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Saddle point energies for atomic jumps and thermodynamic activation energy for ordering and diffusion in intermetallic compounds: Atomistic simulations

Chemical ordering and diffusion are controlled by atomic migration, which in the case of solid intermetallic compounds, proceeds predominantly via elementary atomic jumps to vacancies. The macroscopic rates of both phenomena parameterized by diffusivities (diffusion) and relaxation times (chemical ordering) show temperature dependences quantified by thermodynamic activation energies usually evaluated through the Arrhenius analysis. The atomistic origin of the phenomenon consists of the thermal activation of the atomic jumps described in terms of the "activated-state-rate" theory involving the probability of the atomic displacement from the original lattice site to the intermediate lattice position corresponding to the energetic saddle point. The saddle-point energies are modeled for diverse intermetallic compounds using various concepts and techniques implemented with diverse Hamiltonians. The results are then used as parameters of Kinetic Monte Carlo simulations of ordering and diffusion, whose Arrhenius analysis yields thermodynamic activation energies. Correlation between thermodynamic activation energies for chemical ordering and diffusion and the values and relationships between the saddle-point energies is widely discussed. In particular, the origin of the relationship between the thermodynamic activation energies for ordering and Ni tracer diffusion in NiAl is elucidated in the above terms.

Biography

Rafal Kozubski has completed his PhD from the Jagiellonian University in Kraków in 1984. He has worked as a Post-doctorate at the Strasbourg Institute of Physics and Chemistry of Materials (IPCMS), France (1987 to 1988). He was an Academic Visitor in the Institute for Applied Physics, Swiss Federal Institute of Technology, Zurich, Switzerland (1988 and 1990). He also stayed at the Institute for Solid State Physics, University of Vienna, Austria as a Lise-Meitner Fellow from 1993 to 1995. After completing his Habilitation (DSc) from the Jagiellonian University in Kraków in 1997, he has worked there as an Associate Professor (1997-2006) and in 2006, he was appointed as Full Professor at the same university. 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, 2008, 2009, 2010 and 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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