

MM 33: Transport in Materials: Diffusion, Conduction of Charge or Heat III

Time: Wednesday 10:15–11:30

Location: C 264

MM 33.1 Wed 10:15 C 264

Correlation of structural changes and hydrogen diffusion in polycrystalline WO_3 thin-films by combining in situ transmission measurements and Raman spectroscopy — ●TIM K. HECKER, MARKUS S. FRIEDRICH, ALEXANDER G. STRACK, PAUL TUCHECKER, and PETER J. KLAR — Institute of Experimental Physics I and Center for Materials Research, Justus Liebig University Giessen, Giessen, Germany

To better understand hydrogen diffusion in tungsten trioxide thin films, such samples were microstructured with a PMMA film in such a way that the contact surface with the electrolyte is limited to a narrow stripe-like gap. This allows us to study the lateral diffusion of hydrogen under the PMMA film, increasing the analysable path and time scale by several orders of magnitude and thus significantly improving the spatial and temporal resolution of in-situ transmission and Raman measurements. Spatially resolved transmission measurements in the wavelength range of 633 ± 55 nm show that the investigated diffusion is dependent on the hydrogen concentration. Time-resolved Raman measurements with a 633 nm laser at different distances from the electrolyte contact area show that the transition between the two diffusion coefficients is characterised by a phase transition of the crystal structure to higher symmetry. The results are also supported by a spatially and temporally resolved diffusion simulation. In addition, the measurement method presented here is universally applicable.

MM 33.2 Wed 10:30 C 264

Intermixing of nanoparticle metal alloy — ●YONG LI¹ and JÖRG WEISSMÜLLER^{2,1} — ¹Institute of Hydrogen Technology, Helmholtz-Zentrum Geesthacht, Geesthacht, Germany — ²Institute of Materials Physics and Technology, Hamburg University of Technology, Hamburg, Germany

Metal or its alloy nanoparticles are widely used in catalysis. In this study, the surface diffusion-dominated Brownian motion of nanoparticles at different temperatures is simulated using Kinetic Monte Carlo (KMC). The initial structure of nanoparticles are ordered FCC binary alloy with radii ranging from 2 to 8 nm. It is found that the displacement of the particle centre of mass, R_{cms} , scales with time, t , as $R_{\text{cms}} \propto \sqrt{Dt}$. The diffusion constant, D , has a power law relationship with the particle radius, r , $D \propto r^{-4}$. The Cowley short-range ordering parameter, α_1 , is detected for the first nearest-neighbor shell. The time of α_1 evolves to half of its initial value, $t_{\frac{1}{2}\alpha_1}$, shows a power-law dependence to r with a scaling exponent of 6.

MM 33.3 Wed 10:45 C 264

Interdiffusion in Cu-Ni couples with end-members severely plastically deformed via high-pressure torsion — ●ESAKKIRAJA NEELAMEGAN¹, JASPER BERNDT², STEPHAN KLEMME², GERHARD WILDE¹, ALOKE PAUL³, and SERGIY. V DIVINSKI¹ — ¹Institute of Materials Physics, University of Münster, Münster-48149 Germany — ²Institute for Mineralogy, University of Münster, Münster-48149 Germany — ³Department of Materials Engineering, Indian Institute of Science, Bangalore-560012 India

For coarse-grained polycrystalline alloys, interdiffusion of the Cu-Ni system is investigated, and the composition-dependent interdiffusion coefficients are known to decrease with an increase in the Ni concentration. The present study explores the influence of the end members' microstructure state on the interdiffusion behaviour. Severe plastic deformation via high-pressure torsion is used. We estimate the composition-dependent tracer diffusion coefficients using the augmented tracer-

interdiffusion couple approach. The interdiffusion behaviour of undeformed (coarse-grained) and deformed (ultra-fine-grained) materials are compared. An anomalous diffusion behaviour with respect to the annealing temperature is observed. The comprehensive tracer and interdiffusion data shed light on the impact of plastic deformation on the interdiffusion behaviour.

MM 33.4 Wed 11:00 C 264

Impurity diffusion measurement in liquid Al based alloys using X-ray Radiography — ●MASATO SHINOKI¹, ELKE SONDERMANN¹, and ANDREAS MEYER^{1,2} — ¹Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Köln, Germany — ²Institute Max von Laue - Paul Langevin (ILL), 38042 Grenoble, France

The high accuracy measurements of the impurity diffusion coefficient in liquid metals are indispensable for modeling diffusion theories. The aim of this study is to investigate how the difference in impurity diffusion coefficient in liquid Al is expressed by the hard-sphere model. The impurity diffusion coefficients in liquid Al were measured using the in-situ shear cell method with X-ray radiography technique at 973, 1020, and 1060 K. The concentrations of the two parts of the diffusion couple were chosen to be pure Al and 5 at% Cu, 1 at% Sn, 1 at% Au, 1 at% Ag, and 0.8 at% Bi in Al. The diffusion process was started at connecting each interdiffusion couple after shearing the furnace and concentration profiles were obtained every second. The impurity diffusion coefficients were calculated from the linear fittings to the mean square diffusion distance which is derived from the concentration profiles using Ficks law. The results showed that the excess entropy model using hard sphere reproduced the measured impurity diffusion coefficients in liquid Al better than the hard-sphere model derived from Enskog theory. This excess entropy model reproduces the impurity diffusion coefficients better for other temperatures as well by considering the temperature dependence of the packing density.

MM 33.5 Wed 11:15 C 264

Simulation of Dendrite Growth at the Electrode Interface in Lithium Metal Batteries — ●LEN KIMMS¹, DIDDO DIDDENS^{1,2}, and ANDREAS HEUER¹ — ¹Institut für physikalische Chemie, Universität Münster, Corrensstraße 28/30, 48149 Münster — ²Helmholtz Institute Münster (IEK-12), Ionics in Energy Storage, Forschungszentrum Jülich GmbH, Corrensstraße 46, 48149 Münster

In this talk, we will present a simulation study that investigates the formation and growth of dendrites. The limitations of current commercial battery technologies can be possibly solved by using metallic lithium as electrode material. Lithium metal batteries (LMB) employ lithium metal anchored on a current collector as negative electrode. When charging the battery, cations are reduced at the electrode interface. Controlling the deposition to favor uniform plating is inherently challenging. The high reactivity of lithium metal can form a solid electrolyte interphase (SEI) which together with electric-field effects and a locally varying composition of the electrolyte drive dendritic deposition. A generic coarse-grained model is employed to investigate fundamental driving forces on the dendrite morphology. Not only electric-field effects, transport in the electrolyte, and cation concentration can be evaluated but also the optimization of more intricate procedures is possible. The model allows the exploration of dendrite-suppression techniques like pulse charging, application of an artificial SEI layer, or host structures on the electrode. To understand the complex interplay between microscopic electrochemical conditions, the model may be augmented by insights from molecular dynamics simulations.