Computational Nanoscience

Simo Tuomisto
013456353

Final project - The failure of a copper nanowire

Contents

1 Introduction

In this report I will present results from computer simulations of a copper nanowire under tensile stress. The great strenght of nanoscale objects under stresses has been observed in multiple occations. For practical purposes it is very interesting to know the properties of these nanomaterials when they are scaled towards macroscopic materials.

I have conducted simulations with copper nanowires of varying widths and varying induced stresses. Computed strain-stress-curves will be presented.

Section 2 will deal with the theoretical background of the situation.

Section 3 concerns the computational methods used and the analysis process.

Section 4 has the measured results and the final section will draw conclusions.

2 Theoretical background

Strain is the relative deformation of a material. Strain is a tensor quantity defined as

$$\epsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) \tag{1}$$

where u_i is the displacement towards the i direction. For the interest of this report, a single dimensional relative deformation is sufficient. This is

$$\epsilon = \frac{L - L_0}{L_0} \tag{2}$$

Stress is another tensor quantity that is in turn defined as a force affecting an area element. In this report the main interest is on tensile stress:

$$\sigma = \frac{F}{A} \tag{3}$$

Here the force is perpendicular to the area element and in the simulated case is aligned with the deformation.[**?**]

When a material is deformed to the brink of its fracture, its stress-strain curve will contain much of the important information. Much of the overall dynamics can be summed up in its features and calculated from it. Below is shown an example of a general stress-strain curve[2]

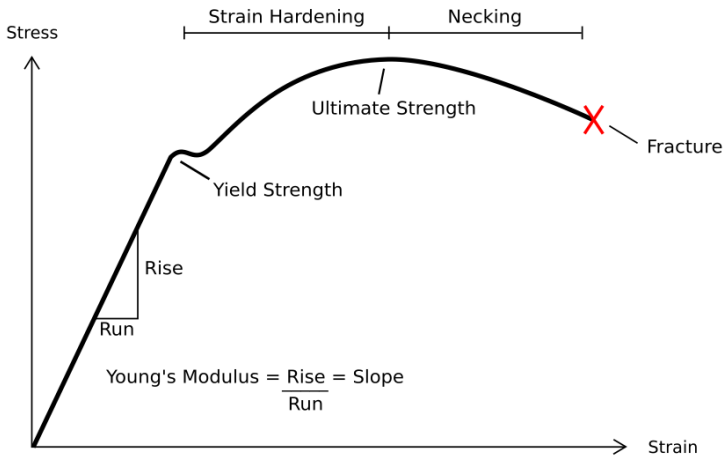

Figure 1: An example of an stress-strain curve

Different materials have different kinds of stress-strain curves. For ductile materials the curve can be much like the one shown in the image. Brittle materials usually fracture before plastic deformation begins 1at the point of maximum yield strength.

The Young's modulus describes the proportionality between strain and stress during the elastic phase in this kind of situation. Thus it is written as

$$Y = \frac{\sigma}{\epsilon} \tag{4}$$

In the following chapters, curves like this will be generated by a computer simulation. Use of molecular dynamics simulations of large number of particles is a very efficient way to check predictions from theoretical models. These, combined with physical measurements, can be combined to a give a clear picture on the properties of materials. Even at their smallest scales.

3 Computational methods

Computations were done using LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator). For each simulation a periodic box was created and a cylinder of copper atoms was created to run through it. Cylinder lenght was 256 Å. This system was relaxed for 1.5 ps with Berendsen temperature control to a room temperature. Time step interval was 0.5 femtoseconds.

After this the state of the system was saved.

A new simulation was done that would stretch the cylinder. Border in the cylinder direction (the z-direction) was changed to a shrink-wrapping border. This means that when the cylinder, under stress, gained length the bounding box would adapt to it. This was to enable a true deformation into empty space.

The tensile stress was accomplished by using LAMMPS force fix "addforce". A force was added to all atoms that were on the top and bottom regions of the cylinder. A region of 100 Å to each direction from origin was left untouched. Suitable added forces were tested in order to get a wire failure inside the simulation timeframe. Final simulated force region was from 0.001 eV/Å to 0.02 eV/Å. Simulation ran for 100000 timesteps of 0.5 fs each and thus simulation time was 50 ps in total. Zero point motion was also removed with a fix. Berendsen temperature fix kept the system at a constant temperature. This had the unfortunate side-effect, that very small force values would not stretch the material.

Batch working was done with a help of a few Python scripts.

Reproducing the data in results is easy. run_relax.py will generate relaxed cylinders and run_stretch.py will reproduce simulations. run_stretch.py has a internal parameter 'lammps_program' that should point to proper LAMMPS executable. In my Windows installation this was 'lmp_serial.exe' and in an Ubuntu workstation that was used for simulation it was 'lammps-daily'.

Analysis of the results was a bit more tedious and it involved a lot of man-

ual labor. For each sample the breaking time of the material had to be found by from Ovito images. Strain and stress values were extracted from LAMMPS-dumps by a Python script. Strain was calculated by measuring the size of the shrink-wrapped bounding box. Stress was calculated from the same dumps by averaging the absolute values of LAMMPS-calculated σ_{zz}-component. Python scripts were written in order to draw pictures from this data. When plotting the stress, an running average was used. Real values for strain were never calculated, as they were not needed.

Included material has calculated strain and stress values and a file that contains measured failure times.

4 Results

Below are two pictures from a typical simulation. The system will, under the stress, deform quite uniformly. The fracture will, however, usually happen near the top or bottom areas. Those are the areas that will have to transfer the induced stress to the center, so this is no surprise. Under lower forces materials would sometimes show beginning of failure in the middle, but the time scale was not long enough for it to happen.

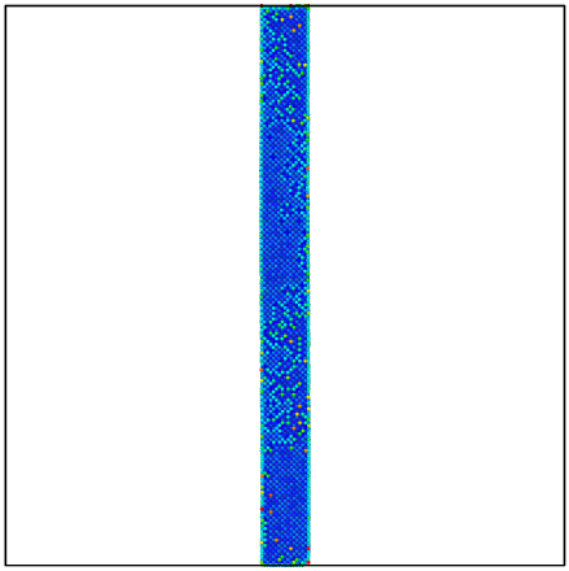

Figure 2: Simulation start, r=15 Å, f=0.007

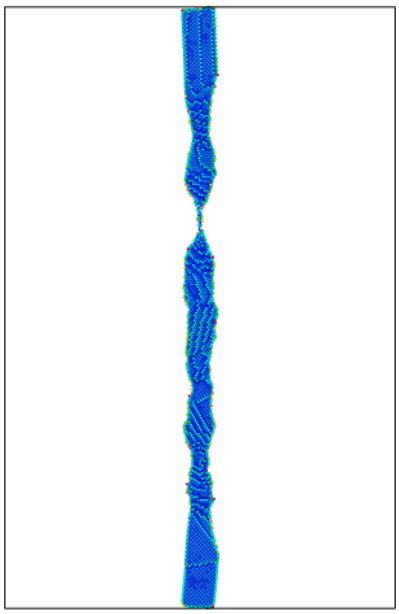

Figure 3: Material failure, r=15 Å, f=0.007, t=30ps

4.1 Stress-strain curves

Usually obtained strain-stress curves look very ductile. After a constant elastic deformation a peak of maximum strength is reached and long plastic deformation follows.

For radius of 5 Å the difference in material behaviour is great around the added force value of 0.010 eV/Å. For value under this (F=0.009 eV/Å), the sample won't break. There will be dislocations and other deformations, but in the timeframe of the simulation it won't break. Thus its strain-stress curve does not remind the others. For forces 0.010 eV/Å and 0.011 eV/Å the system breaks and the curves look ductile.

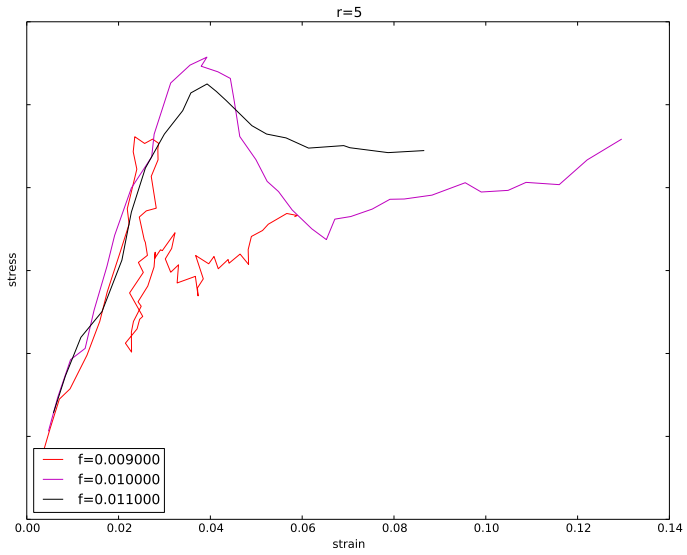

Figure 4: Strain vs. stress-curve, r=5 Å

Simulations with radius of 10 Å were the most fruitful. It is enough to say that when the force reaches a threshhold of 0.011 eV/Å the system ceases to exhibit very peculiar behaviour. This behaviour will be analyzed in detail later on.

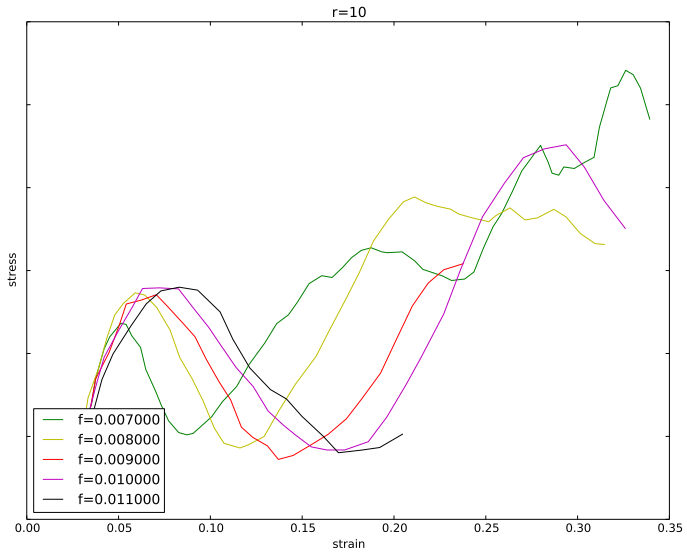

Figure 5: Strain vs. stress-curve, r=10 Å

When the wire radius gets bigger, it starts to present more ductile behaviour. As can be seen from the images below, the location of the maximum strength shifts a little based on the used force. Its value also varies when force changes. The amount of plastic deformation after this strain value is highly dependent on the radius.

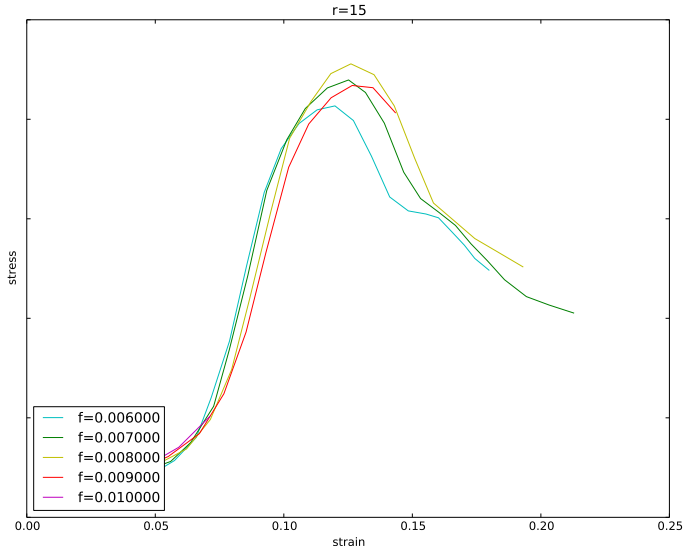

Figure 6: Strain vs. stress-curve, r=15 Å

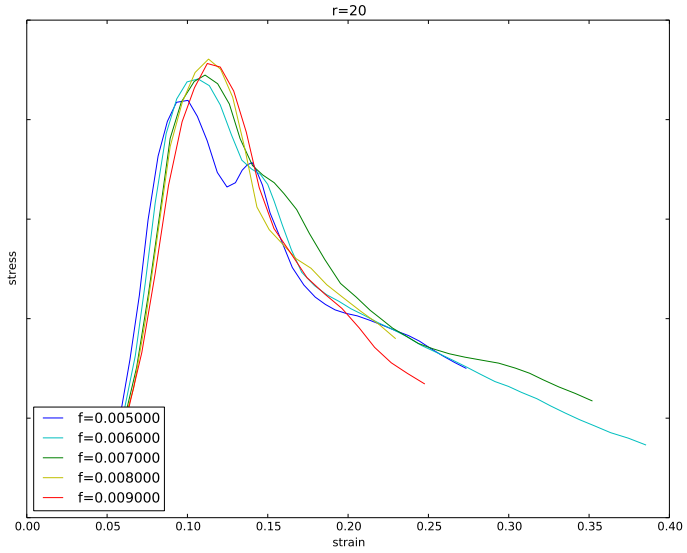

Figure 7: Strain vs. stress-curve, r=20 Å

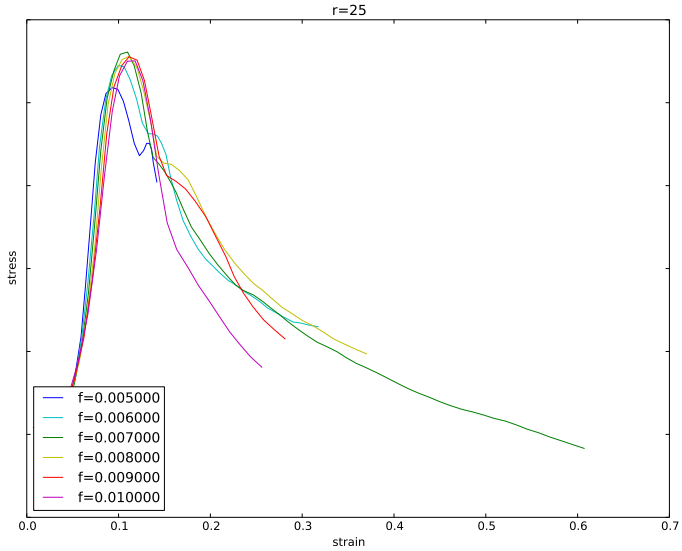

Figure 8: Strain vs. stress-curve, r=25 Å

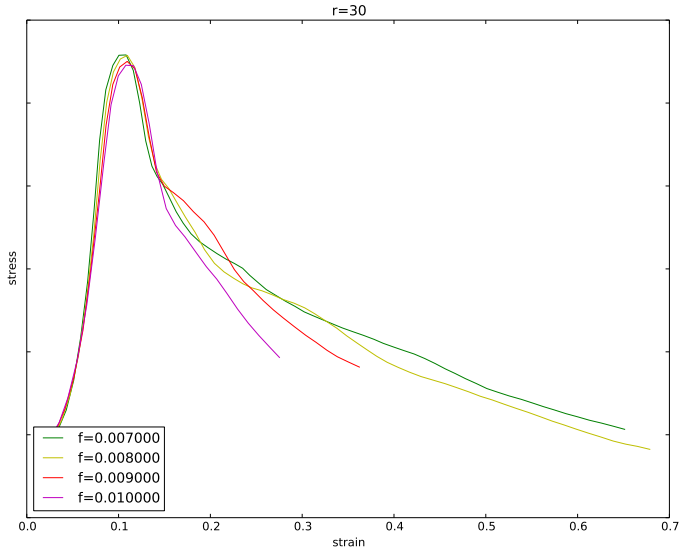

Figure 9: Strain vs. stress-curve, r=30 Å

4.2 A deeper look on the stretch

I will now analyze the stretch dynamics in more detail. This will be done by doing centrosymmetry analysis on a single sample. Sample to be analyzed will be the one with r=10 Å and force parameter of 0.008 eV/Å. This will be because the force parameter seems to be just ideal in order to get many dislocations. Each picture is done by slicing the cylinder in the yz-plane and taking the picture from the x-direction. This enables vision on the radial distribution of dislocations. Color scales goes from blue (normal fcc neighbors) to red (almost no neighbors) through cyan, green and yellow.

Start of the simulation looks like this.

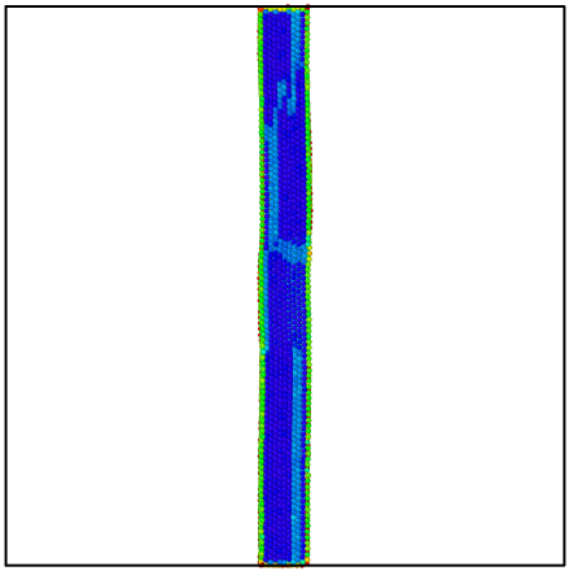

Figure 10: Simulation start

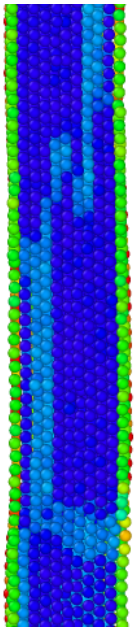

Figure 11: Simulation start (detail)

The interest will be on a detailed region near the center of the cylinder. As can be seen, there are some naturally less dense (warmer) regions in the cylinder.

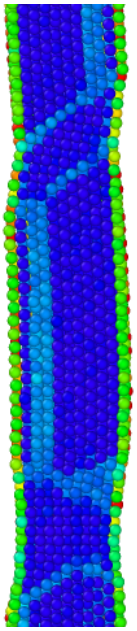

Figure 12: Simulation at 7.5 ps (detail)

After 7.5 ps the region near origin starts to exhibit deformations from the stress. The radius starts to get thinner and there is there are two dislocations just above and below the natural dislocation.

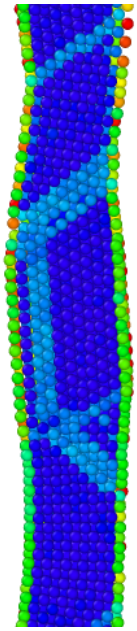

Figure 13: Simulation at 11 ps (detail)

At 11 ps the deformation is very apparent. The dislocations widened and the hexagonal lattice of undeformed material has been deformed into a square lattice. The natural longitudinal less dense are starts to turn into a radial one at the top and the bottom.

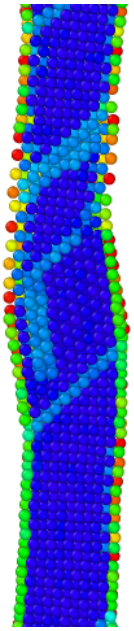

Figure 14: Simulation at 14 ps (detail)

At 14 ps some of the less dense regions have splitted up and disappeared. Most of the central region has been turned into a square lattice.

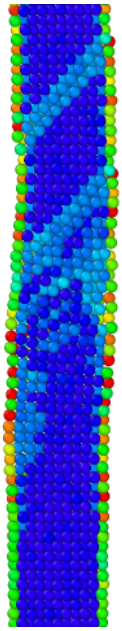

Figure 15: Simulation at 22 ps (detail)

At 22 ps all of the initial less dence areas have packed themselves to an area between the two square lattice regions. At this stage they will break up and the cylinder will widen itself. Those regions will also become part of the square lattice.

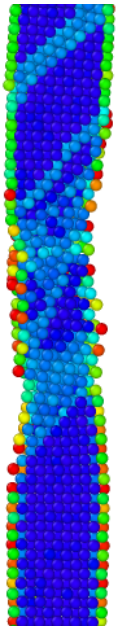

Figure 16: Simulation at 28 ps (detail)

Same thing will happen time and time again. At 28 ps the nanowire has become considerably thinner.

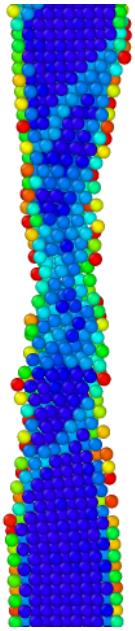

Figure 17: Simulation at 33 ps (detail)

After 33 ps a cascade follows. The material will flow towards the center in order to lengthen the wire, but there is not enough of it. Thus it will become thinner and thinner and at 39.5 ps the nanowire breaks.

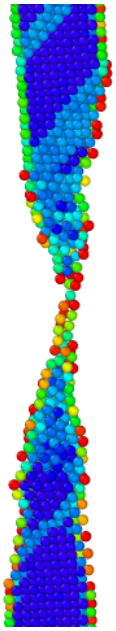

Figure 18: Simulation at 39.5 ps (detail)

What differentiates the 10 Å measurement from the others is the good force parameter scale. While most of the samples break near the stress inducing areas, these samples break near the center.

4.3 Maximum strength

Next picture shows the depedence of stress maximum on the radius of the wire.

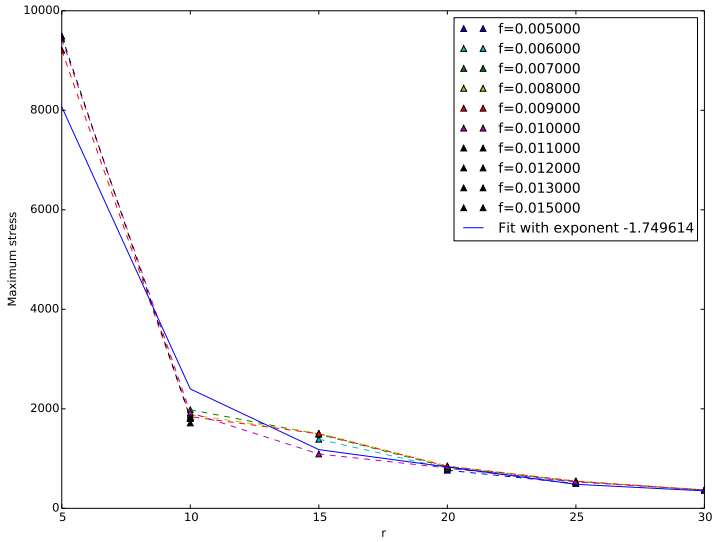

Figure 19: Maximum of stress vs. r

Plotting the data and fitting a polynomial into it gives quite an interesting dependency. Overall exponent found was bit more than -2. As the Young's modulus for elastic strain is proportional to $Y = \frac{\sigma}{\epsilon} = \frac{F}{A\epsilon} \propto R^{-2}$ and the maximum is calculated from data that is a bit lower than the linear value, it is as expected.

4.4 Strain rate

The strain rate of deformation seems to be proportional to the square of wire radius.

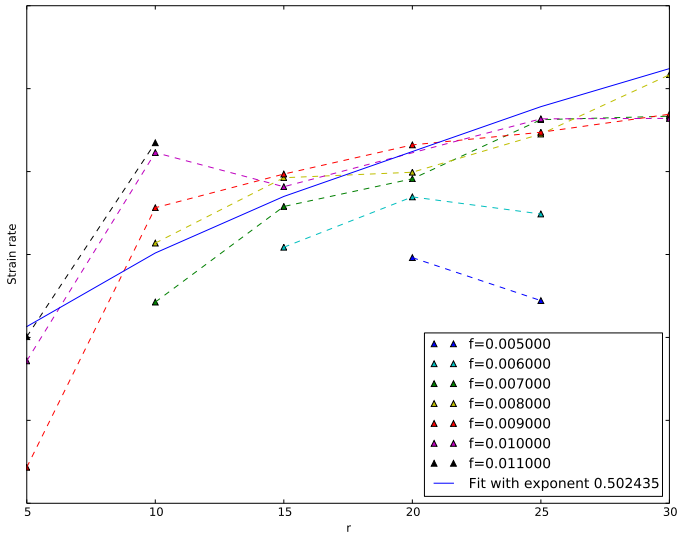

Figure 20: Strain rate vs. r

5 Conclusions

In this report I have done molecular dynamics simulations for copper nanowire. This report has shown that copper nanowire exhibits ductile behaviour under tensile stress. The maximum strain a nanowire can handle depends on the area of the nanowire as $\sigma \propto r^{-1.7}$

References

[1] Lecture material on computational nanoscience, Slides 3, 2013, https://atom.physics.helsinki.fi/courses/s/compnano/lecturenotes/03_mechanical_properties-1x2.pdf

[2] Wikipedia article on strain, http://en.wikipedia.org/wiki/Deformation_%28engineering%29#Elastic_deformation