ME 5329 Homework 4

LAMMPS Cu Nanowire Tensile Test

October 7, 2025

(Corrected October 7, 2025)[0]

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Due: October 13, 2025

Objectives:

- Understand molecular dynamics (MD) calculations using LAMMPS.
- Theoretically generate a stress-strain diagram from an MD tensile test simulation.
- Understand how temperature influence the strength and fracture mechanics of a nanowire.

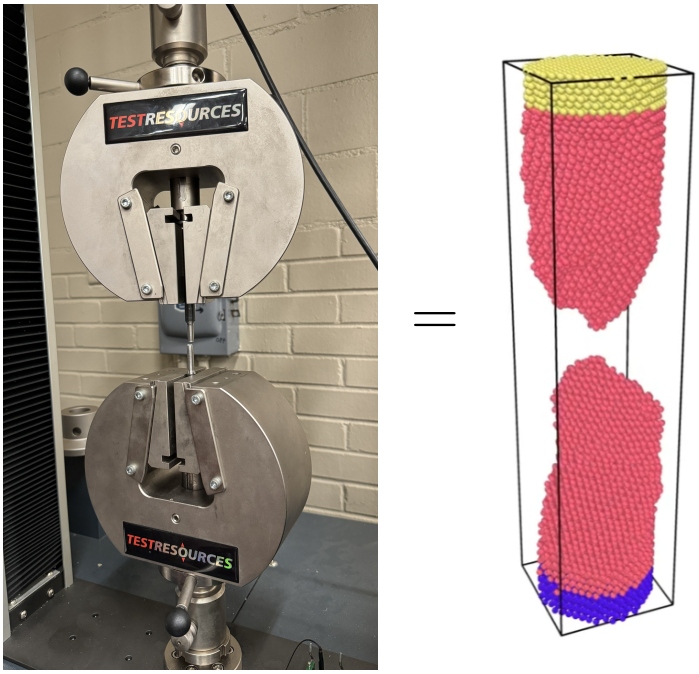

Figure 1: The image on the left shows the tensile test machine in the TTU ME Department, while the figure on the right shows a tensile test simulation in LAMMPS. The length of the bar on the left is 10 cm, whereas the length on the right is 150 nm.

[0]Corrections added October 7, 2025: The LAMMPS data parameter "Lz" should be replaced with "v_box_height" for data processing. The nanowire diameter should be 2 nm for all simulations. Mac users should ensure that the "Cu_u3.eam" potential file is located in their calculation directory before running LAMMPS. This file is linked below in the first assignment section.

Software and Tools Needed for This Homework:

1. First install OVITO Basic by going to the link listed below. This is our visualization code for LAMMPS and we will use OVITO to generate our initial LAMMPS geometries.
   - Go to https://www.ovito.org/
2. If you have a Windows laptop, follow the instructions below to install LAMMPS-GUI:
   (a) (Optional) First, download MSMPI (msmpisetup.exe) from the following link. This allows LAMMPS to run with multithreading: https://www.microsoft.com/en-us/download/details.aspx?id=105289
   (b) Go to this LAMMPS Binary Repository: https://rpm.lammps.org/windows/
   (c) Scroll down until you see the executable named **LAMMPS-64bit-GUI-stable.exe** and download it. The most current version was uploaded on "2025-09-10 21:48".
   (d) After running the executable installer, LAMMPS-GUI should be installed on your Windows machine.
3. If you have a Mac laptop, follow the instructions below to install LAMMPS-GUI:
   (a) (Optional) Install MPI to enable parallel execution if it is not already installed. See the Open MPI Quick Start guide for installation instructions: https://docs.open-mpi.org/en/main/installing-open-mpi/quickstart.html
   (b) Go to this LAMMPS Binary Repository: https://download.lammps.org/static/
   (c) Scroll down until you see the disk image named **LAMMPS-macOS-multiarch-GUI-stable.dmg** and download it. The most current version was uploaded on "2025-09-10 22:00".
   (d) Open the disk image and LAMMPS-GUI should be installed on your Mac machine now.
4. Documentation Links:
   - LAMMPS Documentation: https://docs.lammps.org/
   - LAMMPS-GUI Documentation: https://lammps-gui.lammps.org/
5. The files needed to do this Homework are located here:
   - `Cu.cif` - https://jerschro.github.io/how_to_dft/assets/downloads/me_5329/Cu.cif
   - `cu_nanowire_tensile_test.inp` - https://jerschro.github.io/how_to_dft/assets/downloads/me_5329/cu_nanowire_tensile_test.inp
   - `Cu_u3.eam` (neccesary for Mac users only) - https://jerschro.github.io/how_to_dft/assets/downloads/me_5329/Cu_u3.eam

Creating Initial LAMMPS Structures:

1. Open OVITO and load the Cu.cif file (File → Load File).

2. On the right side of OVITO, there is a drop-down menu labeled **"Add modification..."**. This is where we will modify the pristine copper crystal structure to create a nano-wire.

3. First, let's generate a supercell of Cu (Add Modification Dropdown → Modification → Replicate). For **Number of Images**, choose a reasonable number of replications in each direction. The distance in the **x** and **y** directions should be larger than the diameter of the nanowire, while the distance in the **z** direction should match the length of the nanowire. The unit of distance in OVITO is Å. To determine how many times the unit cell must be replicated the unit cell to reach the desired length, the following equation can be used:

   - The number of replications needed is

   $$N = \left\lceil \frac{L_{\text{wanted}}}{L_{\text{unit cell}}} \right\rceil$$

   - Where:
     - N = number of times to replicate the unit cell
     - L_{wanted} = desired total length (distance)
     - $L_{\text{unit cell}}$ = length of the unit cell along that direction
     - $\lceil \cdot \rceil$ = ceiling function (rounds up to nearest integer)

4. Next, we want to select the cylinder of atoms. To do this, create an **Expression selection** (Add Modification Dropdown → Selection → Expression selection). Make sure that **Operate on** is set to **Particles**. In the Boolean expression box, enter the following, where `D_half_squared` is $\left(\frac{D}{2}\right)^2$ is an integer, in Å, representing the radius squared of the cylinder:

```
Position.X^2 + Position.Y^2 < D_half_squared
```

5. Next, we want to invert the selection (Add Modification Dropdown → Selection → Invert selection). This will select all atoms that are **not** inside the cylinder.

6. Then, delete the atoms outside the cylinder (Add Modification Dropdown → Modification → Delete selected). This leaves only the atoms inside the cylinder.

7. Finally, export and save the structure as a LAMMPS Data File (`.dat`) (File → Export File).

Running LAMMPS Simulations:

1. To run a LAMMPS simulation, create a new directory and copy the initial `.dat` structure along with the LAMMPS input file, **cu_nanowire_tensile_test.inp**, into it. If you are using a Mac, you also need to copy the **Cu_u3.eam** potential file into your this directory.

2. Open the LAMMPS-GUI program and load the input file (File → Open).

3. Modify the `initial_data_file` parameter to match the `.dat` structure you created. Also, set the `sim_temp` parameter to the temperature you wish to simulate. In the provided input file, any other parameter you may want to edit has been declared as a variable; for example: `variable sim_temp equal 300`.

4. To run the simulation in LAMMPS-GUI, click the green button  in the bottom-left corner of the program window. If there are any errors, an error message will pop up.

5. During the simulation, a progress bar appears at the bottom of the program window. The LAMMPS output is displayed in a separate window, and a graph in another window shows the thermo_data variables being saved. You can monitor variables such as **c_Twire** (temperature of the wire), **Pzz** (average stress along the Z-axis), and **v_box_height** (length of the unit cell in the Z-direction).

6. **VERY IMPORTANT:** After your simulation finishes, right-click on the LAMMPS-GUI output window and select **"Save Log to File ..."**. If you do not do this, the data needed to create stress-strain diagrams for this homework will be lost and you will need to rerun the simulation to retrieve the data.

7. Using OVITO, you can watch the tensile test by opening the **"tensile.lammpstrj"** file. If you do not see the nanowire fully break, you may increase the `"tens_run_amt"` parameter to a larger value and rerun the simulation.

Simulations To Run and Deliverables:

1. Create one copper nanowire with a diameter of 2 nm and a length of 10 nm. Screenshot a visualization of the nanowire and report it along with the total number of atoms that are in the structure.

2. Using LAMMPS, equilibrate the system with a Nose-Hoover (NVT) thermostat to the specified temperature for 10 ps, and then perform a tensile test for up to 100 ps at a strain rate of 0.01 $\frac{1}{\text{ps}}$. Apply grips to the top and bottom atoms, each with a thickness of 10 Å. For the nanowire, run the tensile test at the temperatures specified below:

   - 10 K, 300 K, 700 K

3. For each simulation, view the **"tensile.lammpstrj"** file in OVITO. Record the time at which the two fragments are no longer connected, this is the simulation time at fracture. Screenshot a picture of where the necking and fracturing is occurring and report this image. Remember that OVITO reports image numbers, and in this simulation data is dumped every 100 time steps (each time step being 0.001 ps). Thus, for each image, the simulation time can be calculated as:

$$t_{\text{sim}} = \text{image\_number} \times \text{dump\_freq} \times \text{timestep}$$

4. Create a stress-strain diagram from the LAMMPS output (log file) of the simulation, with each temperature reported as a distinct separate line on the same graph and clearly labeled in a legend. Only plot the stress-strain data up to the point of the ultimate tensile strength, $\sigma_{\text{UTS}} = \max(\sigma_{\text{tensile}})$. Take note at what t_{sim} σ_{UTS} occurs at. In the title of the graph, include your name or R-number after giving it an appropriate title. Use a graphing tool of your choice—such as `matplotlib` and `pandas` in Python—to process and plot the data.

   - When reading the LAMMPS output file, the data of interest is located in the section shown below. We will use the *second* data block in the log file, since the *first* data block corresponds to the thermal equilibration step.

```
   Step          Temp          c_Twire          PotEng    ...
     10000   596.06804      685.99857     -86244.496
     10100   606.14347      697.59411     -86237.656
...
...
...
    109900   613.78938      706.39358     -83962.178
    110000   611.18876      703.40059     -83972.569
Loop time of 462.56 on 12 procs for 100000 steps with  ...
```

   - One way to read this data block into a Python data object is to copy the data block (excluding the last line shown in the text box) into a text file named `"log.txt"`, and use the following `pandas` command to read it into a DataFrame:

```
import pandas as pd
df = pd.read_csv("log.txt", delim_whitespace=True)
```

   - The x-axis represents the engineering strain, $\epsilon_{\text{engineering}}$. The `v_box_height` column reports the length of the simulation cell along the z-axis (in Å). The equation for the engineering strain is:

$$\epsilon_{\text{engineering}}(t_i) = \frac{L_z(t_i) - L_z(t_0)}{L_z(t_0)}$$

   - The y-axis represents σ_{tensile} in GPa. The `Pzz` column provides the average stress along the z-axis during the LAMMPS simulation, reported in units of bar. By convention, tension is negative in LAMMPS, so multiply `Pzz` by -1 to follow the standard positive-in-tension convention, and then convert from bar to GPa.

5. Create a table summarizing all simulations. Include the following information for each case:
   (a) ultimate tensile strength (σ_{UTS}) in GPa,
   (b) simulation time at σ_{UTS} (ps),
   (c) simulation time at fracture (ps),
   (d) simulation temperature (K).
6. Discussion questions:
   (a) **Temperature Effects:** How does temperature influence the ultimate tensile strength, σ_{UTS}, of the Cu nanowires?
   (b) **Temperature vs. Necking Behavior:** For the different temperature simulations, do you observe similar necking behavior?
   (c) **Fracture Mechanism:** For the simulations performed in this homework, which simulations exhibit brittle fracture and which exhibit ductile fracture? Can you infer any trends based on temperature?

Submission Requirements:

The only accepted submission format for the report is a Microsoft Word document.

Please submit it under the **'Homework 4'** assignment in Canvas.