



Offer for a diploma/master thesis or a research project

Machine learning assisted ab-initio studies of alloys

Motivation: The objective of this project is the identification and application-tailored design of alloys which optimally match mechanical and thermodynamic requirements, bearing the potential to outperform known materials and open new perspectives for target advanced applications. Nanoscale phenomena such as quantum mechanical binding between atoms dictate the mechanical and thermodynamical properties.

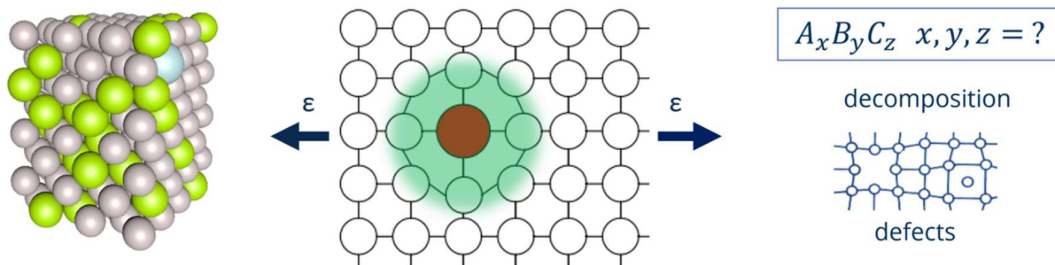


Fig. 1: Alloying elements lead to local strain fields and the overall properties depend on the composition and other effects (like defects, stacking faults etc.)

Goals of the project: Investigation of alloys with first-principle methods, either Density Functional Theory (DFT), Molecular Dynamics (MD), or both. The length scale of the systems is depicted above. The properties of the metal depend e.g. on concentration of alloying elements, local configurations, phase precipitation, temperature. Due to the huge phase space, machine learning methods (e.g. neural networks, kernel regression) will help to accelerate the calculations. A thesis project can go into different directions depending on personal interest and skills. Possible tasks are:

- Thermoelastic properties (DFT and Quasiharmonic Approximation)
- Thermodynamic stability (DFT, MD, phase diagrams)
- Di/par-elastic and chemical locking mechanism in solid solutions (DFT, MD)
- Elastic and plastic properties from stress-strain curves (DFT, MD)
- Machine learning interatomic potentials for molecular dynamics of alloys (DFT, MD)
- Solidification curves, precipitation, heating- and cooling processes of alloys (MD)
- Inverse Design methods (linkage from DFT/MD properties to structure)

Prerequisites are the following completed subjects or modules:

Some knowledge of quantum mechanics, classical mechanics, thermodynamics is an advantage. Interest in computer-based simulations and programming.

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