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

Problem set #1 solution

Instructor: Markus Buehler (mbuehler@mit.edu)
TA: Francisco Martin-Martinez (fmartinm@mit.edu)

---

1. Calculation of diffusion constant and temperature dependence

(a) $D=\frac{1}{2d}\times$ (slope MSD-t) Here d=3 (results are from three dimensional MD)

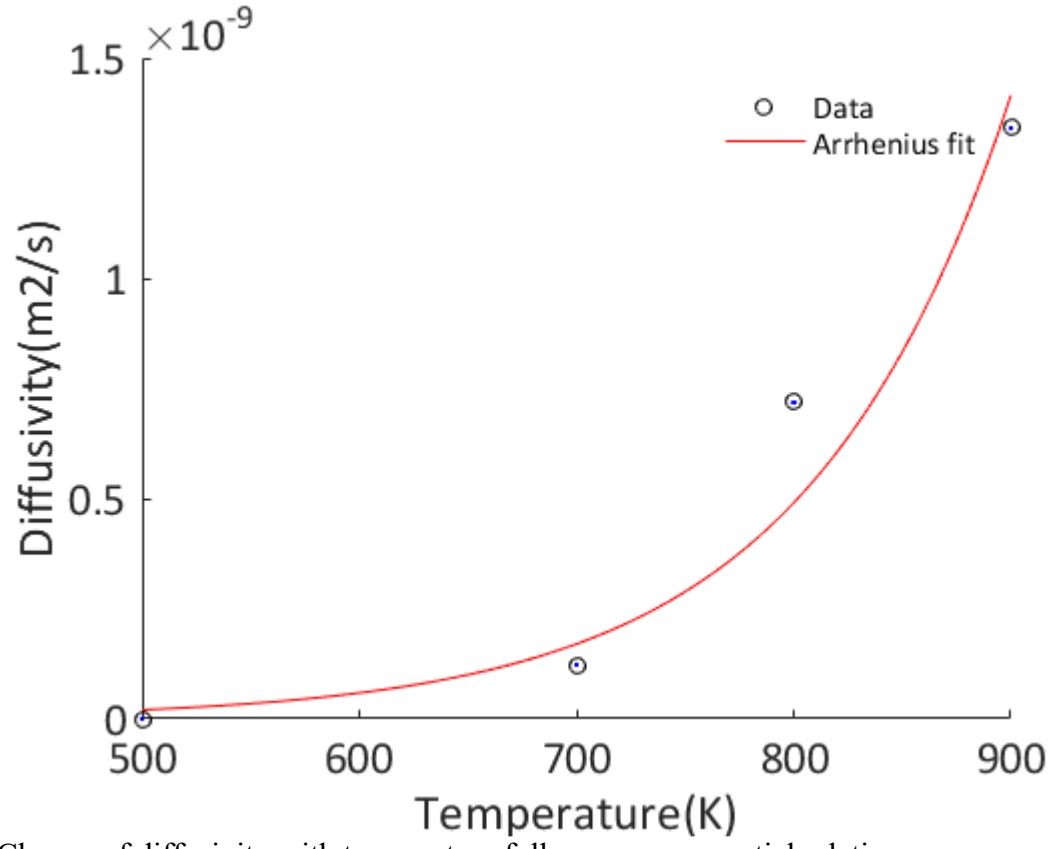
T=500 K D=0

T=700 K $D=\frac{1}{2\times3}\times\frac{7.38\times10^{-20}}{50611\times2\times10^{-15}}=1.22\times10^{-10}\frac{m^2}{s}$

T=800 K $D=\frac{1}{2\times3}\times\frac{43.29\times10^{-20}}{50168\times2\times10^{-15}}=7.19\times10^{-10}\frac{m^2}{s}$

T=900 K $D=\frac{1}{2\times3}\times\frac{81.68\times10^{-20}}{50470\times2\times10^{-15}}=13.42\times10^{-10}\frac{m^2}{s}$

(b)



Change of diffusivity with temperature follows an exponential relation.

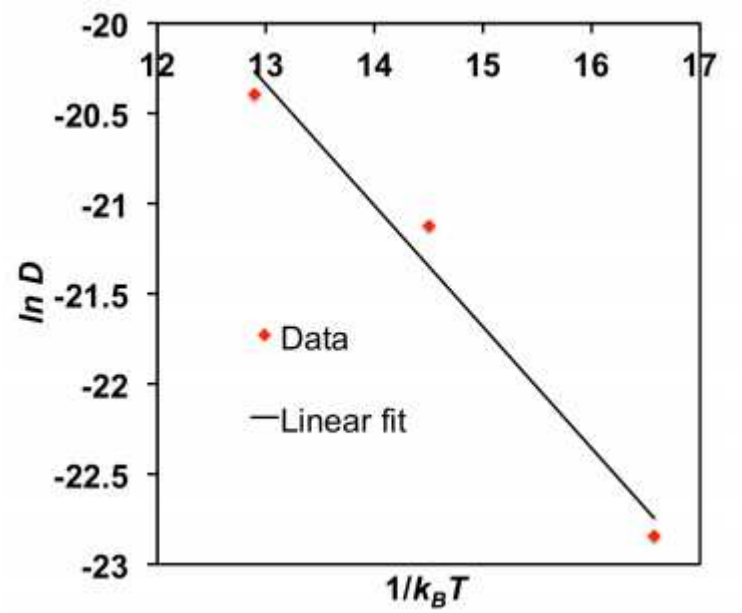
(c)

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

Diffusivity at different temperature follows exponential Arrhenius relation. The exponential form of this relation means that diffusivity grows quickly with temperature.

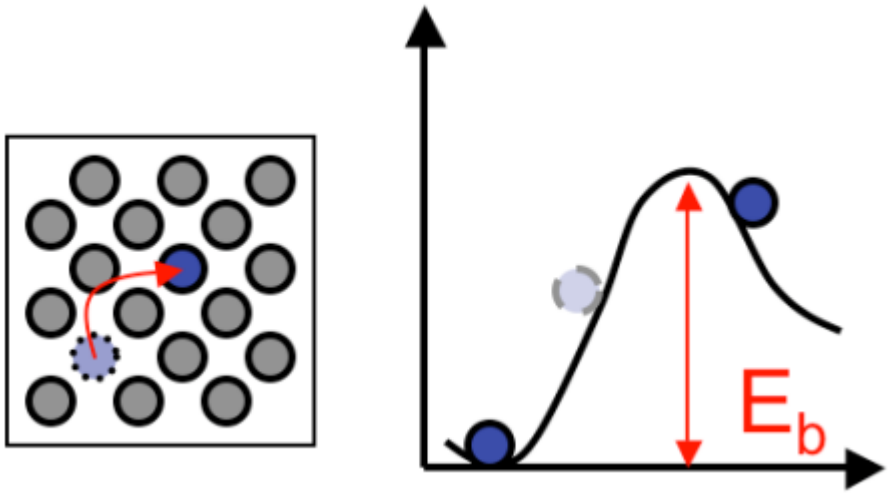
D is the diffusion coefficient (m^2/s)
D_0 is the maximum diffusion coefficient (at infinite temperature; m^2 / s)
Eb is the activation energy for diffusion, per atom (J)
K_B is the Boltzmann constant=1.38×10^{-23} $J.K^{-1}$
T is the absolute temperature (K)

(1) $\rightarrow \ln D = \ln D_0 - \frac{E_b}{K_B T}$ Fit line to lnD- 1/(KB T) data



(2)
$\rightarrow E_b$=0.68 eV and $D_0=0.922\times10^{-5}$ m^2 / s

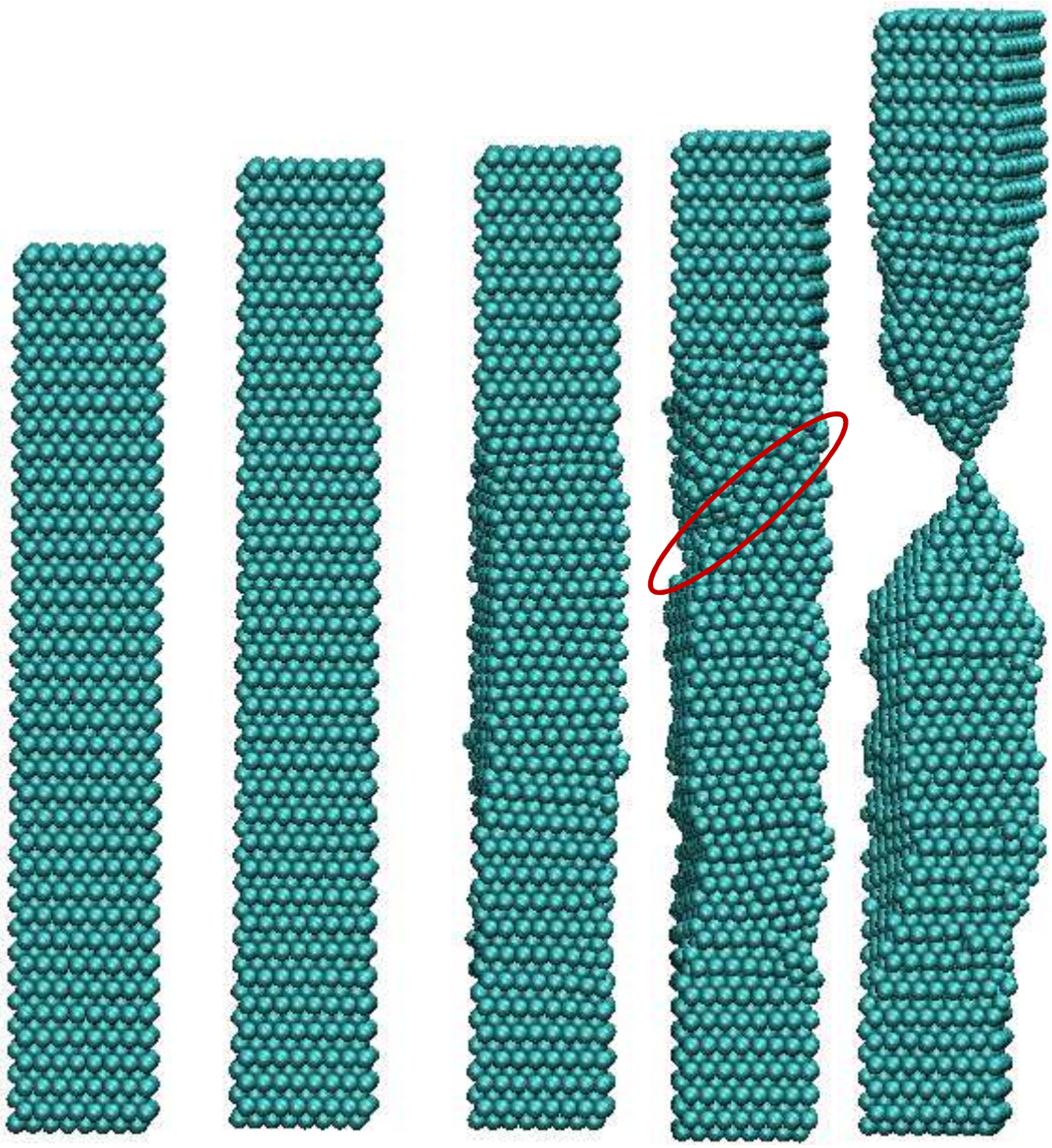
(d)
Since the energy barrier is much larger than thermal energy k_BT, the diffusion mechanism would be site hopping through a relatively ordered lattice. Additional energy added to the system may induce diffusion by Brownian motion.



Diffusion and concept of energy barrier

2. Deformation of a copper nanowire using an EAM potential

(a) .
(b)



step= 0 6000 7000 9000 17500

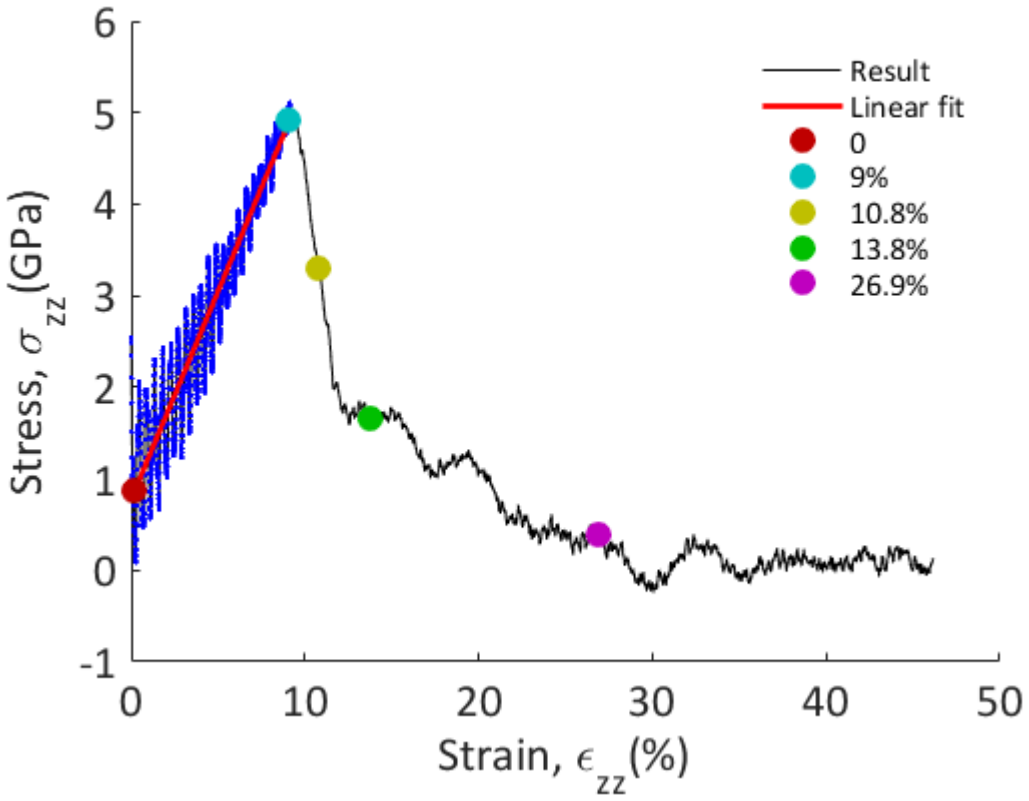
strain=0 9% 10.8% 13.8% 26.9%

→yy

(c)

From the snapshots we see that first the crystal stretches in the elastic regime, which is followed by initiation of necking. The necking continues while some of the crystal planes slide along each other known as slip. Eventually the wire fractures.

(d)



The curve corresponds to the z-direction along which we are straining the wire. Our first and second snapshots (up to %9) correspond to the linear region, where the wire is being strained in the elastic regime. The third and fourth snapshots correspond to the region after the pressure drops and starts to approach zero, which is the region where the wire begins plastically deformed. The final snapshot (26.9 %) is referenced to the region of the plot where the pressure has dropped to zero. In this region the wire has completely fractured.

(e)

$1eV=1.6\times10^{-19}$ J

force×distance=energy & stress=force/distance^2 →stress=energy/distance^3

$1eV/Å^3 = 1.6\times10^{-19}/10^{-30}$ N/m^2 $=1.6\times10^{11}$ Pa=160 GPa

Values of the stress should be multiplied by 160 to be converted to GPa.

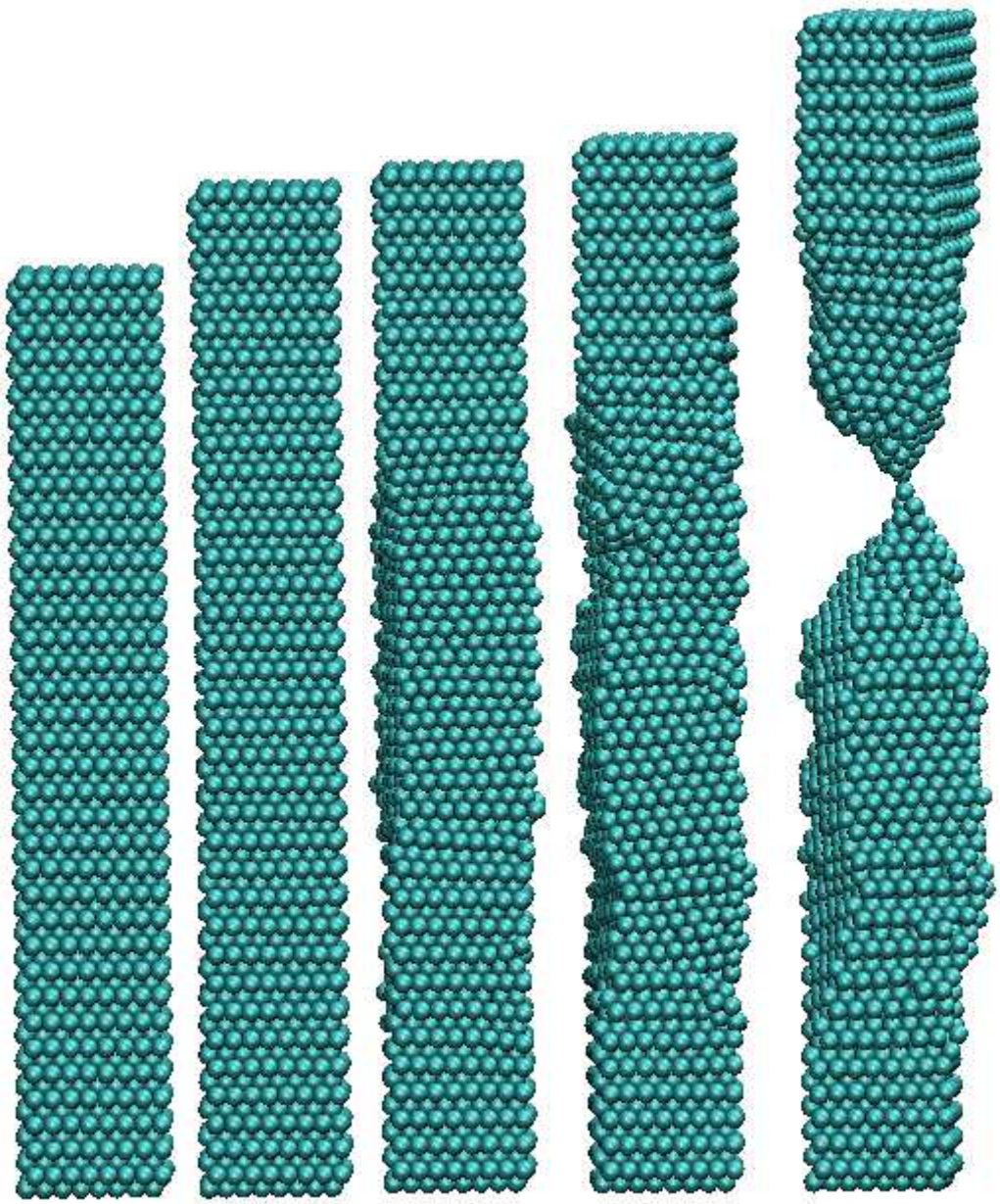
Note: For this case, the Young's modulus is defined as the slope of the stress-strain relationship, $\sigma_{33} = E\varepsilon_{33}$ (index 3 here because load is applied in the *z*-direction).

45.4 GPa

E_{exp} = 130 GPa (for bulk Cu from www.webelemets.com)

(f)

new dimension: 1.414*8≈12 →12 x 12 x 36

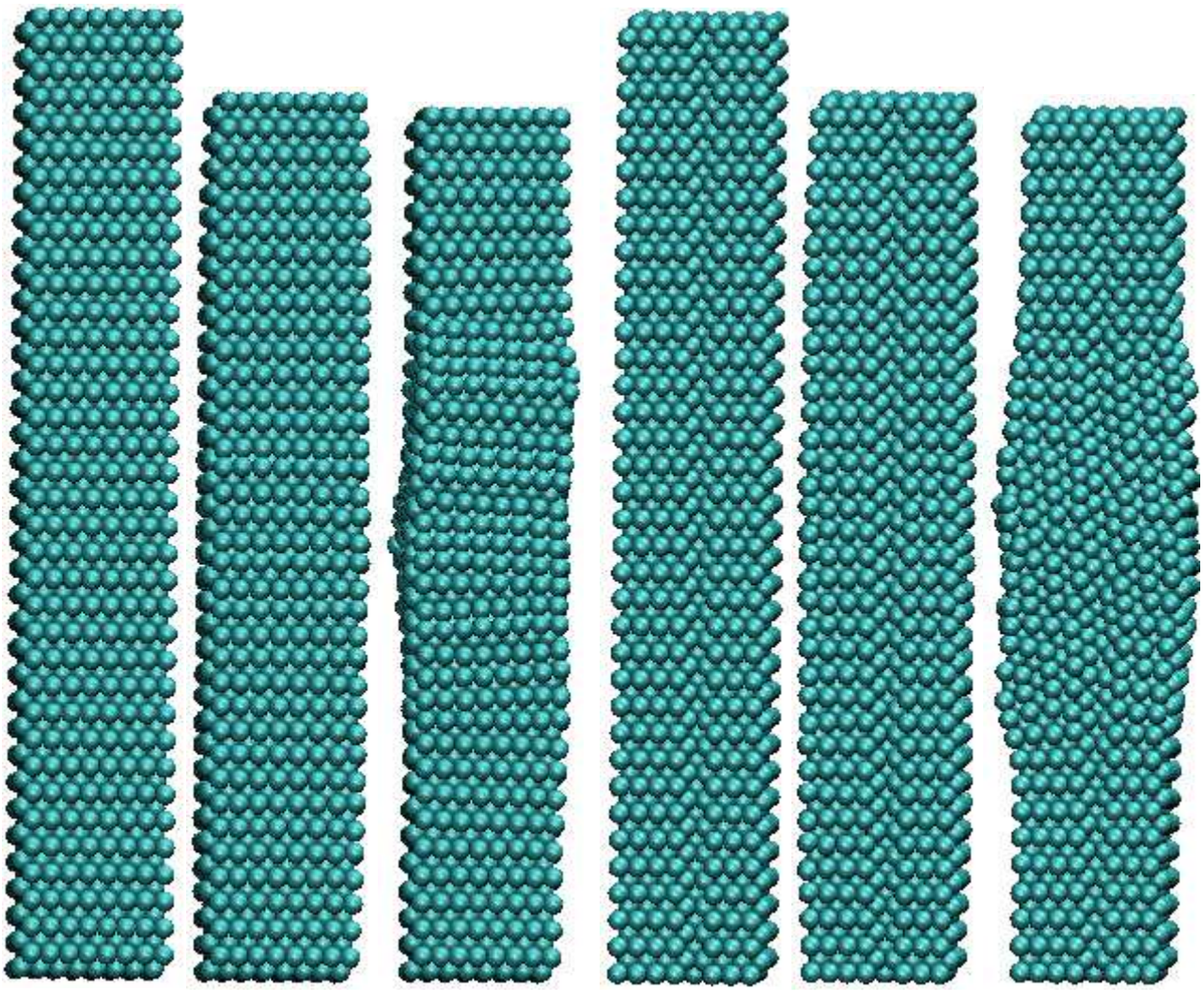


step= 0	6000	7000	9000	17500
strain=0	9%	10.8%	13.8%	26.9%

→yy

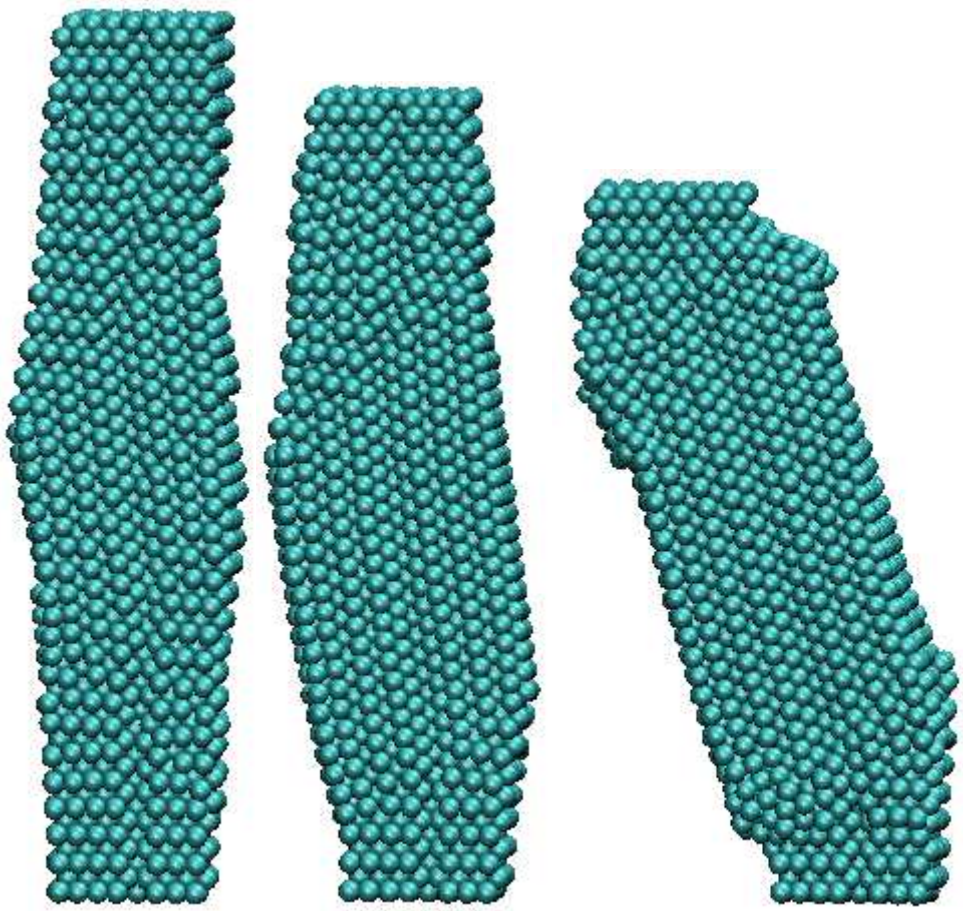
We can see from a comparison of the plots for this thicker nanowire that the elastic regime behaves more or less the same (i.e. The Young's modulus appears to be the same in both cases). However, the plastic deformation regime is more gradual for the thicker wire. This is expected, since the thicker wire is able to deform more to accommodate the increasing strain.

(g)



step= 0 5500 6500 0 5500 6500

→yy →xx

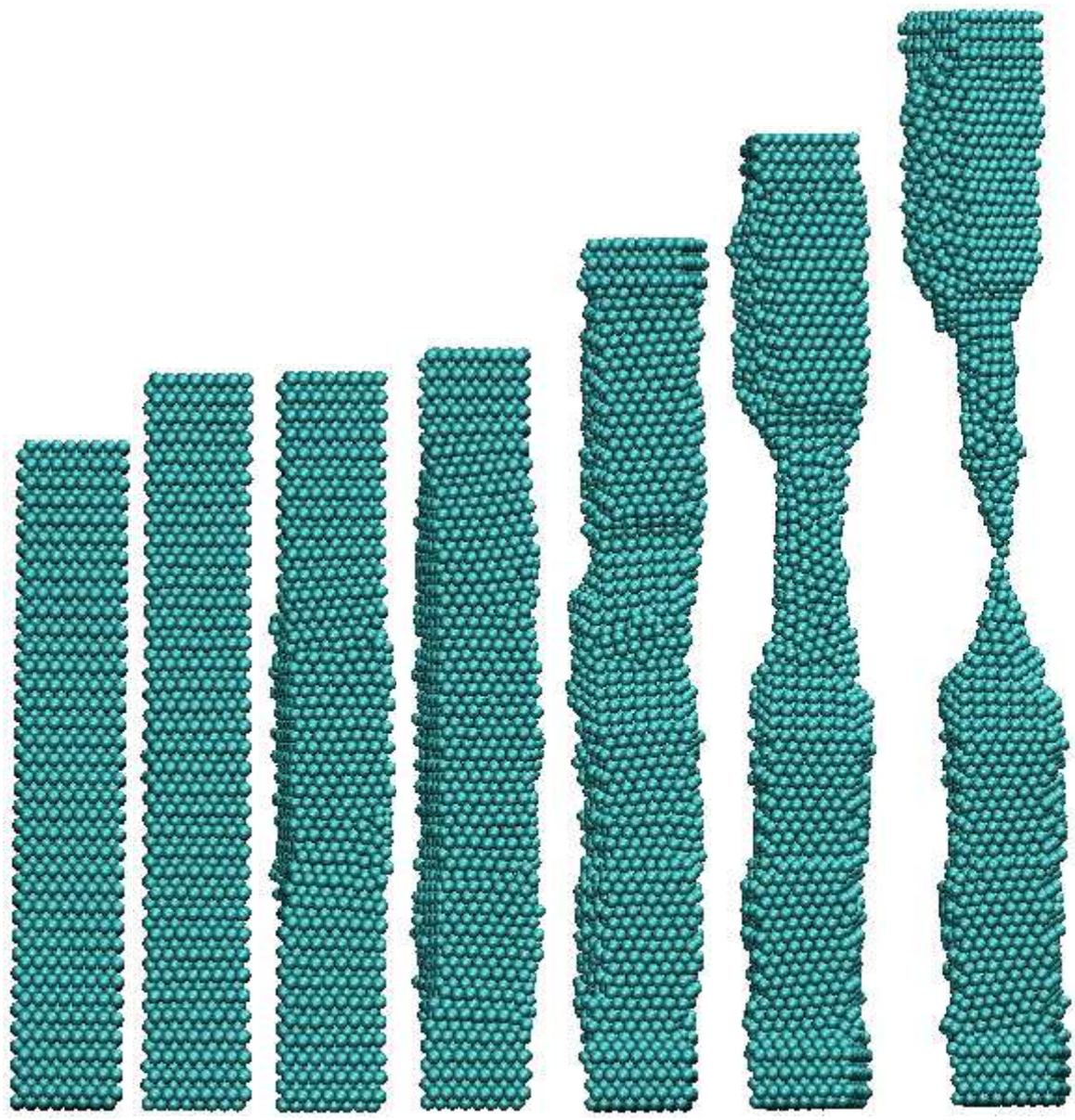


step= 9000 14000 20000
→xx

step= 30000
→xx

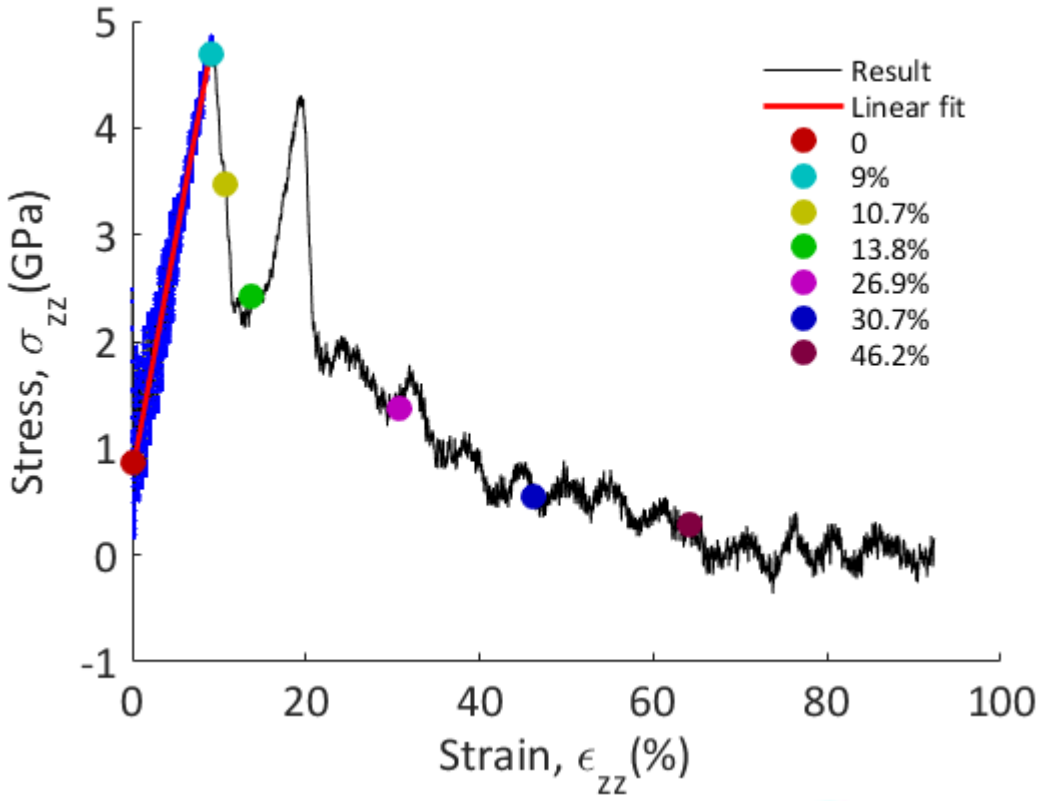
The main deformation mechanism under compression is mechanical slip, this can be seen clearly in the above snapshots.

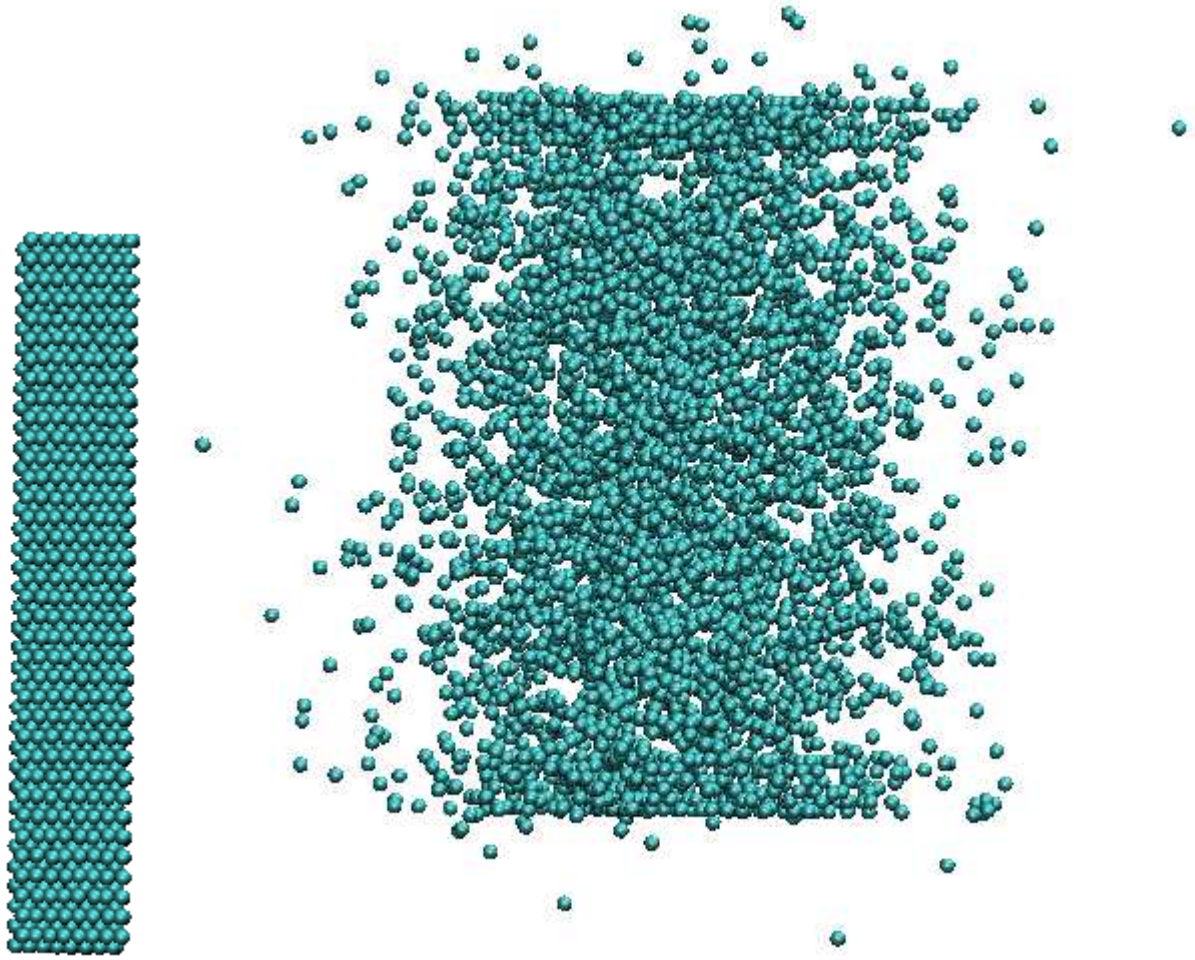
(h) .



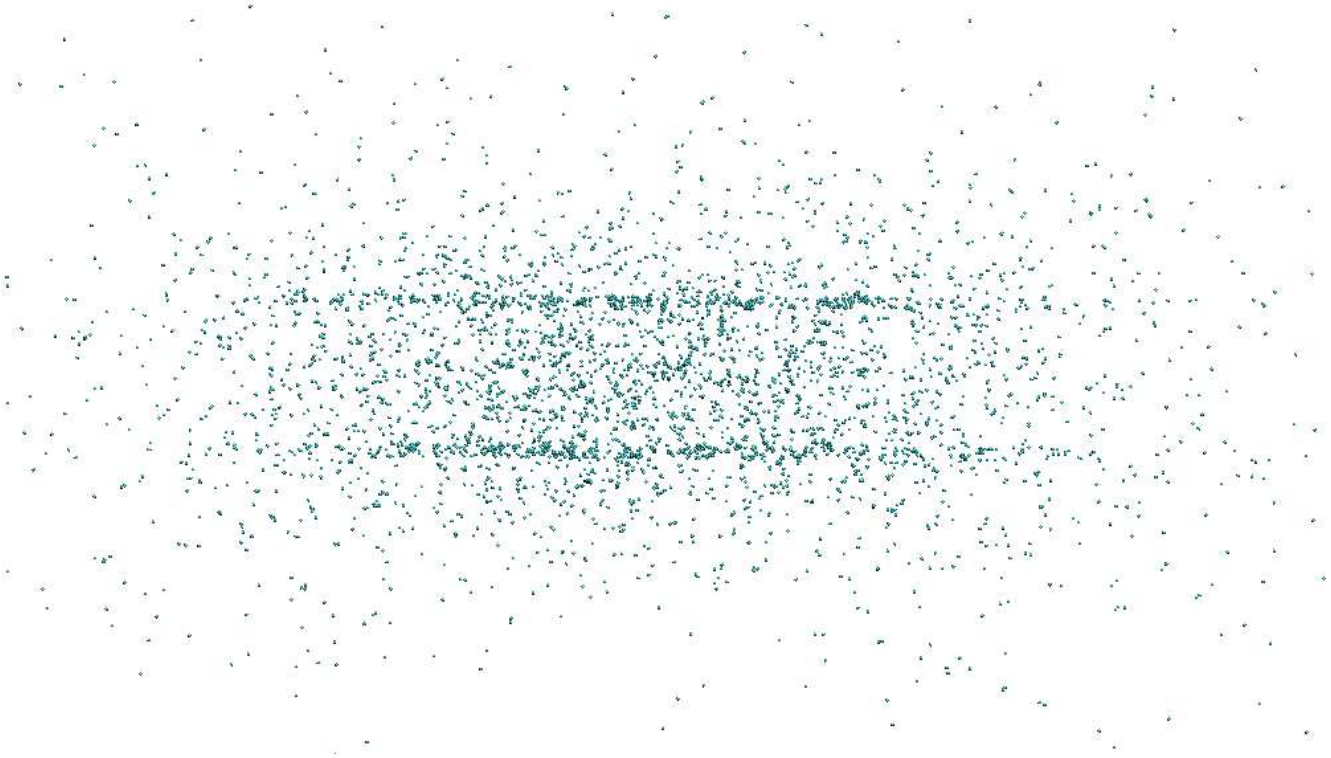
Stiffness = 43.8 GPa

By the increase of temperature stiffness value decreases (from 45.4 to 43.8 GPa) which makes sense. Copper becomes softer by the increase of temperature.


Result
Linear fit
0
9%
10.7%
13.8%
26.9%
30.7%
46.2%
Stress, σ_{zz}(GPa)
Strain, ϵ_{zz}(%)
5
4
3
2
1
0
-1
0
20
40
60
80
100



Step =0 2



Step = 20

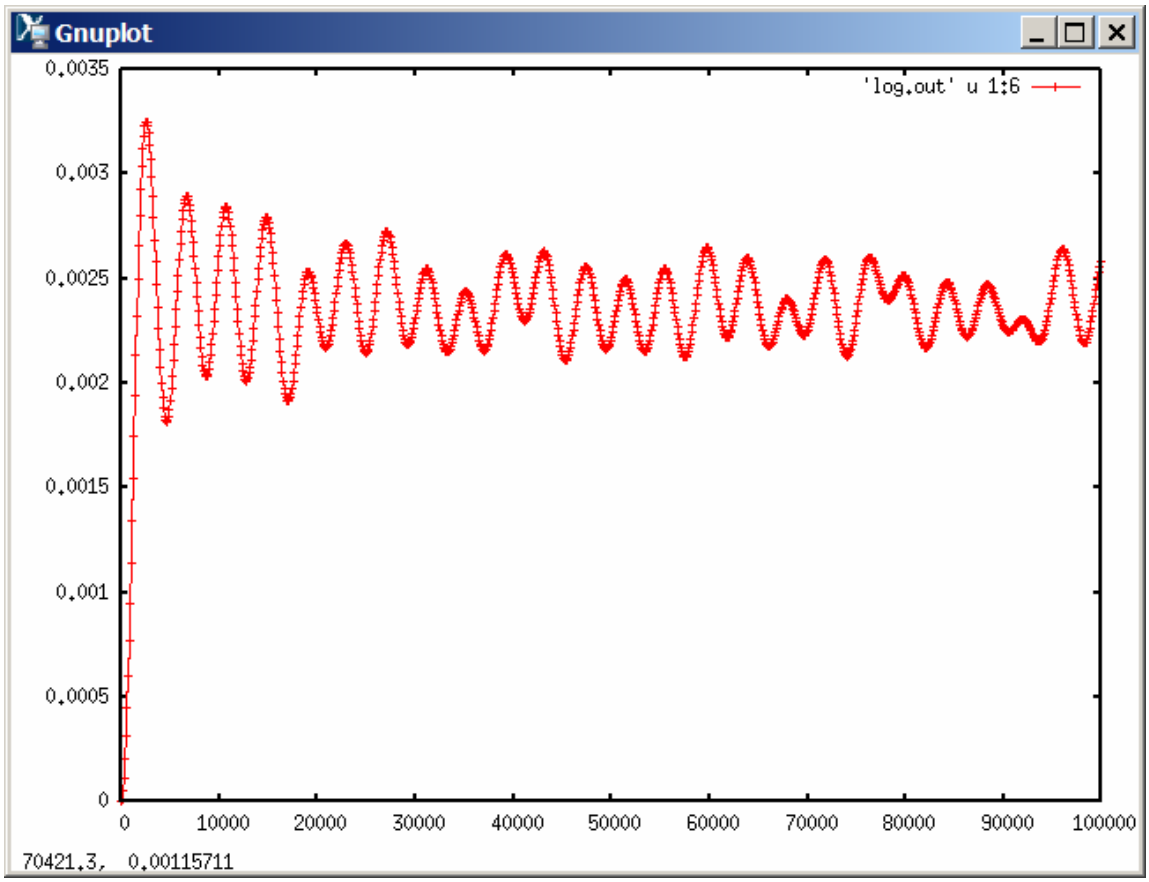
At high temperature, the phase of the nanowire changes to gas. Tensile test is not possible on a gas. Consequently, there is no Young's at this temperature.

(i).

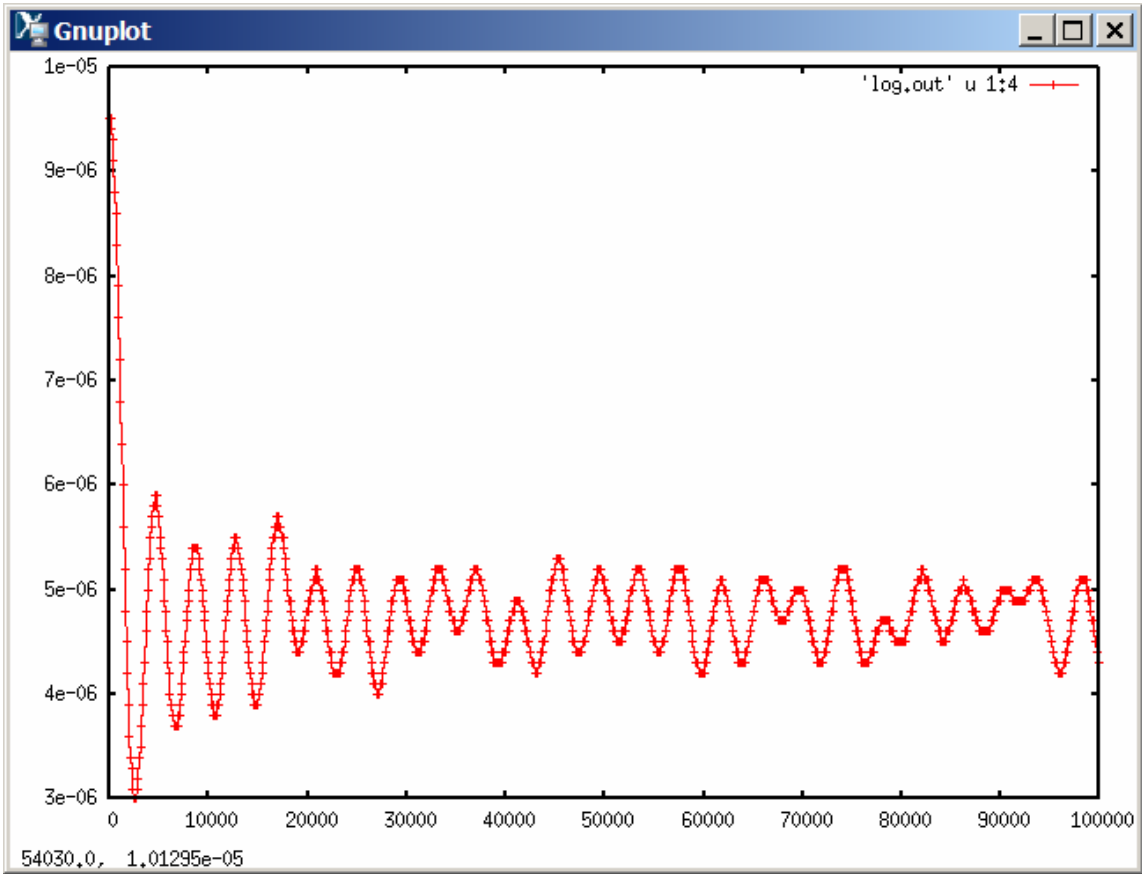
At different time steps the key mechanisms (slipping, shearing, necking) remain the same, they appear sooner (with less number of steps) at larger time step but there is a limit. At very large time step simulation crashes. In theory your time step should be small enough to capture highest frequency of atomic vibrations in your system.

(a)-(f): see code below

(g) **Potential energy plo**t (potential energy increases from zero [since all atoms are in EQ position] to a finite value). All simulations are done with 1,000 atoms.

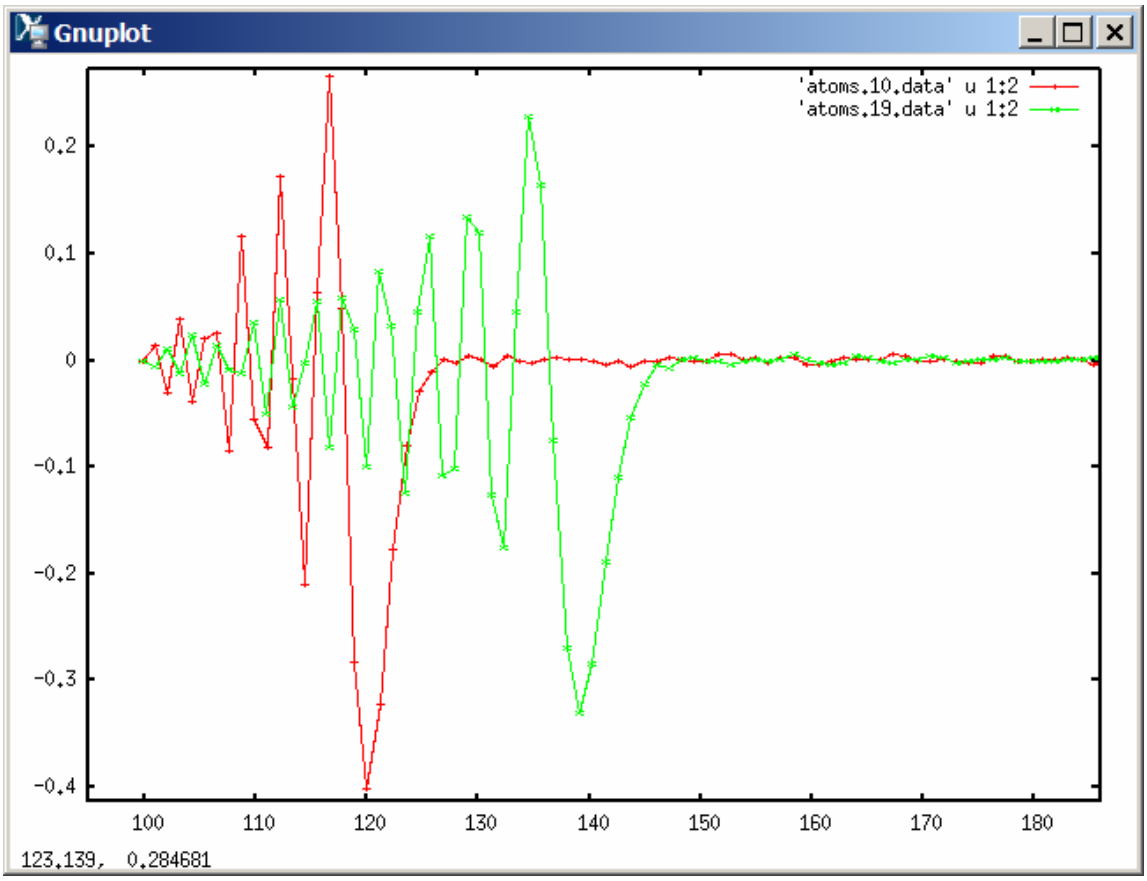


Temperature plot (temperature reaches 1⁄2 of initial value due to equipartition of potential and kinetic energy)



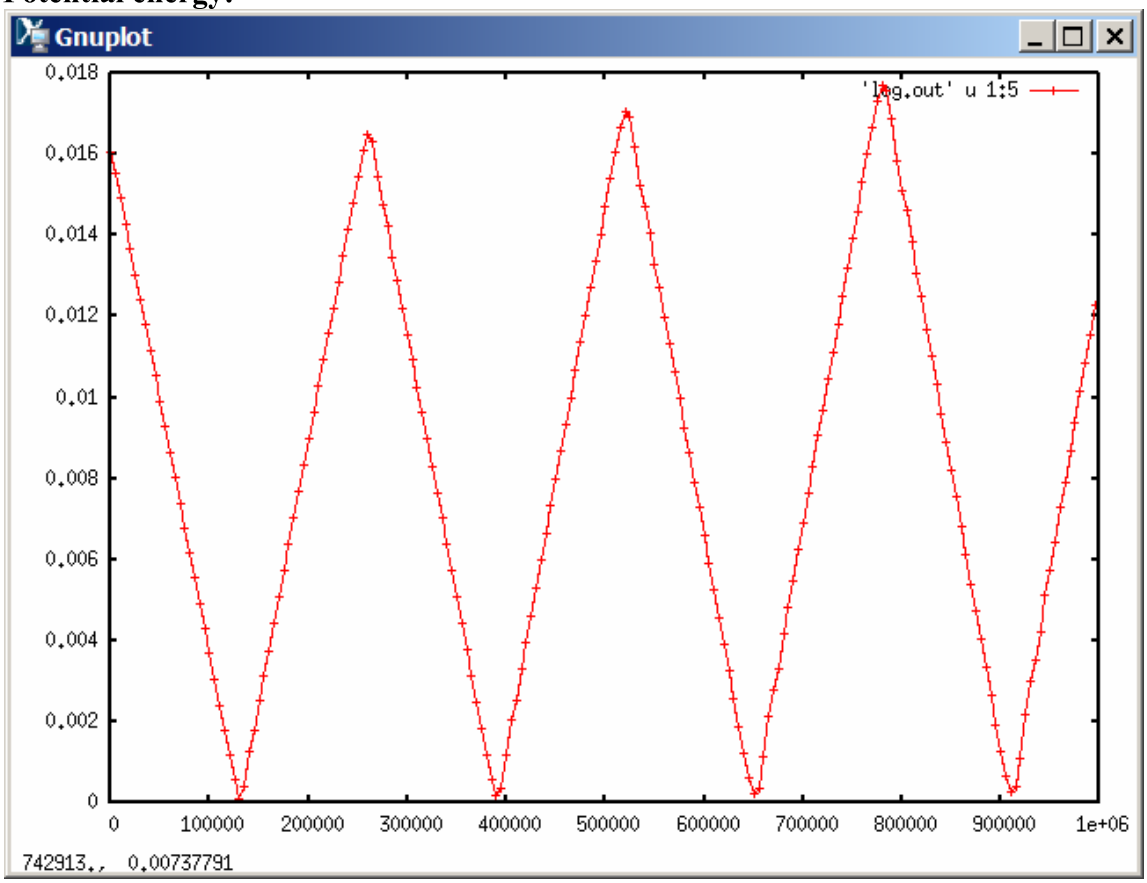
(h) **Wave speed determination** Theoretical prediction: $c_o = \sqrt{E/\rho}$ =6
Numerical solution, e.g. by following a signal generated by plucking the left end and calculating how fast it travels through the string of atoms.
Plot below shows velocity profile at snapshot 10 and 19. Time difference: **3.24**
Position difference: **19** Thus: estimate for wave speed: **5.84** (close to **6**)

Plot of particle velocity distribution (*x*-axis=position of atoms, *y*-axis=velocity), for two different time steps.



(i) **Prestrain system by 3%:** Observe increase in temperature since additional potential energy is moved into particle motion (kinetic energy). Initial potential energy no longer zero since all atoms are displaced from initial position.
This simulation done with 100 atoms (to see wave reflection earlier)
Simulation carried out over 1,000,000 steps (more than required, so that wave reflections can be seen).

Potential energy:



Temperature: