Assignment 2: Mini-Project

Effect of alloying and temperature on fault energies

MM309, MEMS, IIT Indore

Deadline: 4th November

1 Objective

To study the effect of alloying and temperature on the lattice parameters and stacking fault energies (SFEs) of ternary alloys using atomistic simulations and the Diffuse Multi-layer Fault (DMLF) model.

2 Assigned Alloy Systems

Alloy System	T_1 (K)	T_2 (K)	T_3 (K)	Group
Al–Co–Cr	100	550	350	1
Al–Co–Fe	400	200	650	2
Al–Co–Ni	150	500	300	3
Al–Cr–Fe	450	250	600	4
Al–Cr–Ni	100	550	350	5
Al–Fe–Ni	400	200	650	6
Cu–Fe–Ni	150	500	300	7
Al–Mn–Pd	450	250	600	8
Co–Cr–Fe	150	500	300	9
Co–Cr–Ni	450	250	600	10
Co–Fe–Ni	100	550	350	11
Cr–Fe–Ni	400	200	650	12

Each group will consist of four students. Each student must submit their own report.

3 Tasks Overview

3.1 Download Potentials

Download the required interatomic potentials from the NIST Interatomic Potentials Repository: `https://www.ctcms.nist.gov/potentials/`. Choose suitable EAM or MEAM potentials and benchmark them against literature data for pure elements (lattice parameters, cohesive energies).

3.2 Build Supercells

Construct FCC, HCP, and DHCP structures for all compositions. Ensure:

- Comparable/similar box dimensions in all directions.
- Orientation may be along non-conventional axes. dont pick supercells elongated in one direction (e.g. needle, rod shaped as discussed in the class)
- Supercell large enough to minimize periodic boundary effects.

3.3 Simulation Details

Test potentials before you proceed, Use suitable ensembles. Collect averages over sufficiently long trajectories/time steps. Normalize the energies with respect to the system size.

3.4 Estimate Stacking Fault Energies

Compute Intrinsic (γ_{ISF}), Extrinsic (γ_{ESF}), and Twin (γ_{Twin}) SFEs using the DMLF model:
`Refer the publication: M.A. Charpagne, K.V. Vamsi, Y.M. Eggeler, S.P. Murray, C. Frey, S.K. Kolli, T.M. Pollock, Design of Nickel-Cobalt-Ruthenium multi-principal element alloys, Acta Materialia, Volume 194, (2020), Pages 224-235.`

$$\gamma_{\text{ISF}} = \frac{4(E_{\text{dhcp}} - E_{\text{fcc}})}{A_{\text{fcc}}}, \tag{1}$$

$$\gamma_{\text{ESF}} = \frac{E_{\text{hcp}} + 2E_{\text{dhcp}} - 3E_{\text{fcc}}}{A_{\text{fcc}}}, \tag{2}$$

$$\gamma_{\text{Twin}} = \frac{2(E_{\text{dhcp}} - E_{\text{fcc}})}{A_{\text{fcc}}}. \tag{3}$$

3.5 Analyze Results

Discuss the effect of alloying and temperature. Compare the performance of different models and benchmark results with literature.

4 Report Structure (template has to be followed.)

4.1 Introduction / Background

Provide a short background on stacking fault energy (SFE),types, alloy systems assigned, its relevance, and the influence of alloying and temperature. Present a brief literature review. State your objectives clearly. Write down and explain the models/equations used (with references).

4.2 Simulation Methodology and Details

Describe the computational setup and parameters. Specify the potential used. Mention ensembles (NVT, NPT, etc.) and integration schemes. Discuss equilibration and the averaging scheme. List tools used for visualization and analysis. Justify all your choices. Provide sufficient details so that the results can be reproducible.

4.3 Results and Discussion

First benchmark against literature values . Present the main findings. Discuss the effect of alloying and temperature on SFEs. Compare results from DMLF models with other models (Axial Ising models, which you will learn about in class soon). Discuss physical interpretation, limitations, and implications.

4.4 Conclusions

Provide concise takeaways and insights. Summarize how your results improve understanding of SFEs.

4.5 References

Use a consistent referencing style (e.g., `bibtex`) and cite: Original interatomic potential sources, Model references, Key literature on SFEs of alloys from your system.

5 Figures and Data

- Use `mpltern` for ternary plots: `https://mpltern.readthedocs.io/en/latest/index.html`
- Use `matplotlib` for other plots: `https://matplotlib.org/`
- Include units (e.g., eV/atom, J/m^2) and label axes clearly.
- Show error bars where appropriate.

6 Submission Details

- **Deadline:** 4th November
- Each student submit the assignment individually (Google Classroom).
- Folder name: `GroupX_YourName_Assignment2.zip`
- Include:
  - `Report.pdf` (LaTeX-generated)
  - Simulation scripts and input files
  - Results and figures
  - `README.txt` describing workflow

Discussions are encouraged, but **copying will result in penalties.**
All students must understand their own codes and methods, results and analysis as there can be a **viva** on the project :)

Goodluck!!