ENGR 561/861 ICME Homework #1: Bridging Density Functional Theory to Atomistics

Objectives

In this homework, you will bridge information from the electronic scale to the nanoscale by calibrating a MEAM potential to specific DFT data. MEAM potentials can be calibrated with a number of physical quantities, however by downscaling your end goal of modeling the plastic behavior of our material, you can narrow it down to two very important quantities, the energy-volume (EV) curves and the generalized stacking fault energy (GSFE) curve. You can use other quantities to validate your potential.

Target Materials: choose either Al (FCC) or iron (BCC)

For more details, see the assignment on the ICME website: https://icme.hpc.msstate.edu/

Due date: March 11, 2022.

Deliverables

- Write a report that follows a journal article manuscript format (include figures and tables in the text) for your computational study following guidelines mentioned in Details.

Details

DFT Calculations – E-V Curve

1. Plot energy (E) vs. volume (V) and energy (E) vs. atomic separation (A) curves for your material in its reference crystal structure.
2. For your material's reference crystal structure, perform a KPOINT convergence study. Choose the KPOINT grid that reaches a converged solution (think of this as a mesh refinement).
    a. Plot lattice parameter vs. KPOINT grid
    b. Plot bulk modulus vs. KPOINT grid
    c. Plot cpu time vs. KPOINT grid
    d. You should also insure that your results are converged with respect to the energy cutoff (ecutwfc). Note that the energy cutoff value is in Rydberg (Ry), rather than eV.
3. Derive the equilibrium lattice constant, bulk modulus, and cohesive energy using the four equations of state (EOS).
4. Come up with final converged KPOINT grid and plot final E-V and E-A curves.
5. Provide a final set of values using the converged KPOINT and EOS of your choice. This data will be used for calibrating the MEAM potential.

DFT Calculations – GSFE Curve

1. Produce a GSFE curve for your material.
    a. Take care with the slip system and direction you use! You will need to know this when fitting your MEAM potential. (For FCC, typically look at the Shockley partial curve, {111}<112>; for BCC, use {110}<111>)
    b. Use the converged KPOINT and energy cutoff values obtained from the previous section.
2. Report your results.
    a. Plot the change in energy vs. upper atom displacement.
    b. Copy final GSFE curve(s) to your group folder.

MEAM Parameter Calibration

1. Using the MEAM Potential Calibration (MPC) routine determine the MEAM constants by comparing the energy versus atomic separation (E-A) plots from DFT and LAMMPS:
    a. Using DFT results set alat, esub, and bulk
    b. Calibrate the MEAM constants to single crystal elastic moduli found in the literature
    c. Calibrate the MEAM parameters to the GSFE curve obtained from DFT using Cmin, asub, b1, and b3
    d. Plot a comparison of the E-A for the different cases on one plot
    e. Plot a comparison of the GSFE from DFT and GSFE from MPC
2. Conduct a validation check by comparing one of the MEAM calculations available in MPC to a literature value.
3. Sensitivity analysis
    a. Vary several of the parameters (one at a time) up to 50% to show the sensitivity of the parameters on the E-A curve and GSFE curve
    b. Plot the comparisons for E-A and GSFE curves for the different cases on one plot each (one containing the E-A sensitivities and one containing the GSFE sensitivities)
4. Report your results
    a. Place a screenshot of the final fitting routine and parameters in your group folder

Report on your results (upload your report (in a journal article format) and used simulation input on TEAMS).