1.021J, 3.021J, 10.333, 22.00 Introduction to Modeling and Simulation Spring 2018

Problem set #1 (posted Feb. 9, 2018)

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Due: Feb. 26, 2018

Note: You are encouraged to work as a team and submit only one problem set per team. Please indicate all members that participated in the Pset.

Important: Specify all resources you use for your solution (lecture note, book, and web).

The following set of exercises is designed to train you in the basics of atomistic and molecular simulation, focusing on analysis methods, development and application of interatomic potentials and visualization. You will also apply molecular dynamics to study the tensile deformation of a copper nanowire, and generate an animation that visualizes the associated molecular mechanisms. For each exercise, show us how you came to your answer and result. We highly encourage you to make drawings where appropriate. **Note to carefully select the parameters before submitting your job to nanoHUB; the default parameters may not have been adapted to the case you are studying.**

Note: In the analysis you will use in parts 3 and 4, 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 molecular dynamics code is expressed in these units. To facilitate the solution, calculate the units of temperature and pressure (or equivalently, stress) as well as the time unit in terms of the above given reference units.

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1. Calculation of diffusion constant and temperature dependence

A grain boundary (GB) is of great interest from both scientific and technological points of view. The plot below (see Figure 1) provides the mean squared displacement (MSD) of the atoms at an Al GB from simulations at different temperatures, resulting from a three-dimensional molecular dynamics simulation. The goal of this exercise is to practice the application of the MSD to calculate diffusivities, and to study the dependence of diffusivities on temperature.

(a) From the plots, determine the diffusion constant D for the given temperatures.

(b) Plot D as a function of temperature T, and discuss the dependence.

(c) Discuss the temperature dependence and estimate the activation barrier assuming an Arrhenius relationship between D and T:

$$D = D_0 \exp\left(-\frac{E_b}{k_B T}\right) \tag{1}$$

Explain the meaning of all variables in equation (1).

(d) Based on the analysis carried out in part (c), discuss possible mechanisms for atomic diffusion.

Hint: Consider the physical meaning of E_b. Make a simple drawing to illustrate the meaning of eq. (1) and E_b.

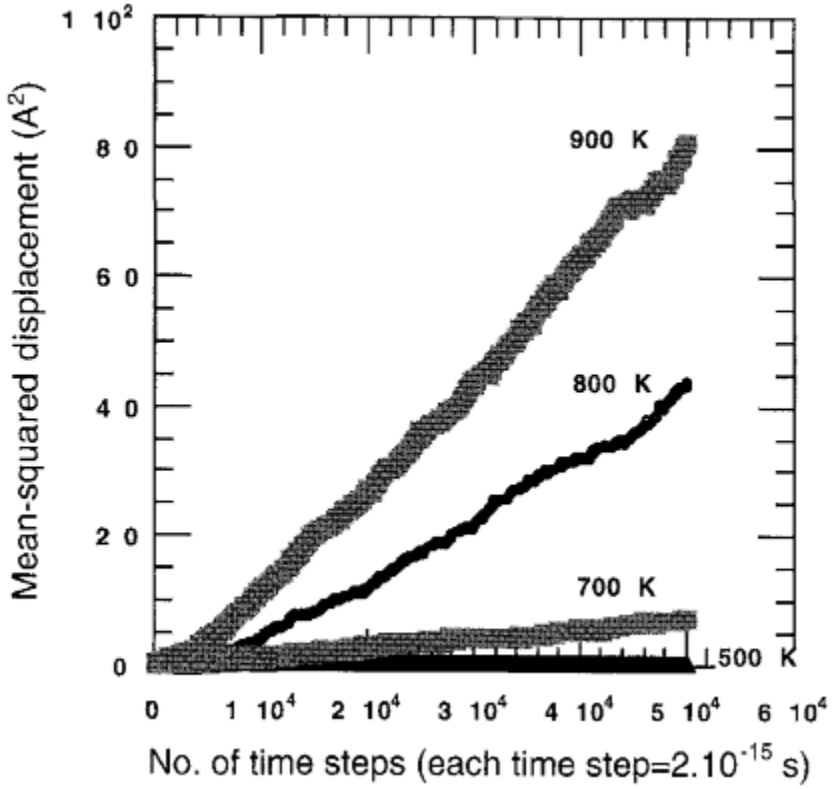

Figure 1: Mean squared displacement for atoms at an aluminum grain boundary, for different temperatures, resulting from a 3D molecular dynamics simulation (Figure courtesy: Liu and Plimpton (1995)).

2. Deformation of a copper nanowire using an EAM potential

Here we focus on deformation and fracture of copper nanowires. Nanowires play a critical role in future electronic devices, serving various needs including interconnects, for electronic devices, waveguides or mechanical sensors. Due to the inherently small dimensions, classical, continuum descriptions of the material behavior are questionable and molecular modeling becomes a reliable modeling tool to understand the mechanical properties of these materials.

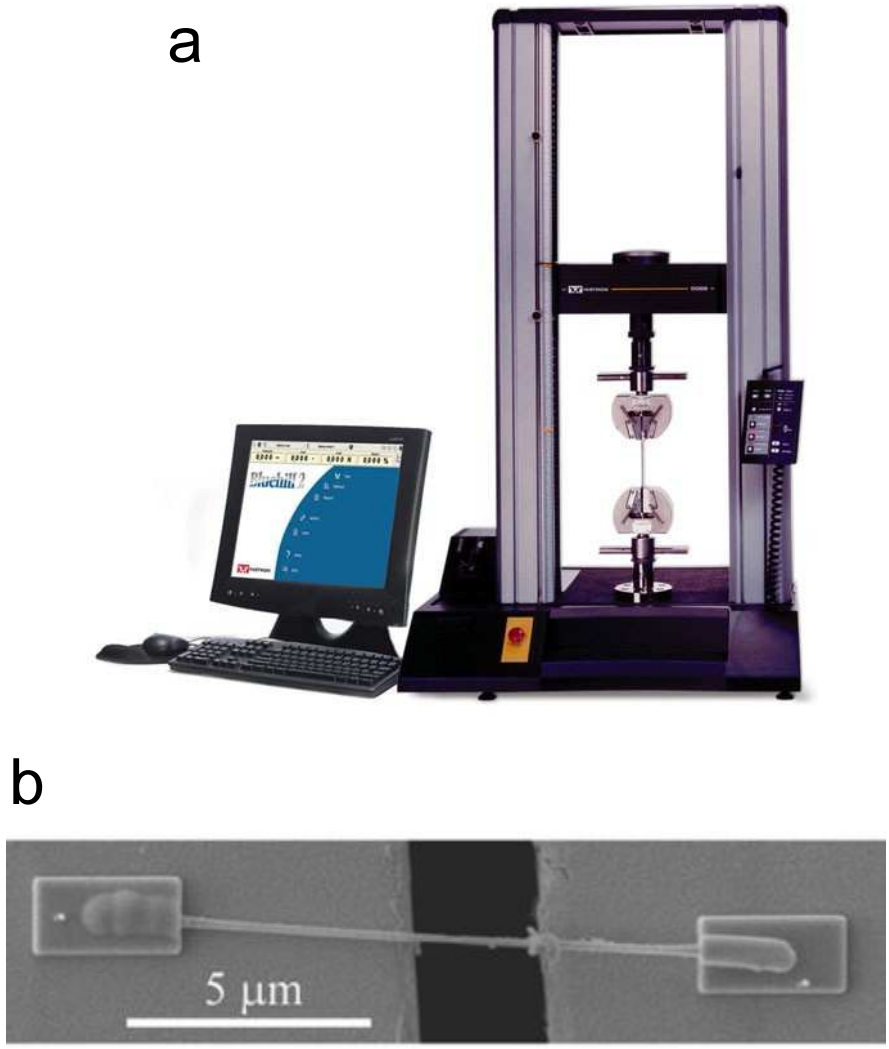

Figure 2: Macro (a) and nano (b) testing of materials. a, Instron tensile test machine, as used for "macroscopic" specimen to measure force versus extension, or stress versus strain. (b), Corresponding tests at the nanoscale can be carried out for nanostructures (e.g. nanowires) by using Atomic Force Microscopes or MEMS/NEMS devices. A test of a nanowire similar as shown in b is carried out using Molecular Dynamics in this problem. Panel b taken from: http://www.sciencedaily.com/releases/2007/09/070927121113.htm

The goal of this exercise is to model a tensile and compression test of a copper nanowire using molecular dynamics simulation with an EAM potential (see Figure 2 for an example of a "macroscopic" tensile test machine and a corresponding nanoscale test of a nanowire).

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

particular, it can accurately represent the chemical bonding at the surface. This is indeed critical to describe the properties of nanowires, since the surface to volume ratio is particularly large.

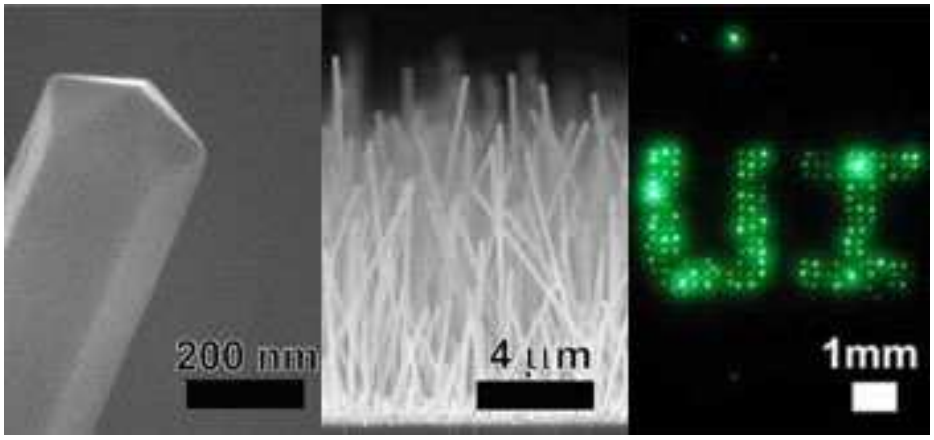

Figure 3: Copper nanowires on different surfaces; each wire is between 70 nanometers and 250 nanometers wide. This figure illustrates a potential application of copper nanowires (note that the specific application is not connected to this problem set). The nanowire arrays could find use in field-emission displays (FED), a new type of display technology that promises to provide brighter, more vivid pictures than existing flat-panel displays. FEDs work in a manner that is similar, in principle, to cathode-ray-tube (CRTs) televisions, but they are only a few millimeters thick and use millions of tiny electron emitters instead of using a single electron gun. In FEDs, the copper nanowires would be used to fire electrons at red, green and blue phosphor particles that are coated on a screen, lighting them up. The nanowires are uniform and have a very pointed tip, and they emit electrons at low voltages, unlike the tungsten filament used in conventional, bulky CRTs, which require many kiloVolts. Source: "*Nanowires Grown for Ultra-Thin Displays*", http://nanoarchitecture.net/article/?c=nano-emissive-displays

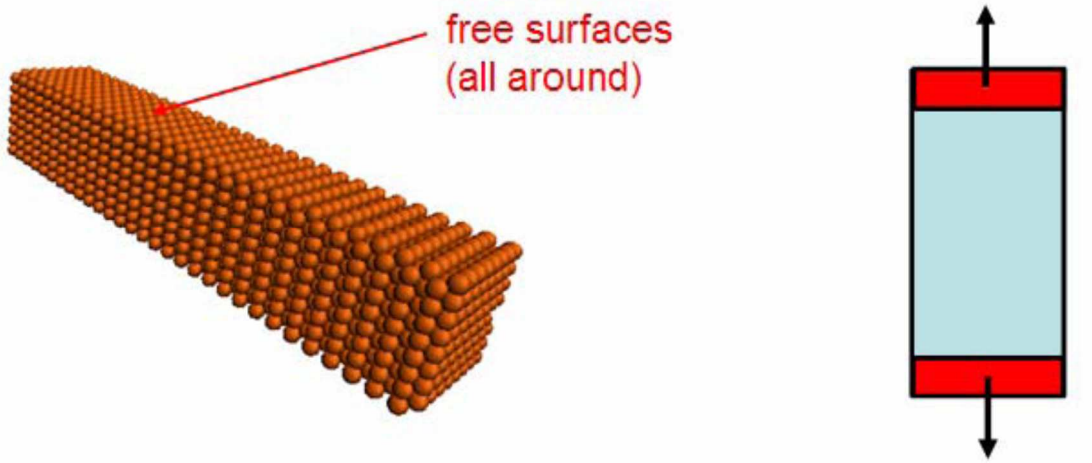

Figure 4: Illustration of boundary conditions for the nanowire simulations carried out here.

Here we will use the nanoHUB module **Nanowire Tensile Deformation Lab** (see notes posted on Stellar) to carry out a tensile and compressive deformation of a copper nanowire as shown schematically above. Note that this module is based on the IMD code (see original manual at: http://www.itap.physik.uni-stuttgart.de/~imd/); it might be helpful to check the meaning of some of the parameters there if needed.

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.

(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.

(g) Describe the deformation mechanics under compression (carry the simulation on until you see significant deformation of the nanowire, using the same deformation rate as above and the same geometry of the nanowire as in part (a) but adapt the parameters for compressive loading). Discuss the results.

(h) Repeat the simulation and analysis in (b-e) with temperature of 0.01 and 10.0. Upon summary of snapshots, thermodynamic outputs, or other analysis, discuss what you observe. You may run additional simulations to prove your hypothesis.

(i) Repeat the simulation and analysis in (b-e) with timestep of 1.0 and 2.0. Upon summary of snapshots, thermodynamic outputs, or other analysis, discuss what you observe. You may run additional simulations to prove your hypothesis. (Hint: You may want to decrease the number of

integration steps to simulate the same period of time. Also, you may want to increase the output frequency to allow same output interval. Anything else you want to change?).

Physical constants:

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

Notes regarding nanoHUB website and Molecular Dynamics codes

For this assignment, we use the ITAP IMD code, suitable for modeling metallic systems with the EAM potential. The ITAP IMD code is made accessible for different applications via the nanoHUB website at:

http://nanohub.org/

The module you need for this pset #1 is **Nanowire Tensile Deformation Lab**.

Visualization: You may use the program Visual Molecular Dynamics or "VMD" (download at http://www.ks.uiuc.edu/Research/vmd/) to visualize the resulting ".xyz" files. VMD is available free of charge. You can directly access a file that contains a series of snapshots, for easy visualization of a movie with VMD. Consider the file "Simulation Movie (XYZ)" that appears as output in nanoHUB.

The nanoHUB website also produces figure files that you can view immediately in your web browser. You can use these or visualize on your own computer using VMD for the final report and analysis of the results.