TECHNISCHE UNIVERSITÄT DRESDEN

DRESDEN concept

Faculty of Mathematics

At the **Institute of Scientific Computing (IWR)** and within the framework of the **Dresden Center for Computational Materials Science (DCMS),** in the newly established interdisciplinary **Mesoscale Material Modeling Group,** two positions as

Research Associate / PhD Student
(Subject to personal qualification employees are remunerated according to salary group E 13 TV-L)

are offered, with 75% to 100% of the full-time weekly hours starting preferably on **March 1, 2021** for a total duration of 3 years. Extensions or variations of the total weekly hours may be considered. The period of employment is governed by the Fixed Term Research Contracts Act (WissZeitVG). The position offers the chance to obtain further academic qualifications (e.g. PhD).

The position is framed within the project entitled "*A mesoscale framework for the modeling of defects and interfaces in crystals*", funded by the German Research Foundation (DFG - Emmy Noether Programme) and headed by Dr. Marco Salvalaglio. This project addresses the mesoscale modeling of crystalline systems. It builds on the phase-field crystal (PFC) model and its amplitude expansion (APFC), which provide convenient coarse-grained descriptions of crystalline structures. It aims at i) delivering novel theoretical tools that bridge micro- and macroscopic features while studying crystals accounting for real material properties, ii) overcoming limitations of current state-of-the-art theoretical approaches in this field through new and hybrid approaches, iii) enabling applications to technology-relevant crystalline systems and related open problems in materials science.

Collaborations with internationally renowned researchers in the field are planned. Exchanges and short research stays abroad may be arranged. Within the DCMS framework, the PhD student will also have the possibility to choose the main subject for her/his PhD (within compatible ones). The activity will be mostly based at IWR, TU-Dresden. This university is among the top universities in Germany and Europe and one of the eleven German "University of Excellence". Moreover, Dresden is one of the most beautiful towns in Germany and evolved in recent years to both an internationally recognized scientific center and a renowned tourist destination. It uniquely combines an outstanding scientific environment, a vivid cultural scene, wonderful nature and affordable costs of living.

Figure: APFC simulation of the growth of a polycrystal *npj Comput. Materials 5, 48 (2019)*

Tasks: **i)** Development of phase-field and phase-field crystal models for studying crystal properties (and complementary methods for selected comparisons); **ii)** Data analysis and quantitative comparison with experiments; **iii)** Implementation of models in computer codes for numerical simulations, in particular exploiting the software environment AMDiS/DUNE; **iv)** Conduct numerical studies, also on HPC facilities. Further specific tasks may be tailored to the attitude and interest of the Ph.D. student.

Requirements: **i)** university degree in Mathematics, Physics, Materials Sciences or related subjects (Master). **ii)** Basic knowledge in computer programming (e.g. Python, Matlab, C++). **iii)** Excellent knowledge of the English language; **iv)** High problem solving ability, motivation/interest in scientific
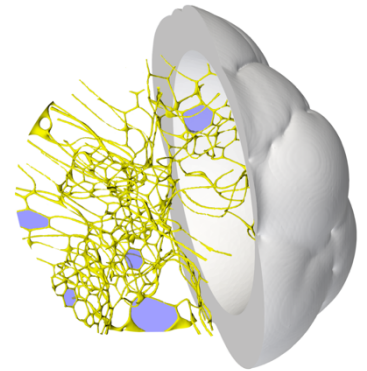
research, willingness to learn, propensity to work in group. Previous experience in numerical methods / simulations and/or theoretical material modelling will be considered preferentially.

Applications from women are particularly welcome. The same applies to people with disabilities. Please send your application including a motivation letter, CV, a letter of recommendation, and university certificates (i.e., list of coursework with grades) preferably via the TU Dresden SecureMail Portal https://securemail.tu-dresden.de by sending it as a single pdf document to **marco.salvalaglio@tu-dresden.de or to TU Dresden, Fakultät Mathematik, Institut für Wissenschaftliches Rechnen, z. Hdn. Herrn Dr. Marco Salvalaglio, Helmholtzstr. 10, 01069 Dresden**. The application deadline is **February 2, 2021** (stamped arrival date of the university central mail service applies). Please submit copies only, as your application will not be returned to you. Expenses incurred in attending interviews cannot be reimbursed.