Phase diagrams computation using the ATAT[1]

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Theoretical determination of phase diagrams of metallic substances is very important in both technological and scientific point of views. In this project, phase diagrams computation using a toolbox ATAT (Alloy Theoretic Automated Toolkit) is carried out to show the practical implementation of first-principles. Two main procedures are included to obtain the phase diagram for a binary alloy system. First, corresponding energy is calculated for each configuration using first principle code. Since computation of phase diagram requires computation of the energy of system with thousands of atom, cluster expansion is implemented to predict the energy for each configuration and further to predict the ground state configuration. Second, Monte-Carlo simulation is performed to compute phase boundaries which sample from a semi-grand-canonical ensemble. Given a target precision, the equilibration time and averaging time are two parameters used to control the calculation of thermodynamic quantity through the MC simulation. Computation results for different systems using ATAT will be compared with the phase diagram from the literature.

References

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[1] MAE715 Final Project Presentation, Spring 2009