MM 68: Transport (Diffusion, conductivity, heat)

Transport II

Time: Thursday 17:30–18:30 Location: TC 010

MM 68.1 Thu 17:30 TC 010

Radiotracer self-diffusion experiments in CoCrFeNi and CoCrFeMnNi high entropy alloy single crystals — •Daniel Gaertner[1], Jonas Lübke[1], Josua Kottke[1], Yury Chumlyakov[2], Gerhard Wilde[1], and Sergiy Divinski[1] — [1]Institute of Materials Physics, University of Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany — [2]Department of Physics of Metals, Tomsk State University, 36 Lenin Ave., Tomsk 634050, Russia

High entropy alloys are multicomponent alloys, which have a large number of constituting elements in equiatomic or nearly equiatomic concentrations. These materials are hypothesized to show significantly decreased self diffusivities. For the first time, diffusion of all constituent elements in equiatomic CoCrFeNi and CoCrFeMnNi single crystals is investigated using the radiotracer technique, thereby the tracer diffusion coefficients of Cr-51, Co-57, Fe-59, Mn-54 and Ni-63 are determined at a temperature of 1100 °C. Two contributions to the long-range atom transport are observed and their nature is elucidated by varying the diffusion times. In addition to the bulk diffusion transport, short-circuit diffusion seems to be prominent due to a high density of grown-in dislocations. The components are characterized by significantly different diffusion rates, with Mn being the fastest element and Ni and Co being the slowest ones.

MM 68.2 Thu 17:45 TC 010

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

High-entropy alloys (HEAs), 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. Hereby, we contribute to a debate about hypothetical sluggish diffusion phenomena in HEAs by investigating self-diffusion in $Al_xCoCrFeNi$ ($x = 0.5$, 1 and 2) alloys.

Tracer diffusion in the $Al_xCoCrFeNi$ alloys is measured between 800 °C and 1100 °C by applying the ^{51}Cr, ^{57}Co and ^{59}Fe radioisotopes. As the Al content x in the $Al_xCoCrFeNi$ alloys is increased, a two-phase FCC+BCC microstructure replaces the single phase FCC one at $x < 0.3$ and the material becomes single phased BCC at $x = 2$. A careful microstructure examination using XRD, SEM and EBSD analysis allowed quantifying the measured diffusion profiles in terms of two separate contributions to long-range diffusion in FCC and BCC phases. The results indicate that the number of alloying elements in HEAs affects diffusion in FCC or BCC HEAs differently.

MM 68.3 Thu 18:00 TC 010

Effect of stoichiometry on self-diffusion in triple-defect binary intermetallics: Semi Grand Canonical and Kinetic Monte Carlo simulations. — •Rafal Kozubski[1], Jan Betlej[1], Piotr Sowa[1], Graeme Murch[2], and Irina Belova[2] — [1]M. Smoluchowski Institute of Physics, Jagiellonian University in Krakow, Lojasiewicza 11, 30-348 Krakow, Poland — [2]Centre for Mass and Thermal Transport in Engineering Materials, School of Engineering, The University of Newcastle, Callaghan, Australia

Vacancy-mediated self-diffusion and chemical short- and long-range ordering in triple-defect binary intermetallics was modelled with Ising nn and nnn pair interactions and simulated in atomistic scale. The Kinetic Monte Carlo (KMC) algorithm was implemented with local-configuration-dependent migration barriers and temperature-dependent equilibrium vacancy concentration determined by means of Semi Grand Canonical Monte Carlo (SGCMC) simulations. The resulting concentration dependence of the component tracer diffusivities in a triple-defect B2-ordering A-B system mimicking Ni-Al was in a very good agreement with the experimental results obtained for that system. In particular, inversion of the relationship between the Ni and Al-diffusivities in Al-rich Ni-Al systems deduced from the features of interdiffusion in Ni-Al was perfectly reproduced by direct self-diffusion simulations. The origin of the phenomenon is elucidated in terms of an increase of the nnn Al jump frequency resulting from specific atomic and vacancy configurations originating from the triple-defect character of disordering.

MM 68.4 Thu 18:15 TC 010

electronic transport coefficients from first principles — •zhenkun yuan, christian carbogno, and matthias scheffler — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6,14195 Berlin

The Kubo-Greenwood formalism has been employed successfully for the first-principles calculation of electrical conductivities at elevated temperature and/or for disordered systems [1]. It relies on *ab initio* molecular dynamics simulations to include electron-phonon scattering, which is the most important scattering mechanism for electronic transport in bulk materials. However, this approach suffers from severe finite-size effects for crystalline solids close to room temperature, since accounting for the dominant scattering with long-wavelength phonons would require extremely large supercells. In this work, we propose possible strategies to overcome this limitation. In particular, we assess to which extent the asymptotically exact extrapolation scheme [2] that we recently developed to correct for finite-size effects in the calculation of vibrational thermal conductivities can be extended to electronic transport. To this end, *ab initio* calculations are performed both for direct (GaAs) and indirect (Si) semiconductors and the obtained results are compared to the existing experimental and theoretical data [3].

[1] M. French and T. R. Mattsson, *Phys. Rev. B* **90**, 165113 (2014).
[2] C. Carbogno, R. Ramprasad, and M. Scheffler, *Phys. Rev. Lett.* **118**, 175901 (2017).
[3] J. Zhou, B. Liao, and G. Chen, *Semicond. Sci. Technol.* **31**, 043001 (2016).