CSC-RUB PhD Project Proposal

Title: Model-based microstructure design for polycrystals with high strength and ductility

Sector of research: Mechanical properties of materials

Degree awarded: PhD

Keywords: Micromechanical modeling, strength, ductility, deformation and failure mechanisms

Supervisor of PhD project: Prof. Dr. Alexander Hartmaier, ICAMS, e-mail: alexander.hartmaier@rub.de

Research focus of supervisor:

- Micromechanical and scalebridging modeling of deformation, fracture and fatigue of multiphase metallic and non-metallic materials
- Micro- and nanomechnical characterization
- Crystal plasticity methods and parameter identification with inverse methods
- Data-oriented methods and machine learning for mechanical systems
- Precision machining and wear of metals and ceramics
- Structural materials (steels, aluminium alloys, copper alloys)
- Simulation methods: ab initio methods, Molecular Dynamics, Monte-Carlo, Dislocation Dynamics, Crystal Plasticity, Finite Element Analysis, Machine Learning

Publications:

Selected publications:

1. S Gao, M Fivel, A Ma, A Hartmaier. 3D discrete dislocation dynamics study of creep behavior in Ni-base single crystal superalloys by a combined dislocation climb and vacancy diffusion model. Journal of the Mechanics and Physics of Solids 102 (2017) 209-223
2. JJ 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 33 (2018) 3750-3761
3. D Reimann, K Chandra, N Vajragupta, T Glasmachers, P Junker, A Hartmaier. Modeling macroscopic material behavior with machine learning algorithms trained by micromechanical simulations. Frontiers in Materials 6 (2019) 181
4. W Amin, M A Ali, N. Vajragupta, A. Hartmaier. Studying Grain Boundary Strengthening by Dislocation-Based Strain Gradient Crystal Plasticity Coupled with a Multi-Phase-Field Model. Materials 12 (2019) 2977
5. L Zhao, J Zhang, J Pfetzing, M Alam, A Hartmaier. Depth-sensing ductile and brittle deformation in 3C-SiC under Berkovich nanoindentation. Materials & Design 197 (2021) 109223

In total: 146 publications with 2671 citations, *h*-index: 28 (source: Web of Knowledge)

Full publication list: https://orcid.org/0000-0002-3710-1169

Public software repositories: https://github.com/AHartmaier

Xtal-Mech – Learning platform for Crystal Mechanics: http://xtal-mech.icams.rub.de/

Summary of research plan

Background: In technical materials strength and ductility are typically contradictory properties, such that increasing one of them will reduce the other one. However, experimental data shows that in some ultrafine-grained materials or in materials with a bi-modal grain size distribution, both properties can be maximized simultaneously. From a materials science perspective such ultrafine-grained or bi-modal microstructures pose a particular challenge because the deformation and failure mechanisms differ quite significantly from those of conventional materials. Furthermore, the microstructure tends to evolve rather dynamically under thermo-mechanical loads. Thus, the stability of these special microstructures needs to be investigated to allow for the design of microstructures with tailored properties.

Study objective: The main scientific objective of this project is to gain fundamental understanding of the deformation and failure mechanisms and the stability of ultrafine-grained or bi-modal microstructures. This understanding shall be employed to derive design guidelines for microstructures with particularly good properties in terms of strength and ductility.

Expected Results: The model-based approach of this project is expected to lead to deformation mechanism maps and also to maps for the microstructural stability of metals with ultrafine-grained or bi-modal microstructures. With the help of such maps, deformation mechanisms and microstructural stability is visualized as function of temperature and applied mechanical load, which is the basis for a purposeful design of microstructures.

Methods: The main method for this project is the phase-field method to study the microstructure evolution under thermo-mechanical loads and physics-based crystal plasticity and damage models that provide an accurate description of the mechanical behavior of the studied materials. In a preliminary study, the combination of these methods has already been proven to yield fundamental insight into the mechanical behavior of polycrystals, see https://doi.org/10.3390/ma12182977.

Candidate Requirements: MSc degree in materials science, mechanical engineering or related disciplines. Experience with numerical modeling. Good English language skills.

Motivation for CSC application: The successful candidate will be a member of the department Micromechanical and Macroscopic Modeling (MMM) at the Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), which is a research center of Ruhr-Universität Bochum. The PhD candidates will also be a part of the ICAMS Graduate School and the Ruhr University Research School, in which they receive a special training on the most important methods of scalebridging and data-oriented materials science and scientific key qualifications. They have access to a powerful computer infrastructure and a modern software environment, in which their research projects can be conducted in an efficient way. The MMM department forms a team with an active and stimulating culture with plenty of scientific and social activities.