MM 14: Transport I: Diffusion

Time: Monday 15:45–17:45 Location: H 0107

MM 14.1 Mon 15:45 H 0107

Diffusion of solutes in Ni-based superalloys: role of vacancies and the treatment of the non-dilute limit — •Sergej Schuwalow, Jutta Rogal, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, 44801 Bochum, Germany

High-temperature properties of Ni-base superalloys are known to be highly dependent on the alloying additives, in particular on the presence of Re. Current knowledge of the mechanisms behind this effect is mostly phenomenological in nature and the details of solute diffusion, interaction with various defects (e.g. interfaces, vacancies, and dislocations) as well as the interplay between composition and microstructure are not well understood.

We have analyzed concentration/temperature-dependent diffusion behavior of selected alloying elements in the dilute limit using a combination of density-functional theory calculations and kinetic Monte Carlo simulations [1]. We found that the diffusion of vacancies, which was speculated to be at the core of the Re effect in literature, is only weakly influenced by the presence of the solute elements at concentrations below 3wt%.

At higher solute concentrations solute-solute interactions need to be taken into account. Here we present developments on a cluster expansion approach for non-dilute systems which allows an ab-initio treatment of diffusion in presence of configurational disorder. We further discuss avenues for the treatment of multicomponent systems.

[1] S. Schuwalow, J. Rogal, R. Drautz, J. Phys.: Condens. Matter 26 (2014) 485014.

MM 14.2 Mon 16:00 H 0107

Phase composition, microstructure and Ni tracer diffusion in FCC FeCrCoNi-based high entropy alloys — •Mayur Vaidya[1,2], Simon Trubel[2], Igor Golovin[3], Buduraju Srinivasa Murty[1], Sergiy Divinski[2,3], and Gerhard Wilde[2] — [1]Department of Metallurgical and Materials Engineering, Indian Institute of Technology Madras, Chennai, India — [2]Institute of Material Physics, University of Muenster, Muenster, Germany — [3]National University of Science and Technology MISiS, Moscow, Russia

High entropy alloys (HEAs) CoCrFeNi, CoCrFeMnNi and CoCrFeMnNiV were prepared by arc melting the constituent elements, followed by homogenization at 1200°C for 50 h. XRD results show that CoCrFeNi and CoCrFeMnNi represent single phase FCC phases, while CoCrFeMnNiV comprises of FCC and tetragonal phases. EBSD analysis confirms a single phase structure, uniform composition and a grain size in excess of 250μm in CoCrFeNi and CoCrFeMnNi alloys. Elemental X-ray maps of CoCrFeMnNiV substantiate its decomposition into a Ni- and Mn-rich phase (located predominantly at grain boundaries) and a V- and Cr-rich phase. Such FCC-HEAs have been explored for high temperature applications, for which creep behavior and in turn the diffusion kinetics of these alloys must be understood. We are studying Ni tracer diffusion in these HEAs using ^{63}Ni radioisotope. Ni diffusion kinetics, amplitude- and temperature dependent mechanical damping in HEAs are reported. Partial support by the Ministry of Education and Science of Russia in the framework of Increase Competitiveness Program of NUST MISiS(K3-2014-045) is acknowledged.

MM 14.3 Mon 16:15 H 0107

Investigating the effect of severe plastic deformation on nickel using radiotracer diffusion and microstructural analysis — •Simon Trubel[1], Sergiy Divinski[1], Martin Peterlechner[1], Gerrit Reglitz[1], Matthias Wegner[1], Christian Simon[1], Ehud Almog[2], and Gerhard Wilde[1] — [1]Institut für Materialphysik der WWU, Münster, Deutschland — [2]Technion, Haifa, Israel

Ultrafine grained and nanocrystalline materials produced by methods of severe plastic deformation (SPD) have roused a growing interest in science and technology. Previous experiments on Nickel of 99.6% purity revealed ultra-fast diffusion rates in ultrafine grained material severely deformed via equal channel angular pressing (ECAP) [1] and high pressure torsion (HPT). This study reports the effect of pre-annealing of ECAP-processed Ni on the grain boundary characteristics and the thermal stability of microstructure. Grain boundary self-diffusion has been analysed using the 63Ni radioisotope in combination with high-precision parallel grinding. The results of the diffusion measurements and of measurements by electron backscattered diffraction (EBSD) and transmission electron microscopy (TEM) are discussed with respect to modifications of grain boundary structures under different routes of SPD processing. Additionally, cold rolled Nickel is investigated as another variant of severely deformed material that has been processed along a different deformation pathway in order to gain insight into the formation conditions of the grain boundaries that act as ultra-fast diffusion paths after SPD treatment. [1] S. V. Divinski, G. Reglitz, H. Rösner, Y. Estrin, G. Wilde. Acta Materialia, 59, 1974 (2011).

MM 14.4 Mon 16:30 H 0107

Kinetics and structural effects induced by liquid Ga penetration into ultra-fine grained Al — •Mehrnoosh Naderi, Martin Peterlechner, Sergiy Divinski, and Gerhard Wilde — Institute of Materials Physics, University of Münster, Germany

One of the spectacular examples of liquid metal embrittlement is the fast penetration of liquid gallium into aluminum and its alloys which occurs even at room temperature, i.e. below the melting point of Ga. Since severe plastic deformation is commonly used for grain refinement and produces a high density of grain boundaries of different types, in this study we focus on the penetration of Ga along grain boundaries of ultra-fine grained Al produced by high pressure torsion (HPT). The volumetric changes and the kinetics of liquid Ga penetration into the Al grain boundary network are investigated. A two-stage process of the excess volume evolution in HPT-processed Al is observed after Ga application. The structural effects are examined by transmission electron microscopy and texture measurements, too. The surface evolution is followed by atomic force microscopy. The results are discussed concerning the underlying mechanisms that control the Ga penetration.

15 min. break

MM 14.5 Mon 17:00 H 0107

Microstructure and Stress Relaxation in Thin Nano Crystalline Platinum Films — •Wolfgang Gruber[1], Florian Strauss[1], Lars Dörrer[1], Michael Horisberger[2], Thomas Geue[2], Jochen Stahn[2], Carsten Bähtz[3], and Harald Schmidt[1] — [1]TU Clausthal, Institut für Metallurgie — [2]Paul Scherrer Institut, Laboratory for Neutron Scattering — [3]Helmholtz-Zentrum Dresden-Rossendorf, Institut für Ionenstrahlphysik und Materialforschung

Various techniques can be used to deposit thin metal films with a thickness in the nanometer range on a substrate. Independent of the method of production residual stress is present in the metal films after deposition. Based on the concept of dilatometry X-ray diffraction and X-ray reflectometry was used to investigate the correlation of strain relaxation and the change of point defect concentration in thin Pt films [1]. In the present work in-situ measurements using synchrotron radiation were performed in the temperature range between 100 °C and 300 °C to investigate strain relaxation in thin Pt films deposited on oxidised silicon substrates via magnetron sputtering and ion beam sputtering, respectively. Self-diffusion of Pt was investigated for samples produced by ion beam sputtering using secondary ion mass spectrometry and neutron reflectometry. The two systems are compared taking the microstructure as revealed by X-ray analysis into account.

W. Gruber, S. Chakravarty, C. Baehtz, W. Leitenberger, M. Bruns, A. Kobler, C. Kübel, H. Schmidt, Phys. Rev. Lett. 117 (2011) 265501.

MM 14.6 Mon 17:15 H 0107

Multiscale modeling approach to occupationally disordered materials: Ion diffusion in Lithium-Titanium-Oxide battery materials — •Hendrik H. Heenen, Saskia Stegmaier, Christoph Scheurer, and Karsten Reuter — Technische Universität München

Lithium-titanium-oxide (LTO) materials have caught a lot of attention as an alternative anode material for lithium ion batteries as they offer high cycling stability, safe operation at high working potentials and a fast charge-discharge behavior. Aiming to link this macroscopic electrochemical performance to the underlying atomic-scale processes, first-principles studies generally offer a unique opportunity to understand the Li ion diffusion and material's structure. In particular for the spinel-type $Li_4Ti_5O_{12}$ LTO they are, however, challenged by the mixed occupancy of octahedral sites by Li and Ti ions [1]. This allows for a high degree of occupational disorder that can not be appropriately

sampled within supercell sizes accessible to present-day first-principles calculations. We address this challenge with a multiscale approach involving interatomic potentials that are parametrized and validated by density-functional theory. This allows to thoroughly sample the configuration space of $Li_4Ti_5O_{12}$ and perform an analysis of the variety of diffusion pathways. Particular focus is placed on the dependency of the average and local Li ion mobility on the thermodynamically accessible configuration space.

[1] B. Ziebarth *et al*, Phys. Rev. B **89**, 174301 (2014).

MM 14.7 Mon 17:30 H 0107

Self-Diffusion in Amorphous Silicon Investigated by Neutron Reflectometry — •Florian Strauss[1], Harald Schmidt[1], Jochen Stahn[2], and Thomas Geue[2] — [1]TU Clausthal, AG Mikrokinetik, Institut für Metallurgie, Deutschland — [2]Paul Scherrer Institut, Villigen, Schweiz

The characteristics of silicon self-diffusion in the amorphous state are still unknown, albeit the material is widely used in solar cells, flat screen displays and is looked at as a promising electrode material in Li-ion batteries. In this model system of a covalent amorphous semiconductor low diffusivities and intrinsic metastability necessitate the use of Neutron Reflectometry (NR) a method capable of determining diffusion lengths of 1 nm and below [1,2]. $^{29}Si/^{28}Si$ isotope multilayer structures are prepared by ion beam sputtering and thermally treated in an Ar atmosphere at temperatures up to 700 °C in order to induce isotope-interdiffusion. The chemical homogeneity and amorphous structure are confirmed by cross-sectional TEM measurements and XRD data. At temperatures between 350 and 500 °C a time dependent short range diffusion process on the length scale of 1 nm is observed and interpreted as a consequence of structural relaxation. At temperatures above 500 °C diffusion over a range of several nanometres is found. Additional measurements by Secondary Ion Mass Spectrometry confirm the data obtained by NR.

[1] H. Schmidt et al., Acta Mater. 56 (2008), 464
[2] E. Hüger et al., Appl. Phys. Lett. 93 (2008), 162104