

IAP 2006: From nano to macro: Introduction to atomistic modeling techniques and application in a case study of modeling fracture of copper (1.978 PDF)

<http://web.mit.edu/mbuehler/www/Teaching/IAP2006/intro.htm>

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Problem set

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We will be using the ITAP IMD molecular dynamics code.

Please see:

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

for instructions and a manual. Compiled versions of the code are provided.

When you compile the code please make sure that the IMDSYS variable is set correctly:

```
setenv IMDSYS ia32-gcc2
```

For the EAM potential:

```
imd_nve_eam4point_glok_homdef_stress  
(EAM energy minimization version)  
imd_nve_eam4point_homdef_stress (EAM NVE version, homdef)  
imd_nve_eam4point_deform_stress (EAM NVE version, deform)
```

For the LJ potential:

```
imd_nve_pair_lj_glok_homdef_stress (LJ energy minimization version)  
imd_nve_pair_lj_homdef_stress (LJ NVE version, homdef)  
imd_nve_pair_lj_deform_stress (LJ NVE version, deform)
```

“deform” – displace regions of atoms, e.g. for application of load by means of displacement BCs

“homdef” – homogeneous deformation according to specified deformation matrix

Please email mbuehler@MIT.EDU in case you have any questions re. compilation or techniques issues.

Visualiuzation: You may use the program “vmd” (download at <http://www.ks.uiuc.edu/Research/vmd/>) to visualize the results.

The output of IMD can be converted as follows to generate an animation with multiple frames:

```
cat OutFile*.chkpt > out.chkpt
python chkpt2xyz.py out.chkpt x.xyz 1.0
```

Then you may use vmd:

```
vmd x.xyz
```

Alternatively, you may use the GNUPLOT program for plotting results.

More information can be found here: <http://www.gnuplot.info/>

A good program to visualize 2D and 3D graphs is MATLAB or Python's MATPLOTLIB (<http://matplotlib.sourceforge.net/>)

1. Unit cells and crystallographic orientations

The first step in atomistic modeling is to define a proper starting geometry, i.e., the positions of every atom in the system.

Here we focus on single 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 the atomic coordinates in Angstrom in proper unit cells for different crystallographic orientations of a FCC crystal of copper:
 - o $[100][010][001]$ (cubical) orientation
 - o $[110][110][001]$ orientation.
2. Calculate the atomic volume and mass density of copper, based on the atomic model.

2. Elastic coefficients of pair potentials and EAM potentials

Pair potentials are one of the simplest potentials to describe the atomic interaction of crystalline materials. Here we derive a simple Lennard-Jones pair potential for FCC copper to fit experimental values of elastic properties of copper.

Results will be compared to more accurate EAM potential formulations.

1. Derive a generally valid analytical expression of the elasticity tensor c_{ijkl} for a pair potential, using a simple analytical form, for nearest neighbor interactions. Assume a $[100][010][001]$ cubical orientation. Please see reference [1].
2. 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 .
3. Derive an expression for the minimum potential well of the LJ potential, corresponding to the cohesive energy stored in each bond.
4. Derive expressions for the elasticity tensor coefficients c_{ijkl} , Young's modulus, shear modulus, bulk modulus and Poisson's ratio, all as a function of the potential parameters in the Lennard-Jones potential (σ and ϵ), for nearest neighbor interactions and considering infinitesimal deformation. Assume a $[100][010][001]$ cubical orientation. Suggestion: Assume isotropic materials behavior and calculate Lamé coefficients λ and μ from the elasticity tensor coefficients, then Young's modulus and Poisson's ratio.
5. How many independent coefficients c_{ijkl} exist for the LJ potential?
6. Does the Cauchy relation hold?
7. 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. Compare the resulting values with the LJ copper potential reported by Cleri and coworkers [2]. Discuss possible disagreement in light of the potential formulation and potential range.

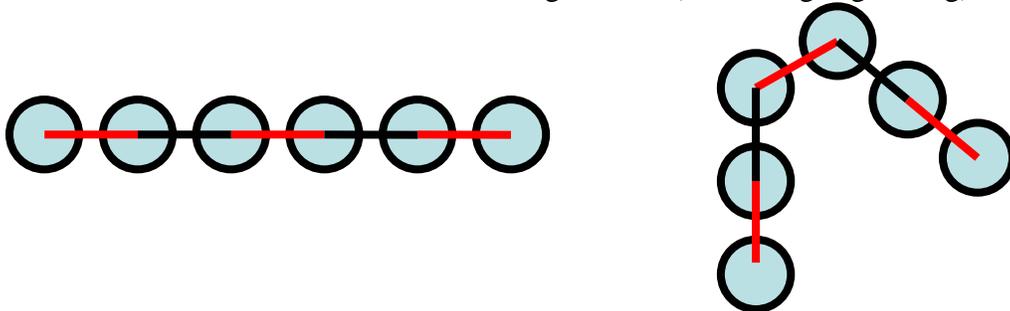
8. Using the ITAP IMD code, calculate the elastic properties of copper using the LJ potential with the LJ parameters developed above, as well as the Mishin's EAM potential [3], including (i) uniaxial strain in the [100] and [110] directions, and (ii) triaxial strain (corresponding to the bulk modulus). Also compare the results with Cleri's LJ potential [2]. Calculate the properties for strains ranging up to the instability strain of the material (zero slope in the stress-strain plot). Summarize the elastic properties for small strains and the instability strain in tables, for different crystallographic directions. Discuss the results obtained with different potentials.
9. Calculate the cohesive energy per atom for the EAM potential.
10. EAM potentials and LJ potentials can be computationally expensive. In regions of small strains, it may be appropriate to use a harmonic approximation to describe the interactions between atoms. Derive expressions for a harmonic potential for FCC copper, assuming a interatomic potential of the form (a is an arbitrary parameter that can be fitted to reproduce the minimum energy depth of the LJ potential)

$$\phi(r) = a + \frac{1}{2}k(r - r_0)^2 \quad (1)$$

Fit the parameters to the LJ potential derived earlier. What are the difficulties of using this potential to describe large-strain elastic properties or fracture?

Can dislocation nucleation and propagation be described using this potential?

11. Assuming the LJ potential with nearest neighbor interactions, what is the energy difference between these two atomic configurations (left=string, right=ring):



The red and black lines indicate an equal distance between atoms corresponding to the equilibrium separation.

Discuss what implications this may have for modeling such a one-dimensional string of atoms.

3. Fracture of a copper nanocrystal with a crack

Having defined interatomic potentials, we can now apply these to model fracture of a nanocrystal of copper.

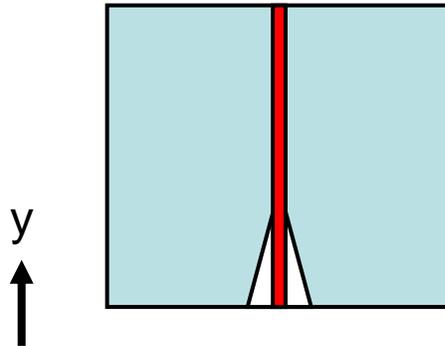
The first step is to become familiar with the ITAP IMD code and its commands related to applying external load to the system by moving part of the atoms.

1. Study the parameter file `Tr_TENSILE` and briefly discuss what each command means. Use the ITAP IMD website to answer this question.
2. Studying the `Tr_TENSILE` file and the other input files, what are the reference units of energy, length and time?
3. How large is the integration step chosen in `Tr_TENSILE` in seconds?
4. What is the reference temperature and reference stress?

Now we will use the EAM potential (EAM1 in Mishin *et al.* [3]) to model deformation of copper.

5. Use the C code “`fcc_110.c`” to build a perfect crystal with $[110][011][001]$ orientations. Visualize the crystal, e.g. using VMD.
6. By using or modifying the C code, insert a macroscopic crack of variable length, assuming a linear wedge-like shape (crack length and opening slope should be a user option). The crack should be oriented in a $[110]$ direction, and the crack surfaces should be orthogonal to the $\{001\}$ plane. In a schematic drawing of the crystal, indicate the glide planes of dislocations.
7. Construct a crystal with dimensions of about 128 \AA in the x -direction and 256 \AA in the y -direction. The crack should extend $1/3$ of the crystal size in the y -direction. The crystal should feature about 18,900 atoms.
8. Perform an energy minimization (GLOK) of the initial structure, holding the boundaries (virtual types 1 and 2) fixed without applying load. Plot the potential energy of the system as a function of iterations. How many iterations are necessary to achieve convergence?
9. It is often convenient to filter surface atoms to study the propagation of cracks. What is a good choice for critical cohesive energy to visualize surfaces of the crystal? Use the “`no_velocities.awk`” code. You can later adjust this value to also visualize dislocations.
10. Provide initial kinetic energy so that the equilibrium temperature is going to be 50K (note that due to the equipartitioning theorem, half the kinetic energy will spill into potential energy, so that the initial temperature needs to be twice as large as the desired temperature).
11. Perform an NVE calculation for ~ 50 ps and plot the temperature evolution (in K) as a function of time. How long does it take until the temperature equilibrates?
12. The next step is to load the crystal with crack under mode I (*i.e.*, orthogonal to the crack extension direction). Use the “`deform_shift`” command to displace the boundary atoms, at a rate of 0.05 \AA every 20 iterations. How fast is the effective displacement and strain rate of the boundary atoms in meters per second?
13. Plot the components of the stress tensor as the applied strain increases. Compare these with the results obtained earlier for the perfect crystal. How can the differences be explained?

14. The presence of a crack and mode I loading leads to failure of the copper crystal. Use the energy method to filter dislocations (modify the value used to display surfaces to visualize dislocations). Describe the mechanisms you observe as the load is increased.
15. Determine the critical strain at which the first dislocation is nucleated or at which the crack propagates (initiation of failure).
16. If you lower or increase the loading rates, how does it influence the critical strain for failure?
17. Looking at the results for mode I loading, obtain a series of checkpoint files *before* and *after* onset of fracture. Use the “no_velocities.awk” script to filter out a thin strip of atoms ahead of the crack, reaching up to the other boundary (see schematic).



Plot the potential energy of all atoms within this strip as a function of their y -position. Plot the evolution of these curves as a function of increase in loading and shortly after rupture.

How would you interpret the results?

18. It has been shown that materials at ultra small scales do not show any stress concentration, regardless of the presence of defects (lecture 4). Calculate the critical length scale for copper, using an estimate for Young’s modulus as obtained above, and using a literature value for the surface energy, as for example found in [4] (e.g. a value of around $\gamma_{Cu(110)} \approx 1.5 \text{ J/m}$).

You may estimate the theoretical tensile strength by assuming $\sigma_{tens,theo} \approx E/10$

(resulting in a value around 10 GPa). Also calculate the result using the value you had obtained earlier. Assume a semi-infinite crack.

Do you expect that the flaw-tolerance mechanism plays an important role in copper?

Discuss situations under which the flaw-tolerance length scale may be important.

4. Fracture and deformation of a copper nanowire

Now we focus on fracture and deformation of a copper nanowires [5, 6]. 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.

1. By modifying the “fcc_110.c” C code, generate a copper nanowire with axial [001] direction, and {110} surfaces (square cross section).
Make sure that you have no periodic boundary conditions since a nanowire should have free surfaces.
Choose dimensions of about 25 Å and 280 Å, resulting in an atomistic system comprising of about 10,000 atoms.
2. Repeat the preparation procedure of GLOK and annealing as before.
3. Using a displacement rate of 0.1 every 20 steps, study the deformation mechanics as a function of increasing strain. Constrain only the z-direction and allow atoms in the boundary to move freely in the x-y plane.
4. How fast is the effective displacement and strain rate of the boundary atoms in meters per second?
5. Plot the components of the stress tensor as the applied strain increases. Compare these with the results obtained earlier for the perfect crystal. How can the differences be explained?
6. Determine the critical strain and stress at the onset of failure. How do these values compare with experiments of macroscopic copper polycrystals?
7. Discuss the observed deformation mechanisms, in particular in light of earlier studies with a cracked crystal (qualitatively). Also, discuss the observations related to macroscopic tensile tests.
8. Estimate Poisson’s ratio ν from these nano-tensile experiments (to do this, measure the contraction as a function of increasing applied strain). How does this compare with experimental values?

5. Additional problems (for additional credit):

1. Repeat the above studies for the LJ potential you developed and discuss difference to the EAM potential. Compare the results for nano-tensile tests with those described in [6], where the authors used a Morse potential.
2. Perform the studies reported in [6] using the EAM potential. Discuss differences in the failure mechanisms observed.
3. The Morse potential is often used as an alternative to the LJ potential [6]. Using similar techniques as above, derive parameters for a Morse potential of the following form:

$$\phi(r) = D \left[\exp(-2\alpha(r_{ij} - r_0)) - 2 \exp(-\alpha(r_{ij} - r_0)) \right] \quad (2)$$

Discuss possible assumptions made. Discuss the meaning of the three parameters. You may train the Morse potential based on the EAM potential. Discuss your parameters in contrast to the parameters described in [6].

4. Study the dependence of fracture mechanics as a function of crystal size and crack length by doubling the system size and reducing the size by a factor of five.

Constants and tables

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

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

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

References

1. Baskes, M.I., *Embedded-atom method: Derivation and application to impurities, surfaces and other defects in metals*. Phys. Rev. B, 1984. **29**(12): p. 6443-6543.
2. 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.
3. Mishin, Y., et al., *Structural stability and lattice defects in copper: Ab-initio, tight-binding and embedded-atom calculations*. Phys. Rev. B, 2001. **63**: p. 224106.
4. Katagiri, M., et al., *The dynamics of surfaces of metallic and monolayer systems: Embedded-atom molecular dynamics study*. Materials Science And Engineering A-Structural Materials Properties Microstructure And Processing, 1996. **217**: p. 112-115.
5. Heino, P., H. Hakkinen, and K. Kaski, *Molecular-dynamics study of mechanical properties of copper*. Europhysics Letters, 1998. **41**: p. 273-278.
6. 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.