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VACANCY MEDIATED SELF- AND INTER-DIFFUSION IN INTERMETALLICS: KINETIC MONTE CARLO SIMULATION

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Methodology of the Monte Carlo simulation of vacancy mediated self- and inter-diffusion is presented and illustrated by the results obtained in the case B2 ordering triple-defect binary intermetallics. The kinetic Monte Carlo (KMC) algorithm was implemented with local configuration dependent migration barriers and temperature dependent equilibrium vacancy concentration determined by means of semi grand canonical Monte Carlo (SGCMC) simulations. The inversion of the relationship between the Ni and Al-diffusivities in Al-rich Ni-Al systems deduced from the features of experimentally investigated interdiffusion in Ni-Al was perfectly reproduced by direct self-diffusion simulations. The origin of the phenomenon was elucidated in terms of an increase of the NNN Al jump frequency caused by the generation of structural Ni-vacancies. KMC simulations of diffusion couple experiment were performed by incorporating physical model of vacancy source and sinks and assuming that equilibrium vacancy concentration in the system is achieved much faster than the equilibrium atomic configuration. Semi grand canonical Monte Carlo (SGCMC) algorithm implemented in the KMC code generated on-line vacancy concentrations locally equilibrated according to the virtual atomic configuration in the sample. The evaluated interdiffusion coefficients, as well as the correlation and Kirkendal effects resulting from the simulation of Ising type models of binary disordered and ordered systems were analyzed.

Biography

Rafal Kozubski has completed his PhD from the Jagiellonian University in Kraków in 1984. He was serving as a Postdoctoral Fellow at the Strasbourg Institute of Physics and Chemistry of Materials (IPCMS), France from 1987 to 1988. He has served as a Lise-Meitner Fellow, the Institute for Solid State Physics, University of Vienna, Austria from Oct' 1993 to Sep' 1995.. In 2006, he was appointed as a Full Professor in the Jagiellonian University in Kraków, Poland. His international experience includes International Fellowship at the Queen's University in Belfast (2006-2008) and Visiting Professorships at the L Pasteur University in Strasbourg/University of Strasbourg, France (2007-2011). In 2016, he was appointed as a Conjoint Professor of the University of Newcastle, Australia. He has published over 100 scientific papers in international reviewed journals and is an Author of over 150 communications on international conferences.

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