MathSys MSc project call 2020/21

Title: Atomistic modelling of magnetic shape-memory alloys

Supervisors: Dr. Mikhail Poluektov, Dr. Łukasz Figiel

Description:

Magnetic shape-memory properties arise from the coupled magneto-mechanical response: mechanical loading leads to a change of material magnetisation, while application of magnetic field leads to large material deformation. Alloys that possess such properties display interesting functional characteristics and have a great potential for applications in sensors and actuators. This project aims at creating a simple mathematical model describing behaviour of such alloys at the atomistic scale.

These alloys have a specific crystal structure, the basic structural unit of which is tetragonal (in simpler terms, it has a shape of a rectangular prism). The spin magnetic moments of the atoms are usually aligned parallel to the short axis of the unit cell. The atomistic crystal structure consists of various phases, each having a different spatial orientation of the basic unit cell. These phases are separated by twin interfaces (also called twin boundaries or phase boundaries), as illustrated in Figure 1. Upon application of mechanical forces or external magnetic field, these twin interfaces move, which leads to reorientation of the unit cells and consequently to material deformation.

To model the behaviour of these materials at the atomistic scale, the magnetic degrees of freedom (atomistic spins) must be correctly coupled to mechanical degrees of freedom (atomistic positions). Furthermore, the coupled magneto-mechanical effects must be modelled over a large range of mechanical deformations, which is non-linear. The model itself is represented by a system of highly non-linear ODEs describing the dynamics of atomistic positions and spins. This is an active area of research and this project aims at considering a specific magneto-mechanical coupling energy term and investigating it computationally. The major activities will involve implementation of the model in MATLAB for a 2D crystal and numerical simulation of the kinetics of the twin interfaces.

This project offers numerous avenues for the follow-up PhD research related to multiscale modelling of magnetic shape-memory alloys. Particularly, at the atomistic scale, there are other energy terms, which will not be considered within this project due to time limitations, but which also play an important role in material behaviour. Furthermore, the correspondence of the atomistic models to the continuum models (represented by PDEs) can be researched and possibly multiscale models can be constructed. Finally, specific simulations at the electronic structure scale (*ab initio* simulations) can be used to inform the atomistic models to describe the shape-memory effect in the most precise way.

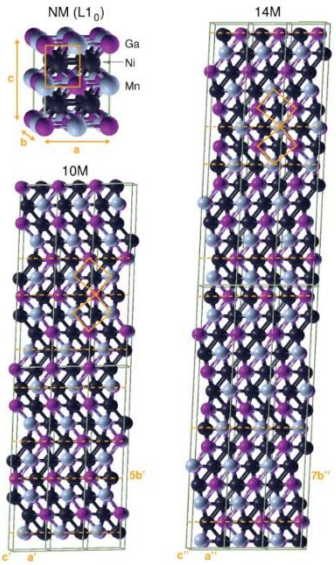

Figure 1: Visualisation of the martensitic crystal structure of Ni_2MnGa ferromagnetic shape memory alloy. The basic building block of these crystals is the tetragonal unit cell, shown in orange squares. The dashed lines indicate the atomically-sharp twin interfaces between differently-oriented unit cells. Image is taken from (Niemann *et al.*, 2012, *Adv. Eng. Mater* 14(8):562-581).