December 15,
16:00 (MSK time)
online

Computational
Materials
Science

Seminar

Atomistic simulation of diffusion phenomena in presence of crystal defects

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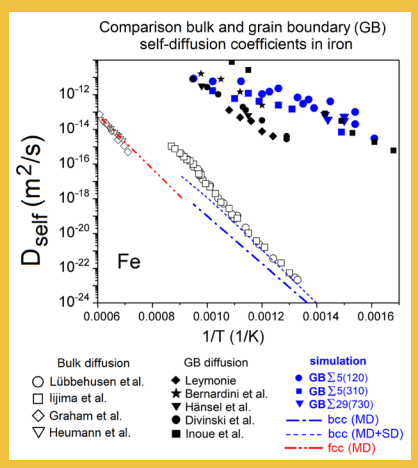
Speaker introduction

Dr. Sergei Starikov is a Project leader in Interdisciplinary Centre for Advanced Materials Simulation (ICAMS, Ruhr-Universitat Bochum, Germany). He obtained his M.Sc. (2007) and Ph.D. (2011) from the Moscow Institute of Physics and Technology with specializations in the computational materials science. In 2016 he was awarded with Medal of the Russian Academy of Science for young scientists for the series of works named “Development of atomistic models and investigation of thermodynamic and kinetic properties of nuclear fuel for new generation reactors”. His work and research interests focus on materials science, development of interatomic potentials, atomic diffusion, and plastic deformation. He is an author of more than 70 peer-reviewed journal publications with personal H-index of 24.

Seminar abstract

The kinetics of many microstructural changes during processing or heat treatment are engaged with diffusion-controlled phenomena. Thus, the atomic diffusion plays a crucial role in many physical processes. It has been recognized that atomic migration in crystalline solids is linked to crystal defects behavior. As the simplest case, the atomistic mechanism of self-diffusion at high temperature is based on the diffusion of point defects (mostly, vacancies). On the other hand, the diffusion phenomena at low temperatures (or in case of highly defected crystal) can be governed by the fast migration of atoms along spatial crystal defects: grain boundaries and dislocations.
The diffusion inside such crystal defects can be caused by the completely different processes than usual vacancy migration. This talk focuses on atomistic simulation of diffusion processes taking place in bcc crystals (Fe, Nb, Mo) in presence of crystal defects.



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