

## MM 20: Topical Session: Interface-dominated phenomena - Diffusion

Time: Tuesday 10:15–11:30

Location: IFW A

**Topical Talk**

MM 20.1 Tue 10:15 IFW A

**The early stage of reactive interdiffusion in the Cu-Al system investigated by in-situ TEM** — ●XAVIER SAUVAGE<sup>1</sup>, FLORENT MOISY<sup>2</sup>, and ERIC HUG<sup>2</sup> — <sup>1</sup>Groupe de Physique des Matériaux, UMR CNRS 6634, University Rouen Normandy, France — <sup>2</sup>CRISMAT, University Caen Normandy, France

The early stage of the reactive interdiffusion in the Al/Cu system was investigated by in-situ TEM at 350°C and 300°C. Original Al/Cu interfaces were created by a purely mechanical process using co-deformation at room temperature by drawing. During the reactive interdiffusion three IMCs were detected: Al<sub>2</sub>Cu and AlCu grew in the Al side and the Al<sub>4</sub>Cu<sub>9</sub> in the Cu side. Systematic comparisons with ex-situ annealed samples and with regions out of the electron beam proved that there was no significant artefact (thin foil or beam effect). Although GBs may act as fast diffusion path, no preferential growth of IMC along these defects could be observed. The mean growth rates of all IMCs follow a classical parabolic law indicating that the kinetic of the transformation is controlled by diffusion mechanisms. A strong deviation was observed however in the early stage of the reaction. Nanoscaled Mg<sub>2</sub>Si particles located in the Al phase strongly interact with the transformation front. It leads to large fluctuations of the velocity of interphase boundaries at the nanoscale. The pinning effect in connection with change in local concentration gradients and driving forces will be discussed.

MM 20.2 Tue 10:45 IFW A

**Influence of atomic interaction on grain boundary self-diffusion in binary solid solutions** — ●VLADIMIR A. ESIN — Centre des Matériaux, MINES ParisTech, PSL University, France

Atomic interaction of solute atoms with solvent ones has been considered to be of the major responsibility for the effect of solute on grain boundary self-diffusion. It is supposed that during diffusion process the diffusing solvent atoms form atomic complex with solute atoms at grain boundary with the formation of chemical bonds [1,2]. A description of solvent GB diffusion is then given for both B- and C-regimes.

Using such an approach, a new equation for the dependence of solvent GB diffusion coefficient on solute bulk concentration is derived for the systems with simple atomic attraction in GB. Theoretical results predict non-linear dependence of solvent GB diffusion coefficient on solute bulk content, which is in agreement with earlier published experimental data regarding the ease of grain boundary diffusion in alloys of different chemical compositions. More importantly, the equation deduced permits to evaluate, on one hand, the characteristics of solute GB segregation from solvent GB diffusion measurements and, on the other hand, GB diffusion coefficient in pure solvent. Such a numerical data analysis for Fe-Sn system is in agreement with experimental results.

[1] V. Esin, B. Bokstein and A. Rodin, Defect Diffus. Forum 309-310 (2011) p. 29.

[2] V.A. Esin and B.S. Bokstein, Acta Mater. 60 (2012) p. 5109.

MM 20.3 Tue 11:00 IFW A

**Development of a copper–nickel embedded-atom potential for a systematic study of grain boundary segregation and grain boundary formation energy** — FELIX FISCHER and ●SEBASTIAN EICH — Institut für Materialwissenschaft, Universität Stuttgart

In this atomistic study [1] on the copper–nickel system, a new embedded-atom potential between copper and nickel is fitted to experimental data on the mixing enthalpy. The resulting phase boundaries of the new potential are in very good agreement with a recent CALPHAD prediction. Using this new potential, a high angle symmetrical tilt  $\Sigma 5$  grain boundary (GB) is chosen for a systematic investigation of equilibrium GB segregation in the semi-grandcanonical ensemble at temperatures from 400 K to 800 K. Applying thermodynamically accurate integration techniques, the GB formation energy is calculated exactly and as an absolute value for every temperature and composition.

Eventually, the thermodynamically unambiguous GB solute excess  $\Gamma$ , obtained from the simulations, is fitted to a recently proposed analytical model for interface segregation [2]. Based on a composition-dependent model curve of the energy of segregation, the solute excess  $\Gamma$  can be described excellently over the entire composition range for all investigated temperatures.

[1] F. Fischer, G. Schmitz, and S. M. Eich, Acta Mater. 176, 220 (2019)

[2] T. Krauß, S. M. Eich, Acta Mater. (submitted)

MM 20.4 Tue 11:15 IFW A

**Mechano-chemical coupling by microstructure evolution of an Al-Sc-Zr-based alloy** — ●BENGÜ TAS, FRIEDERIKE EMEIS, VLADISLAV KULITCKI, MARTIN PETERLECHNER, GERHARD WILDE, and SERGIY V. DIVINSKI — Institute of Materials Physics, University of Münster, Münster, Germany

Al-based alloys are attractive materials for aerospace applications owing to their low density, sufficient weldability and superior strength at room temperature. Severe plastic deformation via equal channel angular pressing at 300°C for 12 passes is applied on a technical AA5024 Al-based alloy in order to produce an ultrafine grained microstructure (UFG) with different types of micro- and nano-precipitates, basically Al<sub>6</sub>Mn and Al<sub>3</sub>(Sc,Zr,Ti). Heat treatments under different external stress fields are subsequently applied using a universal testing machine. The impact of the stress state (pure shear, uniaxial compression or stress-free annealing) on the microstructure evolution including relaxation of residual strains and precipitation is investigated. The mechano-chemical coupling on different scales is examined with a focus on the evolution of core-shell Al<sub>3</sub>(Sc,Zr,Ti) particles. Pure shear results in relatively large grains with a bimodal size distribution, in contrast to smaller, homogeneously distributed grains under uniaxial compression. The impact of the stress state on nano-precipitate evolution is elucidated using analytical and high-resolution transmission electron microscopy.