

PROBLEM A – Nanowire mechanics

For this problem, we use the ITAP IMD code, suitable for modeling metallic systems with the EAM potential or a LJ potential. The ITAP IMD code is made accessible via the GenePattern website at:

<http://starapp.mit.edu:8083/gp/index.jsp>

It is recommended to take a look at the supplementary material in the section “Final project assignment: Part A - Nanowire Mechanics” – in particular the tutorials that provide details about how to run the various codes.

If necessary, you may find additional information regarding the ITAP IMD code at the website:

<http://www.itap.physik.uni-stuttgart.de/~imd/>

including instructions and a manual.

Visualization: You may use the program “vmd” (download at <http://www.ks.uiuc.edu/Research/vmd/>) to visualize the resulting “.xyz” files. “vmd” is available free of charge.

The GenePattern website also produces .png files that you can view immediately in your browser. However, it is recommended to use VMD for the final report and analysis of the results.

A.1 Unit cells and crystallographic orientations, MD units

The first step in understanding the relationship between atomistic structure and its elastic properties is to consider the crystal structure. Here we focus on single FCC crystals of copper composed out of a repeating sequence of unit cells defining the crystal structure.

Copper has a FCC lattice constant of $a = 3.615 \text{ \AA}$.

Assume that all lengths in the atomistic model are given in Angstrom ($1 \text{ \AA} = 1\text{E-}10 \text{ m}$).

1. Define and draw the atomic coordinates in Angstrom in proper unit cells for different crystallographic orientations of a FCC crystal of copper: [100][010][001] (cubical) orientation.
2. Calculate the atomic volume and mass density of copper (defined as mass per volume), based on this atomic model of a perfect crystal.
3. Calculate the units of temperature and pressure (or equivalently, the stress) in terms of the reference units used in the code.
Note that the reference length $l^* = 1\text{\AA} = 1\text{E-}10 \text{ m}$, the reference energy $E^* = 1 \text{ eV}$ and the reference mass $m^* = 1 \text{ amu}$. All output in IMD is in these units.

A.2 Elastic properties of crystals modeled using a LJ pair potential

Pair potentials are one of the simplest potentials to describe the atomic interaction of crystalline materials.

Here we derive parameters for a simple 12:6 Lennard-Jones pair potential for FCC copper to fit experimental values of elastic properties of copper.

1. Assuming a 12:6 Lennard-Jones potential (see lecture notes), derive an expression for the equilibrium position between pairs of atoms (nearest neighbor interactions). Express the LJ length parameter σ as a function of the lattice parameter a .
2. Derive an expression for the minimum potential well of the LJ potential, corresponding to the cohesive energy stored in each bond.
3. Develop a Taylor series expansion of the LJ potential, considering up to second order terms, developed around the equilibrium distance between two atoms, denoted by r_0 . Denote the second derivative of the potential by the parameter $\phi'' = k$.
4. The next step is to determine a set of parameters of the Lennard-Jones (LJ) potential that closely resemble experimental properties of copper. Determine numerical parameters for σ and ϵ based on experimental values for the lattice constant and bulk modulus of copper. Consider only nearest neighbor interactions. Compare the resulting values with the LJ copper potential reported by Cleri and coworkers [1].

Discuss possible disagreement in light of the potential formulation and potential range.

Hint: Take advantage of the following relations – valid for nearest neighbor interactions; shear modulus $\mu = r_0^2 k / 2V$, Young's modulus is $E = 8/3\mu$, and the bulk modulus $K = E / (3(1 - 2\nu))$ where $\nu = 1/4$, and $V = a_0^3 / 4$. The final result is $K = 64\epsilon / \sigma^3$.

Write an expression for K as a function of relevant potential parameters, then determine the unknowns.

5. Using the web based code suitable for calculating elastic properties (Pipeline→IMDElastic), calculate the elastic properties of copper by plotting the stress tensor coefficients σ_{11} , σ_{22} and σ_{33} using (i) the LJ potential with the LJ parameters developed above.

Note: Consider only nearest neighbor interactions by choosing a proper cutoff radius, maybe 10..20% larger than the nearest neighbor distance $a / \sqrt{2}$) and (ii) using Cleri's potential (larger cutoff radius) [1]. Consider equitriaxial strain loading (corresponding to the bulk modulus K).

Calculate the critical strain when the crystal becomes unstable, *i.e.* when the slope of the stress-strain plot approaches zero.

Hint: Look at “engPlot.png” that plots the stress in the three spatial directions.

A.3 Fracture and deformation of a copper nanowire using an EAM potential

Now we focus on fracture and deformation of a copper nanowires [2, 3]. Nanowires may play a critical role in future electronic devices, serving various needs including interconnects, waveguides or mechanical sensors. Due to the inherently small dimensions, classical, continuum descriptions are questionable and molecular modeling becomes the most reliable modeling tool to understand the mechanics of these materials.

Use the web based MD code that uses an EAM potential to model the atomic interactions. As discussed in class, the EAM potential provides a more accurate representation of the chemical bonding in metals than a simple LJ pair potential.

1. Use the web based program to build and model tensile deformation of a copper nanowire (Pipelines→IMDNanowire). Choose dimensions of approximately 20 Å and 260 Å (8x8x60 unit cells).
Model approximately 10,000 integration steps, or until you see significant deformation of the crystal. Use a displacement rate of 0.05 Å per 20 integration steps at the boundaries as a starting value.
Note: Apply the load in the z-direction, the axial direction of the nanowire.
2. Take snapshots of the system as it undergoes deformation and include them in your report for this problem set.
3. Discuss the observed deformation mechanisms. What atomic mechanisms are responsible for deformation?
4. Plot the components of the stress tensor as the applied strain increases, and indicate what regime of deformation corresponds to which snapshot you have shown in 3.
Compare these with the results obtained earlier for the perfect crystal.
How can the differences be explained?
5. Estimate Young's modulus for the nanowire, considering small deformation.
Compare with Young's modulus of copper known from macroscopic tensile tests.
6. Double the dimensions of the nanowire in the cross-section. How does the deformation mechanics and stress-strain response change? Explain differences, if any.
7. Briefly describe the deformation mechanics under compression (select one geometry and perform a simulation under compressive loading).

Constants and units

$$k_B = 1.3806503E-23 \text{ J/K}$$

$$1 \text{ eV} = 1.60217646E-19 \text{ J}$$

$$1 \text{ amu} = 1.660538E-27 \text{ kg}$$

A.4 References

1. Cleri, F., et al., *Atomic-scale mechanism of crack-tip plasticity: Dislocation nucleation and crack-tip shielding*. Phys. Rev. Lett, 1997. **79**: p. 1309-1312.
2. Heino, P., H. Häkkinen, and K. Kaski, *Molecular-dynamics study of mechanical properties of copper*. Europhysics Letters, 1998. **41**: p. 273-278.
3. Komanduri, R., N. Chandrasekaran, and L.M. Raff, *Molecular dynamics (MD) simulations of uniaxial tension of some single-crystal cubic metals at nanolevel*. Int. J. Mech. Sciences, 2001. **43**: p. 2237-2260.

These papers are included on the Project section.