EXMONAN

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Self-diffusion phenomena in triple-defect B2-ordering binary system: Monte Carlo simulation

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The Ni-Al system belongs to the most widely studied and at the same time extremely perspective in terms of design materials. The wide concentration range of B2 NiAl superstructure stability indicates the ability of this compound to accumulate significant amounts of point defects. Off-stoichiometry is compensated in an asymmetric way: Al-rich side is stabilized through vacancies and Ni-rich by passing atoms to anti-structural positions. This phenomenon is known as the so-called long-range disorder with triple-defect type disordering.

An Ising model with nearest neighbors (nn) and next nearest neighbors (nnn) interatomic pair interactions yielding B2 chemical ordering of a binary A-B system mimicking Ni-Al in a wide stoichiometric range was proposed.
A temperature-dependent equilibrium atomic configuration in the system including equilibrium vacancy concentration and distribution was determined by means of Semi Grand Canonical Monte Carlo (SGCMC) simulations. Following the technique developed previously for the same system modeled with nn interatomic pair interactions [1], self diffusion of A and B atoms in equilibrium atomic configuration of the system completed with saddle-point energies for atomic jumps to nn and nnn vacancies was simulated with Kinetic Monte Carlo (KMC) algorithm involving both sorts of the jumps. The evaluated diffusivities of the system components yielded thermodynamic activation energies of the process, which were then analysed in terms of the applied model and the effect of B2 long-range order.

[1] Sowa, P., et. all (2013). Self-diffusion and ‘order–order’ kinetics in B2-ordering AB binary systems with a tendency for triple-defect formation: Monte Carlo simulation. Philosophical Magazine, 93(16), 1987-1998.