MM 7: Diffusion II

Time: Monday 12:00–13:00 Location: H 0111

MM 7.1 Mon 12:00 H 0111

Adaptive jump barrier height in Monte Carlo configuration kinetics. — •Martin Leitner[1], Doris Vogtenhuber[2], Wolfgang Pfeiler[1], and Wolfgang Püschl[1] — [1]Dynamics of Condensed Systems, Faculty of Physics, University of Vienna, Strudlhofgasse 4, A-1090 Wien — [2]Computational Materials Science, Faculty of Physics, University of Vienna, Sensengasse 8, A-1090 Wien

In usual MC simulations of configuration kinetics atom jump probabilities are calculated from energies of the initial and/or final bound states of the moving atom, leaving aside the exact energy of the intermediate saddle point state. This energy may however be critically influenced by the local atomic environment. We propose a strategy to explicitly take account of this influence. The basis is ab initio calculation of representative jump paths in the framework of the nudged elastic band method. From these results, an influence function is derived which modifies the energy of the saddle point and therefore the effective jump barrier height as calculated from the initial and final states according to a cluster expansion scheme. The overall effect is demonstrated on the NiAl system.

MM 7.2 Mon 12:15 H 0111

Frühstadien der Ausscheidungsbildung in AlCu-, AlMgCu-Legierungen : Ab-initio Rechnungen zu Leerstellenbildungsenthalpien — •Iris Kohlbach und Torsten Staab — Helmholtz-Institut für Strahlen- und Kernphysik der Rheinischen Friedrich-Wilhelms-Universität Bonn, Nußallee 14-16, D-53115 Bonn

Durch die Ausscheidung von Fremdphasen kommt es bei Aluminiumlegierungen zur Aushärtung. Während die Ausscheidungssequenz von AlCu-Legierungen sehr gut bekannt ist, liegen die Frühstadien der AlMgCu-Legierungen dagegen noch nahezu gänzlich im Bereich der Spekulation. Zur Untersuchung der Rolle von Leerstellen beim Ausscheidungsprozess im AlCu wurden die Bildungsenthalpien für Leerstellen auf den verschiedenen Untergittern von Al_2Cu (Θ'- und Θ-Phase) mit Hilfe des ab-initio-Codes SIESTA bestimmt. Für Al_2MgCu wurden diese für die S″- und S-Phase berechnet, wobei aus den zahlreichen Vorschlägen zur S″-Phase die Vorschläge von Cuisat bzw. Wolverton [1] ausgewählt wurden. Unsere Ergebnisse zu Leerstellenbildungsenthalpien für AlCu-Phasen zeigen z.B. deutlich, dass sich hier keine Leerstellenagglomerate bilden. SIESTA liefert neben den Gesamtenergien eines Systems zusätzlich relaxierte Atompositionen, die für den Vergleich mit experimentellen Daten von großer Wichtigkeit sind.

[1] Wang/Starink, Int Mater Rev., 2005, Vol. 50, pp 193-215

MM 7.3 Mon 12:30 H 0111

Steady drift-diffusion model of impurity induced subcritical crack propagation — •Mario Koch[1] and Peter Streitenberger[2] — [1]Institut der Feuerwehr Sachsen-Anhalt, Biederitzer Str. 5, 39175 Heyrothsberge, Deutschland — [2]Otto-von-Guericke-Universität Magdeburg, PSF 4120, 39016 Magdeburg, Deutschland

The stress-driven diffusion of point defects to a slowly moving crack under mixed-mode loading is studied by solving the corresponding drift-diffusion equation in a co-moving reference system. Numerical solutions for the quasi-stationary concentration fields and flow field patterns are presented, which reveal important insights into the point-defect migration kinetics near a steadily advancing crack. In particular, it is shown that only impurities within a limited drift-diffusion zone, of which the extension depends on the average crack growth rate, are able to migrate to the crack tip. Considering the existence of a critical impurity concentration per crack length advance as the basic criterion for failure of the material, the crack growth behaviour in form of the crack growth rate versus stress intensity factor curve is calculated. In the case where the size of the plastic zone is very small in comparison with the drift-diffusion zone stage I crack growth is observed, if the size of the plastic zone is very large in comparison with the drift-diffusion zone stage II crack growth is observed.

MM 7.4 Mon 12:45 H 0111

Re-orientation behaviour of c-variant FePt thin films — •Marcus Rennhofer[1], Miroslav Kozlowski[2], Bart Laenens[3], Bogdan Sepiol[1], Rafal Kozubski[2], Andre Vantomme[3], Johan Meersschaut[3], and Gero Vogl[1] — [1]University of Vienna, Vienna, Austria — [2]Jagiellonian University Cracow, Cracow, Poland — [3]Instituut for Kern- en Stralingsfysika

The magnetocrystalline and thermal stability of $L1_0$-FePt makes this alloy suitable for ultrahigh density recording. Various experiments with bulk $L1_0$-FePt dealing with diffusion and ordering dynamics have been performed [1, 2].

Our Monte Carlo (MC) simulations show that the c-variant of the $L1_0$ superstructure (easy axis of the magnetisation out of plane of the thin film samples) is unstable. The monoatomic planes re-orient creating a-domains (easy axis of the magnetic field in the film plane). Our recent conversion electron Mössbauer spectroscopy (CEMS) experiments on -variant ^{57}FePt(50 nm)/MgO(001) thin films show evidence of this re-orientation behaviour. The picture arising from our results is as follows: an re-orientation takes place but reverts after a certain time and then saturates. The effect depends on the annealing temperature. An additional capping of the films suppresses the effect almost completely.

[1] M. Rennhofer et al. Phys. Rev. B. 74(10), 104301 (2006).
[2] R. Kozubski et al J. of Phase Equil. and Diff. 26(5), 482 – 486 (2005).