MM 27: HV Kozubski

Time: Thursday 9:30–10:00 Location: H16

Invited Talk MM 27.1 Thu 9:30 H16

Atomic Migration Phenomena in Intermetallics with High Superstructure Stability — •Rafal Kozubski[1], Véronique Pierron-Bohnes[2], and Wolfgang Pfeiler[3] — [1]Interdisciplinary Centre for Materials Modelling, M. Smoluchowski Institute of Physics, H. Jagellonian University, Reymonta 4, 30-059 Krakow, Poland — [2]CNRS, Institut de Physique et Chimie des Matériaux de Straßbourg, CNRS/ULP, 23 rue de Loess BP 43, 67034 Straßbourg, France — [3]Institut für Materialphysik, Universität Wien, Strudlhofgasse 4, 1090 Wien, Austria

Most of the contemporary materials based on intermetallic phases are either multiple bulk phases, or nanostructured layers deposited on appropriate substrates. In each case, the desired properties of the materials are due to chemical order and the preparation technology consists of a generation of specific processes mediated by atomic migration. It is shown how a nanoscopic (atomistic) image of the atomic migration phenomena results from an indirect experimental technique in combination with Monte Carlo (MC) and Molecular Dynamics (MD) simulations.

"Order-order"relaxations were observed in phases representing three typical cubic superstructures of high stability:
$B2(NiAl, FeAl)$, $L1_2(Ni_3Al)$ and $L1_0(FePd, FePt)$.
Detailed analysis of the atomic-jump statistics yielded by MC and MD simulations elucidated: (i) the origin of the multi-time-scale character of the process, (ii) the atomic-jump correlation effect on the effective activation energy for the relaxations, (iv) the effect of free surfaces on the superstructure stability in $L1_0$ nano-layers; (v) the effect of triple-defect formation on the kinetics of the "order-order"relaxation in B2 binaries.