Contribution ID: **101** Type: **oral**

Thermodynamic activation energy for self diffusion and order-order relaxation in intermetallic compounds: atomistic model and Monte Carlo simulations

Monday, September 4, 2017 3:40 PM (20 minutes)

Self-diffusion and the 'order order' relaxation process in intermetallic compounds is described in terms of effective atomic jump frequencies and the current degree of chemical long-range order. It is demonstrated that the thermodynamic activation energies of self-diffusion and the 'order-order' relaxation can be expressed in terms of the activation energies of more elementary processes. As the derived expressions differ from each other, the values of the thermodynamic activation energies for self-diffusion and the 'order order' relaxation can be different although both processes are controlled by the same vacancy-mediated elementary atomic jumps.
In order to assess the the validity of the derived formulae different B2-ordering binary systems are simulated. The results of the computer experiments are in good agreement with the tested formulae. It is shown that the relationship between the activation energies observed in triple defect B2-ordering binaries, where the value of the activation energy for order-order relaxations is substantially lower than that for self-diffusion, does not hold in the case of non-triple-defect binaries. Using the tested formulae, the origin of the effect is elucidated and attributed to the atomistic origin of the tendency for triple-defect disordering.

P. Sowa, A. Biborski, M. Kozłowski, R. Kozubski, I.V. Belova, G.E. Murch: Atomistic origin of the thermodynamic activation energy for self diffusion and order-order relaxation in intermetallic compounds. Part I and Part II, Philos.Mag., **97**, 1361-1374, 1375-1397 (2017).

Primary author: ABDANK-KOZUBSKI, Rafal (M. Smoluchowski Institute of Physics, Jagiellonian University in Krakow)

Co-authors: BIBORSKI, Andrzej (AGH University of Science and Technology Academic Centre for Materials and Nanotechnology); MURCH, Graeme E. (Centre for Mass and Thermal Transport in Engineering Materials, School of Engineering, The University of Newcastle, Callaghan, Australia); BELOVA, Irina V. (Centre for Mass and Thermal Transport in Engineering Materials, School of Engineering, The University of Newcastle, Callaghan, Australia); SOWA, Piotr (M. Smoluchowski Institute of Physics, Jagiellonian University in Krakow)

Presenter: ABDANK-KOZUBSKI, Rafal (M. Smoluchowski Institute of Physics, Jagiellonian University in Krakow)

Session Classification: Session 2