MM 5: Transport and Diffusion I

Time: Monday 10:15–11:30 Location: H 1029

MM 5.1 Mon 10:15 H 1029

Investigation of Fe diffusion in Cu by Energy Dispersive X-ray Analysis — •Daria Prokoshkina[1,2], Alexey Rodin[2], and Vladimir Esin[2,3] — [1]Institute for Materials Physics, University of Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Deutschland — [2]Department of Physical-Chemistry, National University of Science and Technology "MISiS", Moscow, Russia — [3]"Département Science et Ingénierie des Matériaux et Métallurgie", Institut Jean Lamour - UMR 7198 - CNRS - Nancy-Université - UPV-Metz, Nancy, France

Iron diffusion in copper is of particular interest since anomalies of iron grain boundary (GB) diffusion in copper have been observed recently. Bernardini et al. [1] investigated Fe GB diffusion in Cu at 716 K after annealing during 96 hours in the B-regime, whereas in the work of Ribbe et al. [2] diffusion annealing at 719 K during 20 hours corresponded to the C-regime. Moreover, a strong curvature of the concentration profiles in Fisher's coordinates was observed by both research groups. In the described works the radiotracer technique was applied. The reasons of the observed anomalies remain unknown. To clarify the problem, another method is used in this work: Energy Dispersive X-ray analysis. GB diffusion measurements are performed in the temperature range from 823 to 1073 K. The parameters of the bulk diffusion of Fe in Cu in the temperature range from 923 to 1273 K are also evaluated. The complex approach of investigating Fe GB diffusion in Cu did not permit to observe fast GB diffusion in the temperature range from 823 to 1073 K. [1] J. Bernardini et al. Def. and Diff. Forum. 249(2006)161. [2] Jens Ribbe et al. Def. and Diff. Forum. 289-292(2009)211.

MM 5.2 Mon 10:30 H 1029

Temperature induced transitions of the grain boundary structure studied by radiotracer diffusion — •Sergiy Divinski[1], Henning Edelhoff[1], Sergey Prokofjev[2], and Gerhard Wilde[1] — [1]Institute of Materials Physics, University of Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany — [2]Institute of Solid State Physics, Chernogolovka, Russia

Grain boundary diffusion of ^{110m}Ag in Cu near Σ5 bicrystals is measured parallel and perpendicular to the (001) misorientation axis in both, C and B kinetic regimes after common Harrison's classification. For the first time, the grain boundary diffusion coefficients of a single grain boundary in a true dilute limit of the solute concentration are determined in the C kinetic regime and the values of triple products $P = s \cdot \delta \cdot D_{\mathrm{gb}}$ are measured in the B regime (here s and δ are the segregation factor and the diffusional grain boundary width, respectively). A significant anisotropy of the grain boundary diffusion is established which disappears at the temperatures above 823 K. This temperature corresponds also to a kink in the Arrhenius temperature dependence of the triple product. The phenomenon is discussed in term of a special-to-general transition of the grain boundary structure. The anisotropy of the product $s \cdot \delta$ for a single grain boundary is determined. The effect of non-linear segregation on Ag diffusion in the Cu bicrystal is elucidated via controlled variation of the total amount of the applied tracer material.

The financial support by DFG is acknowledged.

MM 5.3 Mon 10:45 H 1029

Studies of atomic diffusion in crystalline alloys by XPCS — •Markus Stana[1], Michael Leitner[1,2], Manuel Ross[1], and Bogdan Sepiol[1] — [1]Department of Physics, University of Vienna, 1090 Vienna, Austria — [2]Physics-Department E13, TU Munich, 85747 Garching, Germany

X-ray photon correlation spectroscopy is a new method for investigating diffusion on the atomic scale. After our successful application in a Cu-Au single crystal [1], we investigated a Ni-Pt solid solution. As the question of the diffusion mechanism in this system seems settled, the experiment gives good insight in the feasibility and sensitivity of the method. Two samples, a polycrystalline and a single crystal, where prepared and measured at the European Synchrotron Radiation Facility in Grenoble. Activation energy, diffusion coefficient and basic information about the impurity-vacancy interaction has been derived. The talk will give an introduction to XPCS, an overview of our findings and an outlook towards future applications.

[1] M. Leitner, B. Sepiol, L. M. Stadler, B. Pfau, and G. Vogl, Atomic diffusion studied with coherent X-rays, Nature Mat. 8, 717 (2009).

MM 5.4 Mon 11:00 H 1029

Quantitative measurement of the surface diffusion on metallic nanoparticles by aberration-corrected HRTEM — •Alexander Surrey, Darius Pohl, Ludwig Schultz, and Bernd Rellinghaus — IFW Dresden, Helmholtzstr. 20, D-01069 Dresden, Germany

Aberration-corrected high-resolution transmission electron microscopy (HRTEM) allows for the investigation of the atomic diffusion on the surface of a nanoparticle in particular during the coalescence of adjacent particles. The incident electron beam may effectively promote this sintering process, although so far, it is not yet known to which extend. Since the material transport during the inter-particle coalescence occurs via surface diffusion, a quantitative determination of the latter is needed. Thus in the present study, the motion of atoms at the surfaces of Au nanoparticles is characterized by means of aberration-corrected HRTEM with the resolution of individual atomic columns. Subjects of the analysis are Au icosahedra on amorphous carbon substrates and single crystalline Au octahedra whose surfaces extend into the vacuum and which are thus imaged "without a substrate". A method is developed which allows for a quantitative estimation of the diffusion coefficient based on the measured temporal fluctuation of the occupation of individual atomic surface columns as obtained from HRTEM images. The likewise derived coefficient of the surface self-diffusion is in very good agreement with the results of atomic force and scanning tunneling microscopy studies.

MM 5.5 Mon 11:15 H 1029

Diffusion of charged point defects upon long-range coulomb interaction made simple — •Hannes Guhl, Paul Tangney, W.M.C. Foulkes, and Michael W. Finnis — Department of Physics and Materials, Imperial College London, London

Migration of charged point defects has been a long standing issue as it controls mass transport and ionic conductivity in insulators in various technological applications, such as gas sensors and solid oxide fuel cells. However, many stochastic studies aiming to model defect kinetics based on atomistic or first-principles information treat the mutual coulomb interaction only very roughly or neglect it altogether, as the long-range character is awkward to handle within the usually applied lattice models. Therefore, we have developed, on the basis of Debye-Hückel-theory, an intuitive and easy-to-use method to describe the diffusion of fully interacting charged point defects in an otherwise perfect crystal. As an example we apply this to a model oxide material doped with aliovalent foreign atoms. Within a systematic error smaller than one order of magnitude, the proposed formula correctly describes the data obtained from extensive Kinetic Monte Carlo simulations over a wide range of defect concentrations and temperatures. Furthermore, we demonstrate that the long-range character of the coulomb interaction gives rise to a lower bound of the diffusivity as the dopant concentration increases at constant temperature. This suggests that conventional techniques treating the defect-defect-interactions may significantly underestimate the mobility of charged species in ionic materials.