# MM 27 Diffusion I

Time: Thursday 10:15–11:15

Room: IFW B

MM 27.1 Thu 10:15 IFW B

**Transient heterogeneity in long-range order kinetics with limited vacancy mobility** — •David Reith[1], Wolfgang Püschl[1], Ferdinand Haider[2], and Wolfgang Pfeiler[1] — [1]Institut für Materialphysik, Universität Wien, Boltzmanng. 5, AT-1090 Vienna, Austria — [2]Institut für Physik, Universität Augsburg, Universitätsstrasse 1, D-86159 Augsburg, Germany

Limited availability and mobility of vacancies may imprint a heterogeneous character on phase transformations which are otherwise expected to be homogeneous. This effect was investigated by a MC residence time algorithm for disorder-order and order-order transitions in long-range ordered intermetallics of $L1_2$ and B2 structure. The calculation cell was subdivided into coarse graining cells and heterogeneity assessed by the mean square deviation of the local long-range order parameter. A transient increase of this measure over the statistical fluctuation for the respective annealing temperature was observed for the B2 structure, but not in the $L1_2$ case. This can be understood in view of the majority sublattice as an easy diffusion highway. The effect in B2 is even more pronounced when starting from a disordered state. For a homogenous character of the kinetics to be restored, an earlier intuitive criterion relied on the overlap of regions bounded by the mean quadratic random walk distances of neighboring vacancies. Whereas this condition is in fact met at a very early stage in the kinetics, true homogeneity is reached only when a significant fraction of lattice sites has been visited by a vacancy.

MM 27.2 Thu 10:30 IFW B

**Ordering kinetics is affected when jump barrier heights depend on local environment** — •Martin Leitner[1], Wolfgang Püschl[1], Ferdinand Haider[2], and Wolfgang Pfeiler[1] — [1]Institut für Materialphysik, Universität Wien, Boltzmanng. 5, AT-1090 Vienna, Austria — [2]Institut für Physik, Universität Augsburg, Universitätsstrasse 1, D-86159 Augsburg, Germany

Kinetics of order-order transformations in a $L1_2$ long-range ordered model crystal was investigated by Monte-Carlo simulation employing a residence-time algorithm. Atoms were supposed to jump into nearest-neighbor vacancies. In doing so, they have to pass through a rectangular window of atoms which are nearest neighbors to both the initial and the final positions. ab initio calculations of jump profiles [Mat. Res. Soc. Symp. Proc. 842, S5.28 (2005)] for $Ni_3Al$ show that barrier heights are markedly influenced by the kind of atoms occupying this window as well as their relative position. These results were incorporated as a rule into the MC algorithm, with a parameter characterizing the influence of the window atoms. If this parameter is increased from zero, three regimes of kinetic behavior can be discerned: a regime of finite but small influence below a certain threshold, a critical region where behavior changes quickly and in a qualitative way, an asymptotic region where the kinetics is stable against a further increase. It is discussed under which conditions the usual assumption of constant barrier height made in the literature will have to be modified.

MM 27.3 Thu 10:45 IFW B

**Nonisothermal Internal Oxidation of Iron in Palladium** — •Jürgen Gegner — SKF GmbH, Material Physics, Ernst-Sachs-Str. 5, D-97424 Schweinfurt, Germany

Incomplete isothermal-isobaric internal oxidation of dilute homogeneous alloys is a frequently used experimental technique to measure the diffusion coefficient of oxygen in the base metal. Adopting this method, however, derivation of the Arrhenius equation requires a series of anneals at different temperatures. In the present work, a recently introduced [1], simplified experimental procedure is applied to the binary Pd-Fe system: incomplete temperature-controlled isobaric internal oxidation. Mathematical evaluation of the time development of the subscale thickness, which follows from SEM micrographs of samples that are removed from the furnace at several durations of the air annealing, is performed by means of an iterative computer model [2]. In this realistic process simulation, the sought quantity, i.e. the diffusivity $D_O$ of oxygen in palladium, is the fit parameter and found to be:

$$D_O = 0.532 \cdot \exp\left(-18728.27/T\right)$$

Here, $D_O$ is expressed in $cm^2/s$ and temperature $T$ ranges from 1073 to 1473 K. This result is compared with literature references.

[1] J. Gegner: Komplexe Diffusionsprozesse in Metallen. expert-Verlag, Renningen (2006), p. 397-402

[2] J. Gegner: New Computer Model for Internal Oxidation. Proc. MMT-2004, p. 1/28-1/37

MM 27.4 Thu 11:00 IFW B

**Self-diffusion in Amorphous Silicon Nitride** — •Harald Schmidt[1], Mukul Gupta[2], and Michael Bruns[3] — [1]Fakultät für Natur- und Materialwissenschaften, TU Clausthal, Robert-Koch-Str. 42, D-38678 Clausthal-Zellerfeld, Germany — [2]Laboratory for Neutron Scattering, ETH Zürich & PSI, Villigen, CH-5232, Switzerland — [3]Institut für Instrumentelle Analytik, Forschungszentrum Karlsruhe GmbH, D-76021 Karlsruhe, Germany

Amorphous silicon nitride is a model system for a covalently bound amorphous solid with extremely low atomic mobilities where reasonable values of self-diffusivities are still lacking. We used neutron reflectometry on isotope enriched $Si_3^{14}N_4/Si_3^{15}N_4$ multilayers to determine nitrogen self-diffusivities ranging from $10^{-24}$ to $10^{-21}$ $m^2/s$ between 950 and 1250 ℃. Time dependent diffusivities observed at 1150 ℃ indicate the presence of structural relaxation. For long annealing times (relaxed state) the diffusivities follow an Arrhenius law with an activation enthalpy of 3.6 eV. Possible diffusion mechanisms are discussed and the results are compared to the Si and N diffusivities in polycrystalline silicon nitride as obtained by Secondary Ion Mass Spectrometry.