

## PhD Position in Computational Materials Science – Studying and Engineering of Defects

**Project description:** Engineering microstructures usually contain a huge number of planar defects such as grain boundaries (separating grains of different orientations) and phase boundaries (separating different thermodynamic phases). These defects can have great impacts on the properties and performance of the microstructure.

Due to their diverse properties then, structural defects could also open doors for some higher-level engineering approaches. In fact, “crystals are like people: it is the defects in them which tend to make them interesting!”, as Colin Humphreys said. A grain boundary, for instance, can be a weakening point for corrosion attack leading to failure of materials but also it can strengthen the materials by obstructing the motion of dislocations. Planar defects can be modified/engineered by adsorption of solute atoms (segregation), changing their chemical and mechanical properties. Upon segregation, and depending on their thermodynamic changes, defects can even mediate the formation of new, more interesting phases.

In this project, we explore computational methods for designing and engineering planar defects. The segregation behavior and phase stability at the planar defects will be studied using thermodynamic mean-field and phase-field modeling. Based on those pieces of knowledge, a tool will be developed to construct the phase diagrams of planar defects with direct application to microstructure design. The results of the project will contribute to the novel knowledge-based engineering of metallic materials with direct application to data-driven approaches.

**Profile:** The applicant should have a master’s degree in materials science, physics, physical chemistry, or a related field with relevant experiences. A background in computer programming, especially Linux-base experience, C++ programming, and Python programming, is required. The research will be conducted in English and therefore a strong command in written and spoken English is a must. Skills and understandings of thermodynamics and kinetics modeling of materials will be appreciated.

**Funding & contact:** The position is immediately open and closes as soon as filled. The PhD candidate will receive 3 years contract, full time, working in the Federal Institute for Materials Research and Testing ([www.bam.de](http://www.bam.de)) in Berlin. Please send your (i) letter of motivation/introduction (ii) CV, (iii) transcripts of bachelor and master studies, and (iv) the contact info of two references as **a single PDF** file to Dr. Reza Darvishi Kamachali [reza.kamachali@bam.de](mailto:reza.kamachali@bam.de). We are an equal opportunity employer. Please note that only complete applications will be considered.