# CSC-RUB PhD Project Proposal

**Title:** Precision machining of brittle ceramics with diamond cutting: Influence of microstructure and phase transformations

**Sector of research:** Mechanical properties of materials

**Degree awarded**: PhD

**Keywords**: Micromechanical modeling, brittle fracture,

**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. L Zhao, M Alam, J Zhang, R Janisch, A Hartmaier. Amorphization-governed elasto-plastic deformation under nanoindentation in cubic (3C) silicon carbide. Ceramics International 46 (2020) 12470
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:** Diamond cutting of hard and brittle ceramics is a technological challenge because it requires a detailed knowledge about the mechanisms of material removal to guarantee a stable process and a high-quality surface finish. While most ceramics behave in a completely brittle manner in macroscopic tests, micromechanical testing frequently reveals some ductility of the material. During diamond cutting, such a brittle-ductile transition can be observed as a function of the process parameters. It has been shown in the literature that operating the diamond cutting process in the ductile regime offers several advantages and can lead to an ultra-low surface roughness of the machined part. Furthermore, the literature has revealed that phase transformations, as the transition from the crystalline to the amorphous state under the high pressure of the tool, have a strong influence on the material separation process, which is not well understood yet.

**Study objective:** In this research project, the diamond cutting process of brittle SiC ceramics will be investigated on a microstructural scale with the help of numerical models to gain insight into the influence of microstructure and phase transformations on the brittle or ductile nature of the material removal process.

**Expected Results:** It is expected that this project results in several scientific publications in which the conditions for ductile machining and the mechanisms of the material removal process are described in a fundamental way. In particular, the consequences of the formation of an amorphous layer will be elucidated; and the role of grain boundaries on the resulting surface quality is assessed.

**Methods:** The crystal plasticity-finite element method will be employed to study the diamond cutting process, where the material removal is described based on a damage model. An existing model for phase transformation will be adopted to describe the amorphization and other phase transformations that might occur during the cutting process of SiC. In every step, the model is validated based on literature data from experiment and atomistic simulations.

**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.