MM 18: Transport in Materials: Metals, Alloys and Oxides

Time: Tuesday 11:30–13:00 Location: SCH A 118

MM 18.1 Tue 11:30 SCH A 118

Understanding diffusion in high entropy alloys from an experiment-ab initio approach — •Xi Zhang[1], Sergiy Divinski[2], and Blazej Grabowski[1] — [1]Institute for Materials Science, University of Stuttgart, D-70569 Stuttgart, Germany — [2]Institute of Materials Physics, University of Münster, 48149 Münster, Germany

Diffusion in high entropy alloys (HEAs), due to the significant chemical complexity and the severe lattice distortion, has many fundamental features that are extremely important for both basic research and industrial development. The most accurate and direct method to study diffusion is the radiotracer technique whereby a number of intriguing phenomena, e.g., ultra-fast, non-/anti-sluggish diffusion, have been observed. To advance the current understanding of the observed phenomena, accurate theoretical analysis is highly required. The key point of the present approach is the combined measurement of diffusivities and interdiffusion profiles on the one hand and a highly accurate DFT-informed assessment of the diffusion mechanisms on the other. In this way, the long-standing mysteries in HEA diffusion, e.g., "sluggish" diffusion, can be comprehensively examined and understood. Remarkably, we show by investigating an HCP AlScHfTiZr HEA system that the increasing chemical complexity results in a considerably broadened distribution of the defect formation and migration energies which may enhance the mobility of the defects and thus the diffusion rates. The observed "anti-sluggish" diffusion can be traced back to the lattice distortion as revealed by the DFT calculations.

MM 18.2 Tue 11:45 SCH A 118

Composition dependent thermodynamic factor, Manning factor, and impurity diffusion coefficients estimated by a tracer-interdiffusion couple technique — •Esakkiraja Neelamegan[1], Daniel Gaertner[1], Jasper Berndt[2], Stephan Klemme[2], Aloke Paul[3], Gerhard Wilde[1], and Sergiy V Divinski[1] — [1]Institute of Materials Physics, University of Münster, Münster, Germany — [2]Institut für Mineralogie, University of Münster, Münster, Germany — [3]Department of Materials Engineering, Indian Institute of Science, Bangalore, India

The thermodynamic driving force for the diffusion was never validated experimentally. The newly proposed augmented tracer-interdiffusion couple method could be adapted to validate the thermodynamic factor. The approach is demonstrated for a model Ni-Fe binary system, especially for the Ni-rich corner. Pure Ni is diffusion-coupled with a Ni-10 at. % Fe diluted alloy at 1000 C for 24h. The interdiffusion coefficients are estimated from the composition profile measured by an Electron Microprobe Analyser. The composition-dependent tracer diffusion coefficients are estimated following the Belova-Murch approach. Diffusion of the Fe55 and Ni63 isotopes under a chemical gradient is followed. The Fe tracer diffusion coefficients are found to be faster than those of Ni in this composition region. Utilizing the Darken-Manning relation, the thermodynamic factor is estimated and compared with that provided by a ThermoCalc software database. As a result, the composition-dependent impurity diffusion coefficients of Co, Cr, and Mn in these alloys are analysed in detail.

MM 18.3 Tue 12:00 SCH A 118

Control of microstructure in binary alloy thin films by means of electromigration — •Thomas Brede, Reiner Kirchheim, and Cynthia A. Volkert — Universtität Göttingen, Insitut für Materialphysik, Göttingen, Deutschland

Magnetic and electric fields and currents open new and efficient materials processing paths for microstructure optimization than were previously available. For example, it has recently been shown that high DC electric currents can be used to create anisotropic microstructures with elongated ferrite grains in iron-carbon thin films [1]. The elongated grains form in the wake of carbides that migrate due to electromigration induced carbon flux divergences. The underlying mechanisms controlling the microstructural evolution will be presented and will be used to discuss other materials systems that might show this effect and how they could be implemented to achieve precise microstructure control.

[1] Brede, T., Kirchheim, R., & Volkert, C. A. (2020). Anisotropic grain growth in iron-carbon films at high electric current densities. Scripta Materialia, 178, 18-23.

MM 18.4 Tue 12:15 SCH A 118

GP-zone formation and growth in rapidly quenched Al-Cu alloys — •David Stein, Johannes Berlin, Tobias Stegmüller, and Ferdinand Haider — Universität Augsburg, Institut für Physik, 86159 Augsburg, Germany

Natural aging by the formation of Guinier Preston zones in Al-Cu alloys is only possible in the presence of excess vacancies, quenched in from high temperatures. In collision welded samples of Al and Cu, an unexpected high density of GPII-zones was observed in the TEM. In order to obtain similarly high quenching rates of about 104 K/s, meltspinning was used for alloys with a Cu content from 2-5 wt%. After the quenching process, the samples were analyzed after different natural aging times using Differential Scanning Calometry (DSC) , hardness measurements, resistometry and STEM to obtain information about the unmixing kinetics. Additionally EDX and EBSD were used to characterize the microstructure and chemical homogeneity of the samples.

MM 18.5 Tue 12:30 SCH A 118

Theoretical studies on the oxygen migration through crystalline strontium titanate — •Carmen Fuchs[1] and Timo Jacob[1,2,3] — [1]Ulm University, Institute of Electrochemistry, D-89069 Ulm — [2]Helmholtz-Institute-Ulm (HIU), D-89081 Ulm — [3]Karlsruhe Institute of Technology (KIT), D-76131 Karlsruhe

Transition metal oxides with perovskite structure (ABO3) display a range of complex physical phenomena of condensed matter physics, including superconductivity, ferroelectricity, and magnetism. Strontium titanate, SrTiO3 (STO), is the archetypical and most frequently studied representative of perovskite materials. By changing the stoichiometry, major changes in several important properties can be induced including blue light emission,[1] local conductivity,[2] and electron doping.[3] The relationship between the structure and the diffusion behavior of defects in SrTiO3 is studied via DFT calculations using the plane-augmented wave method and the PBE exchange-correlation functional with and without Hubbard U correction. The obtained defect formation energy and activation barriers for oxygen migration through Frenkel- and Schottky-like defects within the crystalline STO structure are discussed and summarized. [1] D. Kan et al, Nat. Mater. 4 (2005), 816-819. [2] K. Szot, W. Speier, G. Bihlmayer, R. Waser, Nat. Mater. 5 (2006), 312-320. [3] A.F. Santander-Syro et al, Nature 469 (2011), 189-193.

MM 18.6 Tue 12:45 SCH A 118

Impact of alloying elements on point defects and diffusion in B2 alloys: an ab initio study — •Aditya Vishwakarma[1], Osamu Waseda[1], Tilmann Hickel[1], Neelamegan Esakkiraja[2], Sergiy Divinski[2], and Aloke Paul[3] — [1]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — [2]Institute of Materials Physics, University of Münster, Germany — [3]Department of Materials Engineering, IISc Bangalore, India

Turbine blades in jet engines are vulnerable to many problems due to the harsh application environments. To prevent oxidation and surface degradation, bond coats of B2 NiAl are most widely used. During the operation at high temperatures, however, the Al content in the bond coat is lost by the formation of an Inter Diffusion Zone (IDZ) between the superalloy (turbine blade) and the bond coat. In this report, ab-initio based studies of point defect formation and kinetics are performed, in order to investigate the diffusion mechanisms and the impact of alloying elements on diffusion in B2 NiAl phase. Our results show that isoelectronic substitutions by Pt and Pd decreases the triple defect migration barriers and increases the Ni vacancy concentration in comparison to pure B2 NiAl. Accordingly, the contribution of the triple defect mechanism increases down the periodic table. These results explain the experimentally observed increase of the thickness of IDZ compared to binary B2 NiAl and have, therewith, an impact on the future design of turbine blades.