Master Thesis: Machine-Learning Algorithms for Simulating Grain Boundary Segregation in Alloys

Reference No.: MCL_233

Materials Center Leoben (MCL) supports numerous companies in the production sector developing high-performance materials, manufacturing processes and products. MCL designs specific computer-aided technologies in order to accelerate innovation processes in manufacturing companies as well as to support the digitalization of the value chain and products. Our portfolio includes cooperative research and development projects with international and national partners from the production and research sectors as well as several consulting, laboratory and simulation services in materials science.
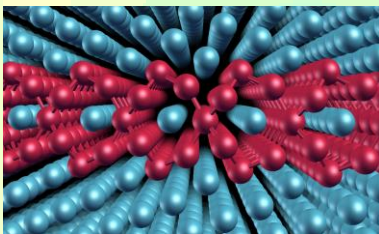
Machine-Learning potentials for Grain Boundaries

These topics inspire you or you are already familiar with them?
Then you are the right person for this position!

What are we looking for….

A motivated master student from materials science, physics, or computational sciences (e.g., computational mechanics, applied mathematics) with one (or more ☺) of the following skills

- crystallography/atomic-scale mechanics,
- atomistic simulation,
- linear algebra/machine-Learning methods,
- programming (Python, C++).

Your challenge…

In this work, you will study grain boundaries—planar defects which influence and determine many mechanical properties of alloys. More precisely, your challenge is to

- develop an algorithm for training machine-learning potentials on grain boundaries,
- develop a Monte-Carlo algorithm for simulating grain boundary segregation as a function of the composition of the alloy,
- develop a machine-learning model that efficiently predicts segregation energies over the whole alloys space.

The precise tasks may depend on your background and personal preferences.

Our offer

An employment with immediate start and a gross salary of € 3.000,- for six months.

Please send your complete application documents by email.
We are looking forward to knowing you!

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We innovate Materials