CSC-RUB PhD Project Proposal

Title: Machine learning based interatomic potential for Magnesium alloys

Sector of research: Computational Materials Science, Physical Metallurgy

Degree awarded: Dr.-Ing. (Phd)

Keywords: metal alloys, machine learning, interatomic potentials

Supervisors of PhD project:

Prof. Dr.-Ing. Markus Stricker, Interdisciplinary Centre for Advanced Materials Simulation

Email: markus.stricker@rub.de; ORCID: 0000-0002-8933-0238

Binglun Yin, Zhejiang University

Research focus of supervisor: My group, Materials Informatics and Data Science at the Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), applies algorithms and methods from data sciences and machine learning to materials science problems. Our background is in Computational Materials Science with a focus on metals and alloys. Specific applications currently include data fusion from simulation and experiment to improve interpretability, the development of interatomic potentials based on neural networks for alloys which are not well described by analytical formulations, and data mining in large defect simulations to improve the understanding of their collective behavior in order to inform coarse-grained models.

Publications:
The choice for relevant publications is based on the objective of the research proposal: code development, defects in metals, interatomic potential fitting

(1) **Stricker, M.** et al. Machine learning for metallurgy II. A neural-network potential for magnesium Phys. Rev. Materials, American Physical Society, 2020, 4, 103602

(2) **Stricker, M.** & Curtin, W. A. Prismatic Slip in Magnesium J. Phys. Chem. C, American Chemical Society, 2020, 124, 27230-27240

(3) Musil, F. ... **Stricker, M.** et al. Efficient implementation of atom-density representations The Journal of Chemical Physics, 2021, 154, 114109

(4) **Stricker, M.** et al. Irreversibility of dislocation motion under cyclic loading due to strain gradients Scripta Materialia, 2017, 129, 69 – 73

(5) Roters, F. ... **Stricker, M.**; et al. DAMASK – The Düsseldorf Advanced Material Simulation Kit for modeling multi-physics crystal plasticity, thermal, and damage phenomena from the single crystal up to the component scale Computational Materials Science, 2019, 158, 420 - 478

Summary of research plan:

Background: The macroscopic mechanical behavior of metals is dictated by its microstructure and defects. Assessing those defects and their behavior is often tedious or impossible experimentally but powerful computational methods such as density functional theory (DFT) and molecular dynamics (MD) allow to observe defect behavior in simulations quantitatively. DFT simulations are very accurate but severely limited in size and time scales which prohibits, e.g., the simulation of fracture behavior. Therefore MD simulations with interatomic potentials are routinely used to asses those material conditions. The

Achilles' heel of MD simulations is the interatomic potential which describes the energies and forces of atomic systems. Most classic potentials fall short in quantitatively describing atomic systems, especially multi component alloys. Recent methodical developments resulted in so-called machine-learned (ML) interatomic potentials, where the analytical form is replaced by structural descriptors and a regression method to map from an atom in its environment to its energy contribution. These ML-based approaches are particularly promising for the description of alloys containing more than 2 elements. The research in this project will consist of fitting an ML interatomic potential on DFT data for Magnesium based alloys (e.g. Mg-Al-Ca), validating its material properties and assessing it using MD simulations of defects and fracture properties.

Study objective: The main objective of this project is to fit and assess a ML based interatomic potential for Magnesium based alloys. Pure Magnesium is brittle, it exhibits low ductility and low toughness. Alloying can markedly improve these properties which qualifies an alloy for real world use in fabrication with high fatigue resistance. The final potential will be used to predict component size mechanical behavior based on MD simulations of dislocations and fracture properties. These results are then used to mechanistically understand the role of alloying elements in improving the ductility of Magnesium to guide materials development.

Expected Results: Magnesium alloy interatomic potential; prediction of mechanical properties; publication of results in peer-reviewed journals; participation and presentation of results at international conferences

Methods: The methods used include density functional theory, ML-algorithms, MD simulations; computational infrastructure is available through powerful personal workstations at ICAMS and through access to a high performance computing cluster.

Candidate Requirements:

- An excellent Master's degree in Engineering or Materials Science with a computational focus
- Basic experience in programming, preferably (in order of importance): Python, C++
- A high level of spoken and written English (IELTS band score of 6.5 or higher)

Motivation for CSC application: The successful candidate will work at the Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), a central facility for Scale-Brigding Materials Modeling at Ruhr-University Bochum. She or he will have access to high performance computing facilities. He or she will benefit from existing collaborations and work groups of Prof. Stricker's group at RUB and with international collaboration partners. Most notably in the context of CSC is the possibility to have a second Phd supervisor from Zhejiang University (Chinese national) with extensive international experience. She or he further will participate in the ICAMS Graduate School for Scale-Bridging Materials Modeling which includes interdisciplinary lectures, a graduate seminar, and soft skill training such as scientific presentation and writing.