Master thesis

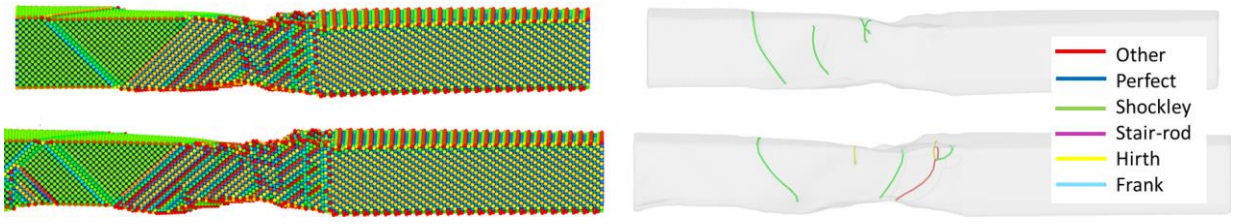
Division of Mechanics

Lattice dislocation density influence on properties in tungsten modelled by MD simulations

Master theses 30hp

The European Spallation Source (ESS) will be the world's brightest neutron source facility, and is presently under construction in Lund, Sweden. The target material providing neutrons is pure tungsten. Tungsten is a metal with high strength and has the highest melting point of all metals. However, its low ductility and a high ductile to-brittle transition temperature are of concern. By the irradiation of the tungsten target, different lattice defects and dislocation structures are induced. The proposed project aims at determining the impact of the lattice dislocation density on the tensile behavior and the thermal conductivity, properties that presumably also are temperature dependent. Therefore. different temperatures, mimicking different post-irradiation annealing temperatures, will be studied.

Simulations of structures at the atomic scale is a new and very attractive research topic since many material properties that we observe on the macroscale changes as the geometrical dimensions decreases to the nanoscale. A commonly used numerical method to extract and understand such phenomena at the nanoscale is molecular dynamics (MD) modelling, which will be employed in this project using the free software. LAMMPS is a classical MD code and an acronym for Large-scale Atomic/Molecular Massively Parallel Simulator. It integrates the Newton's equations of motions for collections of atoms that interact via short- and long-ranged forces, and allows for a variety of initial and boundary conditions.



The work is suitable for 2 students and can start in January 2021.

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