Bachelor / Master - Thesis

Computation of material properties using Density Functional Theory

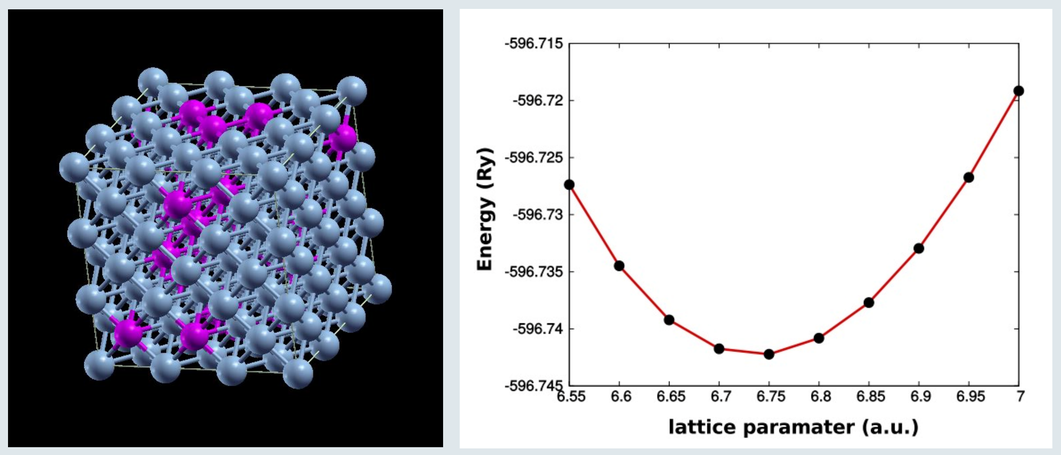
Helmholtz-Zentrum Hereon, Institute of Materials Mechanics, Solid State Materials Processing (WMP)

Introduction

The ICME (Integrated Computational Materials Engineering) approach partially involves model development for various materials phenomena namely phase transformation, crack propagation, dislocation dynamics, corrosion, etc. The synergy between the multi-scale simulation models and performance analysis is responsible for the effectiveness of ICME. Within this framework, it is possible to cover a wide spectrum of length and time scales by employing suitable methods for the purpose. Starting from ab-initio methods at electron level, molecular dynamics and kinetic Monte Carlo methods at the nano level, phase-field method, and crystal plasticity at the micro and mesoscale to macroscale process modelling simulations; the multi-scale approach has a lot to explore.

The aim of this work is to determine the material properties such as lattice parameter, elastic constants, interfacial energy etc. using ab-initio calculations similar to Figure 1. The computed values serve as input to various mesoscale models designed for microstructure evolution as shown in Figure 2. An opportunity to establish the thermal dependence of material properties also exists within the scope of the work. The computations would majorly use Density Functional Theory to predict the properties. The specific alloys that are of interest here are the Al-rich binary and ternary systems.

The place of employment would be Helmholtz-Zentrum Hereon located in Geesthacht.



Material crystal structure — Energy calculations for computing properties

Figure 1: Illustration of a sample material crystal structure and corresponding energy calculations leading to property prediction through DFT.

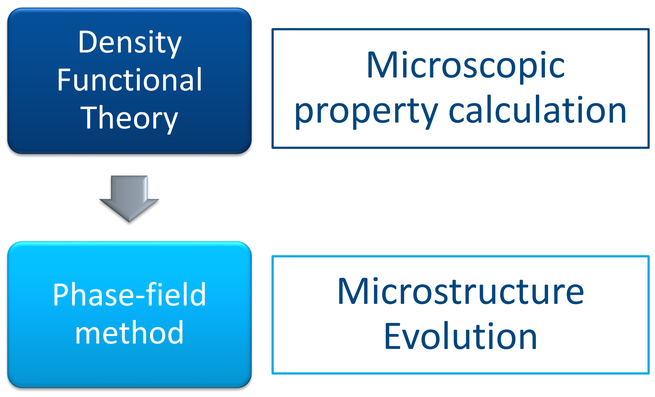


Figure 2: Schematic showing a simplified hierarchical portrayal of various modelling approaches. The present work deals with the first step of the flowchart.

Tasks

- Comprehensive literature research on the Al alloy system, Density Functional Theory, elastic constants prediction using DFT, and finite temperature DFT.
- Design of various shell scripts and input files required for the computations.
- Energy calculation and subsequent estimation of properties using DFT.
- Presentation of results and documentation of the work (in English).

Expectations

- Adequate grasp of crystal structure, and aluminium alloy systems in general.
- Basic knowledge of Density Functional Theory.
- Familiarity in working with linux, shell scripting is advantageous.
- Willingness to learn new software, skills and punctually deliver as per the project requirement.

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