MM 28: Transport I - atomic transport

Time: Tuesday 10:15–11:45 Location: IFW D

MM 28.1 Tue 10:15 IFW D

Volume diffusion in high-entropy $Al_xCoCrFeNi$ alloys — •Josua Kottke[1], Simon Trubel[1], Matthias Wegner[1], Louis J. Santodonato[2], Sergiy V. Divinski[1], and Gerhard Wilde[1] — [1]Institute of Materials Physics, Unversity of Münster, Germany — [2]Department of Materials Science and Engineering, The University of Tennessee, Knoxville, USA

High-entropy alloys, i.e. multicomponent alloys with a large number of constituting elements in equiatomic or nearly equiatomic composition, attract an increased attention as potential structural materials due to their favorable mechanical and physical properties, especially at elevated temperatures. In the present study, the tracer diffusion of Cr, Co, Fe, and Ni is measured in the $Al_xCoCrFeNi$ alloys at 1000°C and 1100°C applying the ^{51}Cr, ^{57}Co, ^{59}Fe and ^{63}Ni radioisotopes, respectively. The addition of Al to the CoCrFeNi FCC alloy is known to induce the appearance of a two-phase, FCC+BCC, microstructure which is examined using EBSD and EDX analyses. A correlation between the phase decomposition tendency and the tracer diffusivities of constituent elements is discussed.

MM 28.2 Tue 10:30 IFW D

Novel method to predict effects of structural changes on energy barriers in NASICON materials — •Kaustubh Bhat, Stefan Blügel, and Hans Lustfeld — Peter Grünberg Institut (PGI-1) and Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich GmbH, D-52425 Jülich, Germany

Among ionic conductors, NASICON [1] materials are receiving renewed attention because of their compositional diversity, particularly for large-scale energy storage applications. We first use the Nudged Elastic Band (NEB) method for calculating the energy barrier for sodium ion transport in $Na_6Sc_4(PO_4)_6$. Small changes in structure cause changes in the energy barrier. We model this using the second-order force constant matrices at the ground state and at the saddle point, and have developed a method to calculate the new ground state, the new saddle point state and thus the new energy barrier without performing a new NEB calculation. We propose a method to find the new force constant matrices and their corresponding eigenvalues at the new extrema. We validate this method using several materials eg. $Na_6Sc_4(SiO_4)(PO_4)_5$ [2].

[1] H.Y.P. Hong, Mat. Res. Bull. **11**, 173-182 (1976).
[2] M. Guin and F. Tietz, J. Power Sources **273**, 1056 (2015).

MM 28.3 Tue 10:45 IFW D

Chemical and tracer diffusion in the Fe-Ga binary couple — •Bengü Tas-Kavakbasi[1], Aloke Paul[2], Igor Stanislavovich Golovin[3], Gerhard Wilde[1], and Sergiy V. Divinski[1] — [1]Institute of Materials Physics, University of Münster, Germany — [2]Department of Materials Engineering, Indian Institute of Science, Bangalore, India — [3]National University of Science and Technology "MISiS", Moscow, Russia

In the present study, Manning's "sandwich interdiffusion" approach is applied to the Fe-Ga binary system and the interdiffusion measurements are directly combined with a tracer diffusion experiment. The ^{55}Fe radioisotope is deposited on the outer surfaces of a Fe-8Ga/Fe-24Ga interdiffusion couple (the concentrations are given in at.%) and on the initial interface between the two alloys. The couple was subsequently annealed at 900°C. The interdiffusion coefficient at 900°C is determined using electron probe profiling and the standard Sauer-Freise analysis. A strong composition dependence of the interdiffusion coefficient was found and its dependence on the molar volume is evaluated. The composition dependence of the ^{55}Fe tracer diffusion coefficient in the Fe-8Ga/Fe-24Ga interdiffusion couple has been determined, too.

MM 28.4 Tue 11:00 IFW D

Diffusion and ionic conductivity from ab initio non-equilibrium molecular dynamics — •Sergei Simak — IFM, Linköping University, SE-58183 Linköping, Sweden

Even fast diffusion and ionic conductivity in solids are too slow for studies from accurate ab initio equilibrium molecular dynamics (MD). The use of the nonequilibrium color-diffusion algorithm allows one to substantially speed up the simulations. Our recent implementation of the algorithm has been applied to the problem of oxygen diffusion and ionic conductivity in doped ceria, a promising electrolyte material for intermediate temperature solid oxide fuel cells (IT-SOFCs). The application of the methodology speeds up the simulated oxygen transport by a factor 60 compared with standard equilibrium MD. The calculated conductivity values agree with the available experimental data, and the experimental temperature trend is well reproduced [1-2]. The developed methodology might be useful for a large number of problems related to diffusion.

REFERENCES.

1. J. Klarbring, O. Yu. Vekilova, J. O. Nilsson, N. V. Skorodumova, and S. I. Simak, "Ionic conductivity in Sm-doped ceria from first-principles non-equilibrium molecular dynamics", Solid State Ionics, 296, 54 (2016).

2. J. O. Nilsson, O. Yu. Vekilova, O. Hellman, J. Klarbring, S. I. Simak, and N. V. Skorodumova , "Ionic conductivity in Gd-doped CeO2: Ab initio color-diffusion nonequilibrium molecular dynamics study", Phys. Rev. B 93, 024102 (2016).

MM 28.5 Tue 11:15 IFW D

Grain boundary diffusion and segregation of ^{57}Co in high-purity copper: Radiotracer measurements in B- and C-type diffusion regimes — •Daniel Gaertner, Gerhard Wilde, and Sergiy Divinski — Institute of Materials Physics, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster

Grain boundary diffusion of ^{57}Co in high-purity polycrystalline copper is investigated using the radiotracer technique in Harrison's B- ($850 - 1150$ K) and C-type ($550 - 950$ K) kinetic regimes. The triple product $P = s \cdot \delta \cdot D_{gb}$ (s is the segregation factor and δ the grain boundary width) and the grain boundary diffusion coefficient D_{gb} of Co in Cu are determined to obey the Arrhenius laws with the activation enthalpies of $Q_{gb} = 66.2$ kJ/mol and $H_{gb} = 100.9$ kJ/mol, respectively. Using the experimental estimate of δ, $\delta \cong 0.5$ nm, Co is found to segregate strongly at Cu grain boundaries and the corresponding segregation factor follows an Arrhenius dependence with the segregation enthalpy of $H_s = -34.7$ kJ/mol . Co-diffusion experiments with the ^{57}Co and ^{110m}Ag isotopes support a 'sub-interface'-type of grain boundary segregation of Co in Cu.

MM 28.6 Tue 11:30 IFW D

Modeling hydrogen diffusion in amorphous and polycrystalline thin films of tungsten trioxide — •Simon Burkhardt[1], Matthias Thomas Elm[1,2], and Peter Jens Klar[1] — [1]Heinrich-Buff-Ring 16, 35392 Giessen — [2]Heinrich-Buff-Ring 17, 35392 Giessen

The mandatory development of efficient energy management also will advance the commercialization and industrialization of electrochromic fenestration. Most of these devices are based on the electrochromic behavior of thin films such as tungsten trioxide (WO_3) induced by reversible insertion and extraction of ions and electrons into the films. A consistent fundamental understanding of the coloration processes is still lacking up to now but is needed to systematically enhance device performance and to increase their cyclability. To elucidate the transport behavior of protons and electrons in WO_3 thin films, we performed spatially and temporally resolved in situ transmission measurements on lithographically structured samples during electrochemical hydrogen insertion into amorphous and polycrystalline thin films. The experimental results show a significant influence of film morphology on lateral hydrogen diffusion and are compared with different simulations of theoretical models. These models are based on one dimensional diffusion problems in different continuous media and describe the experimental data qualitatively very well.