

## MM 33: Diffusion and point defects II

Time: Thursday 11:45–12:45

Location: H6

MM 33.1 Thu 11:45 H6

**Thermal vacancies in metallic nanoparticle** — ●MICHAEL MÜLLER and KARSTEN ALBE — TU Darmstadt, Institut für Materialwissenschaft, FG Materialmodellierung, Petersenstr. 23, D-64287 Darmstadt

The influence of particle size on the concentration of thermal vacancies in metallic nanoparticles is investigated. By analyzing the contributions of surface energies and surface stresses to the vacancy formation energy, a particle size dependent model is derived. The vacancy concentration in metallic nanoparticles is predicted to be smaller than the bulk value. The results are verified by Monte Carlo simulations using a broken bond model and by molecular statics calculations with embedded atom method potentials. The combination of both methods allows to study the influence of surface energies and stresses, separately, and to verify the proposed model description.

MM 33.2 Thu 12:00 H6

**Stöchiometrische Leerstellen in Ausscheidungsphasen von Al-Legierungen** — ●IRIS KOHLBACH und TORSTEN STAAB — Rheinische Friedrich Wilhelms Universität Bonn, Helmholtz Insitut für Strahlen- und Kernphysik, Nussallee 14-16, 53115 Bonn

Beim Aushärtungsprozess von Aluminiumlegierungen werden Fremdphasen ausgeschieden, die z.T. metastabil sind. Die Legierungen werden lösungsgeglüht und abgeschreckt und die Leerstellen dabei eingefroren. Daraus ergibt sich die Fragestellung ob Abweichungen von der Stöchiometrie in einzelnen Ausscheidungsphasen durch diese Leerstellen kompensiert werden. Dazu wurde für Al-Kupfer-Legierung und AlMgSi-Legierung mit Ab-Initio-Methoden die Leerstellenbildungsenthalpie für die verschiedenen Untergitter, z.B.  $Al_2Cu$  oder  $Mg_2Si$  berechnet. Die Berechnungen wurden mit Hilfe des ab-initio Codes SIESTA vorgenommen. SIESTA nutzt hierbei die selbst konsistente Dichtefunktionaltheorie (DFT) für die Berechnung der elektronischen Strukturen. Neben den Leerstellenbildungsenthalpien erhält man bei den Berechnungen mit SIESTA auch die entsprechenden Atompositionen. Die so gewonnenen Atompositionen werden mit experimentellen Ergebnissen aus der Positronenvernichtung verglichen.

MM 33.3 Thu 12:15 H6

**Ab-initio modelling of defect properties in B2 NiAl** — ●DANIEL LERCH, KERRIN DÖSSEL, STEFAN MÜLLER, and KLAUS HEINZ — Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen

The strongly ordering B2 phase of the intermetallic compound NiAl is

known to be stable for a broad concentration range off its stoichiometry. Evidently this is due to the existence of constitutional defects. Experimental studies have shown that the dominant defect types in Al rich and Al poor parts of the B2 phase are Ni vacancies and Ni antisites (Ni atoms on the Al sublattice) respectively. We elucidate the ordering and ground state properties of defects in B2 NiAl on the basis of ab-initio calculations. We have applied the Cluster-Expansion (CE) formalism with Density Functional Theory (DFT) and the nudged elastic band method (as implemented within the computer code VASP) supplying the required input energies, as well as activation barriers for defect diffusion. Consistent with the existence of vacancies a full description of defects in NiAl bulk is only possible if vacancies are included by treating them as a third independent component within the CE formalism. One possible choice for a complete orthonormal basis set of point functions, required in such a ternary CE, are the first two Chebychev polynomials which were chosen in this case.

This work is supported by the "Studienstiftung des deutschen Volkes" which is gratefully acknowledged.

MM 33.4 Thu 12:30 H6

**Ab initio study of the carbon-carbon interaction in iron** — ●OLGA KIM, MARTIN FRIÁK, and JÖRG NEUGEBAUER — Max-Planck-Institut für Eisenforschung, Max-Planck-Strasse 1, 40237, Düsseldorf, Germany

The difference in solubility of carbon between the austenite and ferrite is the basis for the solid solution hardening of steels. The C-solubility is determined by the C-C interaction energy that influences the distribution of carbon atoms in both phases. The interaction energy in austenite is easily measurable and well known. However, in ferrite it could not be deduced experimentally due to the very low solubility of carbon in ferrite. In order to gain a detailed insight into this issue we have theoretically determined the dependence of the C-C interaction energy in ferrite as function of the C-C separation by employing density functional theory (DFT) in the generalized gradient approximation (GGA). Our results show that interstitial carbon atoms strongly repel each other. This effect gives rise to the experimentally observed low solubility of carbon in ferrite. The theoretical data provides also direct insight into ordering tendencies of carbon atoms and thermodynamic stability. In a second step the analogous calculations have been performed for austenite. Using these data the temperature dependent carbon activity in austenite is derived and compared to results obtained by the quasi-chemical approximation (R. B. McLellan and W. W. Dunn: J. Phys. Chem. Sol. 30, (1969) 2631) and with available experimental data.