Master thesis

# Division of Mechanics

## Electro-magnetic field influence on the mechanical properties of nanosized crystal structures modelled by MD simulations

## Master theses 30hp

Simulations of structures at the nanoscale is a new and very attractive research topic, since many mechanical properties of materials that we observe on the macroscale changes as the geometrical dimensions decreases to the nanoscale. A commonly used numerical method to extracted and understand the mechanical behavior at the nanoscale is molecular dynamics (MD). It is well known phenomena that an electro-magnetic field influences the deformation of nanosized crystal structures. The goal of this project is to develop a simulation model of a nanobeam under influence from an electro-magnetic field and extract mechanical properties changes and deformation patterns. The software LAMMPS will be used for the simulations. LAMMPS is a classical molecular dynamics code and an acronym for Large-scale Atomic/Molecular Massively Parallel Simulator. It integrates Newton's equations of motions for collections of atoms that interact via short- or long-range forces with a variety of initial and/or boundary conditions.

**Contact:** Prof. Aylin Ahadi, Division of Mechanics, aylin.ahadi@mek.lth.se