Solid state diffusion: Atomistic simulation and phase field modeling

Rafal Kozubski[1*], Helena Zapolsky[2*], Gilles Demange[2], Piotr Sowa[1], Jan Betlej[1]

[1]M.Smoluchowski Institute of Physics, Jagiellonian University, Krakow, Poland
[2]GPM UMR 6634, University Rouen Normandy, Saint-Etienne du Rouvray, France

rafal.kozubski@uj.edu.pl
helena.zapolsky@univ-rouen.fr

The workshop is composed of two main parts: the first part devoted to atomistic Monte Carlo simulations and the second part devoted to the Phase Field modelling. In each part a lecture will be accompanied by exercise activities.

The first lecture will present: (i) the foundations of the implementation of Monte Carlo techniques in equilibrium and non-equilibrium Statistical Thermodynamics; (ii) equilibrium and kinetic aspects of steady-state tracer diffusion; (iii) models and MC techniques adequate for the determination of equilibrium configurations of solids including defect concentration; (iv) principles of Kinetic MC. The exercise activities including: (i) visualization of the MC generation of equilibrium configuration of a system within the Shapink model (spectacular SGCMC simulation of phase equilibria in a lattice gas composed of atoms and vacancies); (ii) KMC simulation of steady-state vacancy-mediated tracer diffusion and demonstration of the fulfilment of Einstein-Smoluchowski relation and (iii) simulation of a diffusion couple and the evolution of its concentration profile – will yield illustration of the lecture.

Over the past three decades, phase field model (PFM) have become one of the main tools for the modeling the microstructure of alloy at mesoscale. This method based on the non-linear Allen-Cahn and Cahn-Hilliard kinetics equations provides a way to model the non-equilibrium dynamics such as spinodal decomposition, precipitation or morphological evolution of microstructure in a wide range of materials.

In this part of the workshop, a lecture is planned which detail the formalism of PFM with emphasis on the thermodynamic fundamentals behind the formulation of this approach. The lecture will also include a new extension of the PFM at atomic scale. Several examples of applications of PFM will be done. During the workshop, the participants will not only get the basic principles of PFM, but also hands-on experience on the computational implementation of the PFM to solve different problems in material science. The aim is to reach a level of understanding among the participants, which will allow them to develop phase-field modeling solutions for their own problems.

The lecture will be followed by computer exercises: (i) PFM modeling of spinodal decomposition in binary alloys; (ii) PFM modeling of microstructural evolution in Ni-based alloys and (iii) Interpretation of the PFM results for microstructural evolution and comparison with the classical Lifshitz, Slyozov and Wagner theory of coarsening.