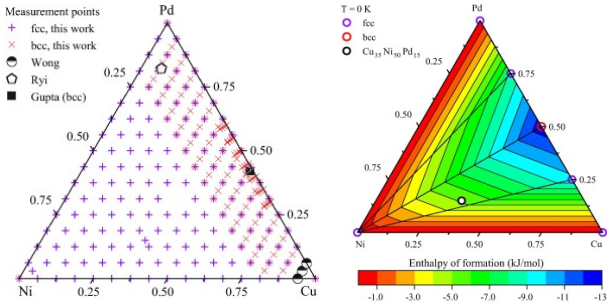
DFT SIMULATIONS OF ALUMINIUM ALLOYS



MOTIVATION:

In studies of light metal alloys there are challenges when it comes to establishing relations between the nano-structure and the mechanical properties, as for example strength and ductility. In Al-Mg-Si/Ge-(Cu) alloys, which are industrially relevant due to their superior mechanical properties (high strength / weight ratio and good corrosion properties), the hardness increase is due to precipitation of nanometre-sized metastable phases that form from solid solution during heat treatment. The goal of our group is to develop a computational platform for studying Al-based alloys at atomistic level and with high accuracy (DFT level) which will enable efficient simulations and investigations of different intermetallic compositions. The proposed MSc work is part of this larger scheme.

WHAT THE STUDENT WILL DO IN THE PROJECT:

The student will perform benchmark DFT simulations for Al-based alloys which will be used for training the Cluster Expansion (CE) method for interatomic interactions. In addition, the student will perform migration path mapping (by DFT) for selected atomic transitions. The obtained information (energetics, migration barriers) will be fed into kinetic Monte Carlo (KMC) simulations. The DFT simulations will be performed on local supercomputers using an existing code (GPAW). Input to the simulations will come from close collaboration with other researchers and students working experimentally with transmission electron microscopy.

REQUIRED FROM THE STUDENT:

Background in materials physics (solid state physics), and interest in materials science would be an advantage. We need a student interested in modelling and programming, and working independently in a larger group of scientists. An interest in using and developing simulation tools is required. Experience with C++ or Python is essential.

OTHER ASPECTS:

There are many people working on aluminium alloys at NTNU, and we have several ongoing external projects, including two Centres of innovation (CASA and SFI Manufacturing) where we work in close collaboration with SINTEF, Hydro and other companies producing aluminium products. A few of the companies involved are, in addition to Hydro Aluminium, Benteler Automotive, Steertec, Neuman Aluminium, Nexans, SAPA and Gränges. See the video made in CASA here! The students will participate in project meetings in these consortiums in Trondheim or/and at industry sites. Students get their own problem which fits well into the rest of the work done. Within this field there are possibilities for continuation as a PhD student and summer job. This topic is closely related with another project where these alloys are modelled by kinetic Monte Carlo (see the announcement by TEM Gemini Centre). As part of the initial DFT training, a visit at the Tampere University of Technology and/or Aalto University in Finland is likely.

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