MM 14: Diffusion and Point Defects III

Time: Monday 14:45–15:45 Location: H6

MM 14.1 Mon 14:45 H6

Atomic Study of Pipe Diffusion in Al and AlCu alloys — Jan-Michael Albina[2], Christian Elsässer[2], •Thomas Gnielka[2], and Peter Gumbsch[1,2] — [1]izbs, Karlsruher Institut für Technologie , Kaiserstr. 12, 76131 Karlsruhe — [2]Fraunhofer IWM, Wöhlerstr. 11, 79108 Freiburg

The formation energies of vacancies and activation energies for vacancy diffusion in the core of an edge dislocation in Al are investigated by means of atomistic simulations. With the climbing image nudged elastic band method it is possible to find exact saddle points for a diffusion path. The calculated formation energy for a vacancy at the core of an edge dislocation ($E_{f,v} = 0.51\ eV$) is in agreement with already published data. For the important migration step we found however a higher value of $E_{mig} = 0.43\ eV$. Based on the path of minimal activation energies, a model for the quasi 1-D diffusion will be presented.

Furthermore the influence of Cu impurity atoms on activation energies will be shown.

MM 14.2 Mon 15:00 H6

Computing ab initio free energy contributions of point defects — •Blazej Grabowski, Lars Ismer, Tilmann Hickel, and Jörg Neugebauer — Max-Planck Institut für Eisenforschung, Düsseldorf, Deutschland

A common assumption when computing defect concentrations is that the dominant entropy contribution is due to configurational entropy. Other entropy contributions such as harmonic and anharmonic lattice vibrations are assumed to be second order effects and are computationally expensive to calculate. Thus, such contributions have been rarely considered in defect calculations. With the increasing capability of ab initio approaches to e.g. provide accurate free energies to macroscopic approaches (e.g. CALPHAD), the inclusion of the aforementioned smaller entropy contributions will become more and more important. We have therefore developed a hierarchical scheme to coarse grain the configurations space allowing to efficiently calculate harmonic and anharmonic contributions to vacancy formation [PRB 79, 134106 (2009)]. In the present talk we will discuss the application of this approach to vacancies in aluminum and show that the inclusion of anharmonic contributions has a dramatic effect on the entropy of vacancy formation.

MM 14.3 Mon 15:15 H6

Vacancies in aluminium and dilute Al alloys - an investigation by positron annihilation spectroscopy — •Meng Liu, Benedikt Klobes, and Karl Maier — Helmholtz-Institut für Strahlen- und Kernphysik, Rheinische Friedrich-Wilhelms-Universität Bonn, Nußallee 14-16, D-53115 Bonn

Aluminium and its alloys are widely applied in our daily lives as construction material, food packages and so on due to their unique properties, namely light weight and high strength. In case of age-hardenable Al alloys used e.g. in automotive and aviation industry they are greatly influenced by precipitates which are usually formed through vacancy driven diffusion. In Al alloys quenched-in vacancies will be trapped by solute atoms, but in pure aluminium they diffuse to the surface, grain boundaries, dislocations and disappear at room temperature. In this study HCl solution cooled to 203 K is used instead of water as quenching medium in order to optimize quenching rate, and to freeze vacancies at such temperature. Based on this quenching method a vacancy reference in pure aluminium is obtained by using positron annihilation techniques, which are especially suitable for the investigation of open volume defects, since positrons are highly sensitive to vacancies. The results are then compared to dilute Al alloys. In this way information about solute concentration around vacancies and/or their relaxation can be obtained.

MM 14.4 Mon 15:30 H6

Comperative study of diffusion in n-type TCO materials — •Péter Ágoston and Karsten Albe — Technische Universität Darmstadt, Institut für Materialwissenschaft, Petersenstr. 32, 64287 Darmstadt

In this contribution we present first-principles calculations on atomic migration for several n-type transparent conducting oxide (TCO) materials. We focus on the migration in the typical TCO materials In_2O_3 SnO_2, ZnO, CdO and Ga_2O_3. We have conducted total energy calculations within the framework of density-functional theory on a local level and in conjunction with the nudged elastic band method to obtain the formation and migration energies for all relevant defects in several charge states. We observe pronounced differences in the diffusion behavior for the investigated materials. This is partly caused by the different defect equilibria present in the different materials but also connected to the crystal structures and the resulting geometries of the migration processes.