Paul-Drude-Institut für Festkörperelektronik

Master Thesis Topic

Elastic strain fields of dislocation and dislocation networks as derived by numerical extended FEM (XFEM) and analytical tools

Background and Motivation:
The strain field by a single dislocation can be calculated based on text-book knowledge, however, more complex arrangements usually require numerical approaches. Numerical extended finite element methods (XFEM) may serve as a versatile tool to consider highly realistic geometries and full elastic anisotropy (particularly in 2D layered materials or materials with low crystal symmetry or high anisotropy). A detailed knowledge of the resulting strain landscape contributes to a better understanding of the elastic properties and potentially provides the key to drive plastic relaxation pathway.

Objectives:
Creating XFEM cases for single and multiple dislocation arrangements in various crystallographic systems (e.g., isotropic, cubic and trigonal) and compare results to analytical calculations.

Methodology:
- Making familiar with FEM simulation package (which offers many-fold applications of static and dynamic processes otherwise unable to treat analytically)
- Finding suitable boundary conditions and model dimensions
- Getting knowledge on the strain-stress relation

Skills and Requirements:
- Background in semiconductor physics, materials science, or related fields.
- Experience in numerical data treatment as e.g. python but not necessarily Finite Element code

Opportunities and Benefits:
- Modern computational infrastructure
- Supportive environment with experts for various scientific sub-fields
- International and culturally diverse community
- Location in the heart of Berlin with excellent public transport connections
- Subsidized travel ticket

Contact:
Dr. habil. Michael Hanke
+49 30 20377-287
hanke@pdi-berlin.de