Ordering kinetics and self diffusion in bulk and nano-layered B2-ordering AB binary systems: effect of temperature-dependent tendency for triple defect formation

A. Biborski, P. Sowa and R. Kozubski
M. Smoluchowski Institute of Physics, Jagiellonian University in Krakow, Poland
E.V. Levchenko, A.V. Evteev, I. V. Belova, G.E. Murch
School of Engineering, The University of Newcastle, Callaghan, Australia

Kinetic Monte Carlo (KMC) simulations of ordering kinetics in bulk and nano-layered triple-defect B2-ordering AB binary systems revealed sequential operation of two relaxation processes dramatically differing in rates. Initial extremely fast process consisting of almost exclusive triple defect formation and running with very high driving force is abruptly stopped and followed by extremely sluggish relaxation leading the system to equilibrium configuration. The sluggish relaxation stage is associated with experimentally observed “order-order” kinetics in NiAl. In AB (001)-oriented nano-layers the isothermal evolution of atomic configuration is affected by the above complex relaxations combined in addition with vacancy and B-atom segregation on free surfaces.

The present contribution is focused on the atomistic origin of the sudden change of relaxation rate in the system. Detailed study of the evolution of atomic energy profiles due to antisite defect generation allow to elucidate this origin in terms of a decrease of disordering efficiency of the atomic jumps. The KMC results are compared with conclusions following from a mean-field-type analytical model of the phenomenon.

Temperature dependence of the tendency for triple-defect formation in the modelled system was an opportunity for studying an effect of this tendency on self diffusion of its A- and B-components.