Brief report on the research stay at UC Berkeley

I visited the group of Prof. Mark Asta in UC Berkeley from 10.04.2016 to 10.07.2016 under the DFG priority programme SPP-1713. The aim of SPP-1713 programme is to understand the mechano-chemical coupling during the precipitate formation in Al-based alloys. This understanding requires an investigation of the elasticity effects onto the chemical composition and morphology of the precipitates during their temporal evolution. As particles precipitate out starting from a solid solution, the strain field around the precipitates grow owing to the particle-matrix lattice mismatch which in turn affects their chemistry.

The basic idea to understand this coupling phenomena during the precipitate formation is to incorporate the elasticity and chemical effects within the kinetic Monte Carlo simulations. Prof. Asta's group developed a hybrid scheme on the similar lines to estimate the coherent phase boundaries for a Ti-O system where they used cluster expansion to consider the local chemical effects and the Khachaturian's microscopic elasticity theory (MET) to calculate the elastic strain energy. To learn and test the applicability of this hybrid scheme to the Al-Sc system was the main goal of my UCB visit.

The underlying assumption of MET is the linear concentration dependence of the lattice parameter. In the dilute solid solution limit (Sc being the solute in Al matrix), we observed a near perfect linear trend (cf. Fig. 1) but in the limit of precipitate phase (Al_3Sc – 25 % Sc), we observed a huge deviation of the calculated precipitate lattice parameter (4.103 Å) from linearity. This deviation rendered MET inapplicable for studying the mechano-chemical coupling during the precipitate growth in Al-Sc system.

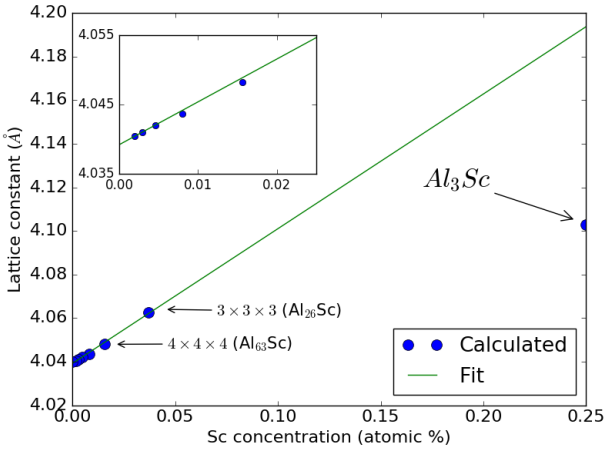

Figure 1: (Main): Variation of the lattice parameter of Al-Sc system with the Sc concentration. The points are the calculated lattice parameter and the green line is the linear fit. (Inset): Zoom for low Sc concentration.

We decided to use an alternative approach of including the elasticity effects via embedded atom method (EAM) since the EAM potentials are typically fitted to elastic constants. To include the short and medium range interactions and the local chemical effects, we opted to perform a cluster expansion (CE) on the difference of EAM and density functional theory (DFT) energies which would then be applied as a correction term to the EAM energy for the short and medium range interactions.

As a starting point, I learned how to perform the CE using ATAT code for which Prof. Asta's group has an expertise. I then learned how to perform total energy calculations using EAM-based code LAMMPS. The next step is to perform kMC simulations combining LAMMPS and ATAT with the kMC code in order to atomistically derive the TTT-diagrams fully accounting for the strain and chemical effects. This is still ongoing work and the collaboration with Prof. Asta will continue during the course of this work.

– Ankit Gupta