnitude, significantly improving the spatial and temporal resolution of the in-situ transmission measurement. Spatially resolved transmission measurements in the wavelength range of 633±55 nm demonstrate that the investigated diffusion is dependent on the hydrogen concentration. The results are also supported by a spatially and temporally resolved diffusion simulation. Furthermore, the measurement method presented here is universally applicable to electrochromic thin film samples.

MM 35.3 Fri 10:45 H22

Diffusion and activation energies of hydrogen and its isotopes in boron structure — •Bianca Solomonea[1,2], Calin Pantis-Simut[2,3], Mihaela Cosinschi[2,3], Paul Dinca[1], Corneliu Porosnicu[1], and George Nemnes[2,3] — [1]National Institute for Laser, Plasma and Radiation Physics (INFLPR), Atomiştilor Street 409, 077125 Măgurele, Ilfov, Romania — [2]Faculty of Physics, University of Bucharest, Atomistilor 405, Magurele-Ilfov 077125, Romania — [3]Horia Hulubei National Institute for Physics and Nuclear Engineering, Reactorului 30, Magurele-Ilfov 077125, Romania

The retention and release of hydrogen isotopes in plasma-facing materials (PFM) is a critical concern for the ITER project. The decision to construct the Tokamak reactor as a fully tungsten-based machine presents challenges regarding plasma ignition and stability, particularly due to impurities in the working gases. Boronization is applied to retain impurities by forming covalent bonds with oxygen and nitrogen. This study uses ab initio calculations via Density Functional Theory (DFT), molecular dynamics (MD), and the nudged elastic band (NEB) method in the SIESTA code to examine boron structures in crystalline and amorphous forms. Activation energies for trapping, detrapping, and diffusion processes are determined. Given the difficulty of defining hydrogen-isotope diffusion in boron structures, and its importance for retention and desorption in redeposited or co-deposited layers of the PFM, we focus on identifying the potential diffusion trajectories of hydrogen within the boron structure. This includes mapping a potential landscape and locating local minima and saddle points.

MM 35.4 Fri 11:00 H22

Diffusion behavior of Li ions in crystalline and amorphous Li-Zr-O and Li-Nb-O phases — •Daniel Mutter[1], Diego A. Pantano[2], Christian Elsässer[1], and Daniel F. Urban[1] — [1]Fraunhofer IWM, Wöhlerstraße 11, 79108 Freiburg, Germany — [2]TotalEnergies OneTech, 2 place Jean Millier, 92400 Courbevoie, France

Li containing transition metal oxides are known as good ionic conductors. Performing classical molecular dynamics simulations with a Morse potential model based on the Bond Valence method, the diffusion behavior of Li ions is investigated in crystalline and amorphous phases with the stoichiometries Li_2ZrO_3 and $LiNbO_3$. The diffusivities are obtained from a statistical Arrhenius analysis of mean square displacement curves at different temperatures. The crystalline phase of Li_2ZrO_3 exhibits two well-defined migration mechanisms: vacancy-mediated migration is dominant below and a collective site exchange of Li ions above a crossover region between about 1700 and 1800 K. The latter mechanism, which is related to the formation of Frenkel pair defects and subsequent rotation of Li-Li pairs, also prevails in the amorphous phases with a strongly reduced activation energy. This is explained by a smaller equilibrium separation of Li ions in the amorphous phase than in the crystal structure. The demonstrated methodology and the discussed results shed light on a hitherto rarely described diffusion mechanism in ionic metal-oxide materials relevant for ion-battery applications.

MM 35.5 Fri 11:15 H22

Ag bulk and grain boundary diffusion in AlCoCrFeNi2.1 compositionally complex alloy — •Heng Zhang, Mohan Muralikrishna Garlapati, Sergiy V Divinski, and Gerhard Wilde — Institute of Materials Physics, University of Munster, Wilhelm-Klemm-Str. 10

Bulk and grain boundary diffusion of Ag in a eutectic Al-Co-Cr-Fe-Ni multi-principal element system is measured using the radiotracer technique and applying the 110Ag radioisotope. An equilibrium microstructure was produced by rotary forging and annealing of cast and homogenized initial casting ingot material. Ag diffusion is measured in the temperature interval from 673K to 1373K accounting for volume (at high temperatures) and short-circuit (at moderate and low temperatures) diffusion contributions. In the present case, interphase boundaries can potentially contribute in addition to grain boundaries to the short-circuit diffusion. The grain- and interphase-boundary diffusion experiments were performed in the B-type kinetic regime based on Harrison's classification. The results are analyzed with respect to constituent phases (FCC and B2) and different interface types. The contribution of interphase boundary diffusion is analyzed in detail.

MM 35.6 Fri 11:30 H22

Mechano-chemical coupling induced by Co grain boundary diffusion in SIGMA5(310) Cu bicrystals — •Esakkiraja Neelamegan[1], Anoosheh Akbari[1], Hui Ding[2], Harald Rösner[1], Daniel Gaertner[1], Christian Liebscher[2,3], Gerhard Wilde[1], and Sergiy Divinski[1] — [1]Institute of Materials Physics, University of Münster, Münster-48149 Germany — [2]Max-Planck-Institut für Sustainable Materials, Düsseldorf, Germany — [3]Faculty of Physics and Astronomy, Ruhr University Bochum, Bochum, Germany

Grain boundary diffusion of 57Co in pure copper SIGMA-5(310)[001] bicrystals is investigated using the radiotracer technique. Experiments are conducted under both the type-B and type-C kinetics regimes, as classified by Harrison. By varying the amount of applied 57Co tracer solution, characteristic changes in the shape of the penetration profiles are observed and attributed to Co segregation induced changes of the grain boundary structure. The structural changes due to the Co addition are examined by scanning transmission electron microscopy. The elastic strains near the grain boundary are measured using nano-beam diffractions with a nanometer resolution. The Co-induced variations of the GB structure provide an intriguing picture, particularly when considering their influence on the diffusion behaviour in the presence of deliberately introduced solute atoms.