591V Multiscale Materials Modeling
Fall 2015
Homework 4
Due on 12/11/2015

1. Deformation of a copper nanowire using an EAM potential

Here we will use the nanoHUB module Nanowire Tensile Deformation Lab (see notes posted on blackboard) to carry out a tensile deformation of a copper nanowire as shown schematically below (see Figure 1). The crystal orientation for the nanowire is x=[110], y=[1-10] and z=[001]. The dimensions given in x, y and z (in the **Nanowire Tensile Deformation Lab module**) are directly in units of the unit cell, which is in the x and y direction 2.556 Angstrom and in the z-direction 3.615 Angstrom. Thus to get the correct dimensions of approximately 20 x 20 x 130 Angstrom^3 you will need to choose dimensions of 8 x 8 x 36 in nanoHUB.

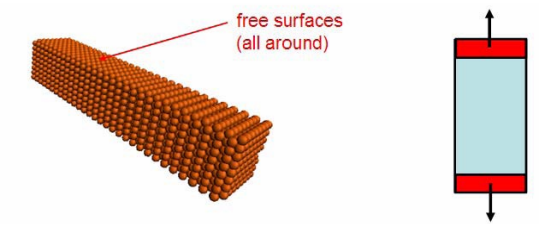

Figure 1: Illustration of boundary conditions for the nanowire simulations.

(a) Use the web based program to build and model tensile deformation of a copper nanowire. Choose dimensions of 20 Å and 130 Å. Run the simulation for 30,000 integration steps, or until you observe significant deformation of the nanowire. Use a displacement rate of 0.02 Å per 20 integration steps at the boundaries (both at lower and upper part). Note: Apply the load in the z-direction, the axial direction of the nanowire.

(b) Take snapshots of the system as it undergoes deformation and include them in your report for this problem set, clearly labeled and clearly explained. The visualizations should be done carefully as they assist you in analyzing the microscopic details of the simulation results.

(c) Discuss the observed deformation mechanisms in detail. What atomic mechanisms are responsible for deformation? Do you see any particularly interesting mechanisms, such as rotation of the end points relative to each other, shear, slip, necking, or others? Hint: Generate a movie of the deformation process within JMol or VMD (recommended for the analysis) and watch the simulation results from different angles as the structure undergoes deformation.

(d) Plot the components of the stress tensor as the applied deformation (strain) increases, and clearly indicate what regime of deformation corresponds to which snapshot you have

shown in part (b).

(e) Estimate Young's modulus for the nanowire, considering small deformation. Compare with Young's modulus of copper known from macroscopic tensile tests. Note: For this case, the Young's modulus is defined as the slope of the stress-strain relationship, $\sigma_{33} = E\varepsilon_{33}$ (index 3 here because load is applied in the z-direction).

(f) Double the cross-sectional area of the nanowire while keeping the length the same. How does the deformation mechanics and stress-strain response change? Explain the differences, if any.

Notes: In the molecular modeling code you will use for the simulations, the reference length is L=1Å =1E- 10 m, the reference energy is E =1 eV and the reference mass m =1 amu. All input and output from the simulation code is expressed in these units.

Physical constants:

k_B =1.3806503E-23 J/K 1 eV = 1.60217646E-19 J 1 amu = 1.660538E-27 kg

2. Nanomechanics of a tropocollagen molecule

Collagen is an important structural protein in vertebrates and is responsible for the integrity of many tissues like bone, teeth, cartilage and tendon. The mechanical properties of these tissues are primarily determined by their hierarchical arrangement and the role of the collagen matrix in their structures (see reference [1] for an overview of the structure).

The goal of this exercise is to use MD for analyzing and understanding the behaviour of a single tropocollagen molecule. We will use the Steered Molecular Dynamics (SMD) technique to apply a tensile load to the ends of the molecule. This computational approach is implemented in the **stretching simulation of an alpha-helical protein domain** module in nanoHUB (use the CHARMM force field parameters for collagen).

(a) What is the initial length of the tropocollagen molecule?

(b) Implement and perform a protein stretching simulation of the collagen segment (all input files provided on blackboard), using the SMD method, to simulate the following boundary conditions (see Figure 2 below):

Figure 2: Geometry of load application under tensile deformation.

Use the following parameters:

DCD Frequency	= 150
Velocity	= 0.0005
Number of Steps	= 150000
Number of Averaging Bins	= 300

What stretching velocity does this correspond to (in m/sec)? What is the total simulated time (in seconds)?

Note: A run with 100,000 steps for this system takes approximately 6-8 hours. Also make sure that you implement the correct SMD stretching direction; it should be the **direction of the initial molecular axis**.

(c) Plot snapshots of the tropocollagen molecule as it undergoes tensile deformation. Describe the observations and clearly label your graphs. Choose visualizations that allow you to gain insight into the mechanisms of deformation.

(d) Plot force vs. displacement. Indicate regimes of deformation and explain based on the plots you generated in part (c). Estimate the Young's modulus of the tropocollagen molecule under small deformation (assume a circular cross-section of the molecule). Compare with published values, e.g. those cited in reference [1].

1. A. Gautieri, *et al.*, "Hierarchical structure and nanomechanics of collagen microfibrils from the atomistic scale up," *Nano Letters*, Vol. 11(2), pp. 757-766, 2011