CSC-RUB PhD Project Proposal

Title: Atomistic simulations of nanoscratching across grain boundaries in metals

Sector of research: Computational Materials Science

Degree awarded: PhD (Dr. Ing.)

Keywords: Molecular dynamics simulations, mechanical properties, metallic microstructures, defect-defect interactions

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: Nanoindentation and nanoscratching are state-of-the art mechanical testing methods, which provide access to the local hardness, friction and wear behaviour of a microstructure. With the increase of computational power, large-scale molecular dynamics simulations of these experiments have become attractive, since they enable us to monitor the evolution of plasticity on the atomistic level and can therefore help us to understand the defect-defect interaction mechanism that govern deformation and wear of metallic materials. In particular the effect of dislocation-interface interactions, and how these interactions are influenced by the nature of the interface (e.g. misorientation, lattice misfit, local chemistry) can be revealed. As demonstrated by recent investigations on nanoscale hardness using atomistic simulations, it is now possible to directly correlate dislocation interactions to the measured hardness in nanoindentation simulations. This implies that the influence of dislocation pile ups, slip transmission and crystal anisotropy can be determined in a systematic way.

Study objective: Characterize the influence of interface structure of twin and grain boundaries on slip transmission as part of wear mechanisms in metallic microstructures.

Expected Results: Structure-property relations which describe the effect of interface geometry on dislocation slip transfer as well as dislocation and/or microcrack nucleation

Methods: Large-scale molecular dynamics simulations, 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 mechanical deformation
- 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.