CSC-RUB PhD Project Proposal

Title: Ab-initio investigation of grain boundary segregation in metallic microstructures

Sector of research: Computational Materials Science

Degree awarded: PhD (Dr. Ing.)

Keywords: Ab-initio density functional theory calculations, metallic microstructures, segregation engineering, cohesion and fracture

Supervisor of PhD project: PD Dr. habil. Rebecca Janisch, ICAMS, e-mail: rebecca.janisch@icams.ruhr-uni-bochum.de

Research focus of supervisor:

I want to understand the mechanical properties of material microstructures "from the bottom up", where the starting point can be the behavior of atoms or even of electrons in the microstructure. In my group we use ab-initio density functional theory calculations and molecular dynamics simulations to investigate the impact of defects (mainly phase and grain boundaries) in metals and alloys on the mechanical properties of microstructures, and we relate these effects to the fundamental defect properties like structure, stiffness and strength. Ideally, these relationships can be captured by analytic expressions which can serve as constitutive relationships for multiscale mechanical modeling.

Publications:

(1) A. Chauniyal, G. Dehm, **R. Janisch**, *On the role of pre-existing defects in influencing hardness in nanoscale indentations—Insights from atomistic simulations*, Journal of the Mechanics and Physics of Solids (2021), 154, 104511.

(2) A. Neogi, **R. Janisch**, *Twin-boundary assisted crack tip plasticity and toughening in lamellar γ - TiAl*, Acta Materialia (2021), 213, 116924.

(3) A. Azócar Guzmán, J. Jeon, A. Hartmaier, **R. Janisch**, *Hydrogen embrittlement at cleavage planes and grain boundaries in bcc iron—revisiting the first-principles cohesive zone model*, Materials (2020), 13, 5785.

(4) J. Möller, E. Bitzek, **R. Janisch**, H. ul Hassan, A. Hartmaier, *Fracture ab initio: A force-based scaling law for atomistically informed continuum models*, Journal of Materials Research (2018), 33, 3750 – 3761.

(5) H. Dette, J. Gösmann, C. Greiff, **R. Janisch**, *Efficient sampling in materials simulation - Exploring the parameter space of grain boundaries*, Acta Materialia (2017), 125, 145-155.

Summary of research plan

Background: Nanocrystalline materials exhibit unique structural and functional properties due to the dominant presence of grain boundaries (GBs). The stability of these GBs plays a crucial role in determining the plastic deformability and hardness of metallic materials, especially with extremely fine grains. Grain growth during annealing is influenced strongly by the grain boundary character, especially the inclination of the grain boundary plane and chemistry, and so are the resulting mechanical properties, e.g. the creep behaviour, or the fracture toghness. Therefore, there is a strong interest in manipulating the structure and energy of grain boundaries in metals and alloys, and a large demand for extensive data on grain boundary properties in multicomponent systems. Ab-initio density functional theory calculations provide the means to explore the relation between grain boundary chemistry, structure, and grain boundary energy, but also properties such as grain boundary mobility and cohesion.

Study objective: Characterize the influence of interface structure and chemistry of twin and grain boundaries on the mechanical properties and provide quantitative data and understanding as basis for segregation engineering of metallic microstructures.

Expected Results: Structure-property relations which quantify the impact of chemistry and geometry on grain boundary energy and derived properties.

Methods: Ab-initio density functional theory calculations, parallel computation on the ICAMS computer cluster.

Candidate Requirements:

- excellent master's degree in materials science or a related discipline
- solid knowledge of physical metallurgy, especially about defects in microstructures
- strong interest in atomistic modeling of defects
- excellent spoken and written English (IELTS band score of 6.5 or higher)

Motivation for CSC application: The candidate will work in an international environment at the interdisciplinary centre for advanced materials simulation (ICAMS). At ICAMS, state-of-the-art computational methods are being developed and applied to understand and design modern materials. The candidate will be trained in atomistic simulation methods, as well as the use of a modern computational infrastructure.