Au Nanowire Deformation using MD Simulations

MSE 203: Introduction to Computational Materials

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INTRODUCTION

- Au nanowires provide exceptional properties due to their high surface-to-volume ratio, and they are used in nanoelectronics and other biomedical devices.

- Deforming the nanowire under uniaxial tension and analysing the changes in stress-strain at different strain rates and temperatures helps us to improve the designs for further applications.

Concepts

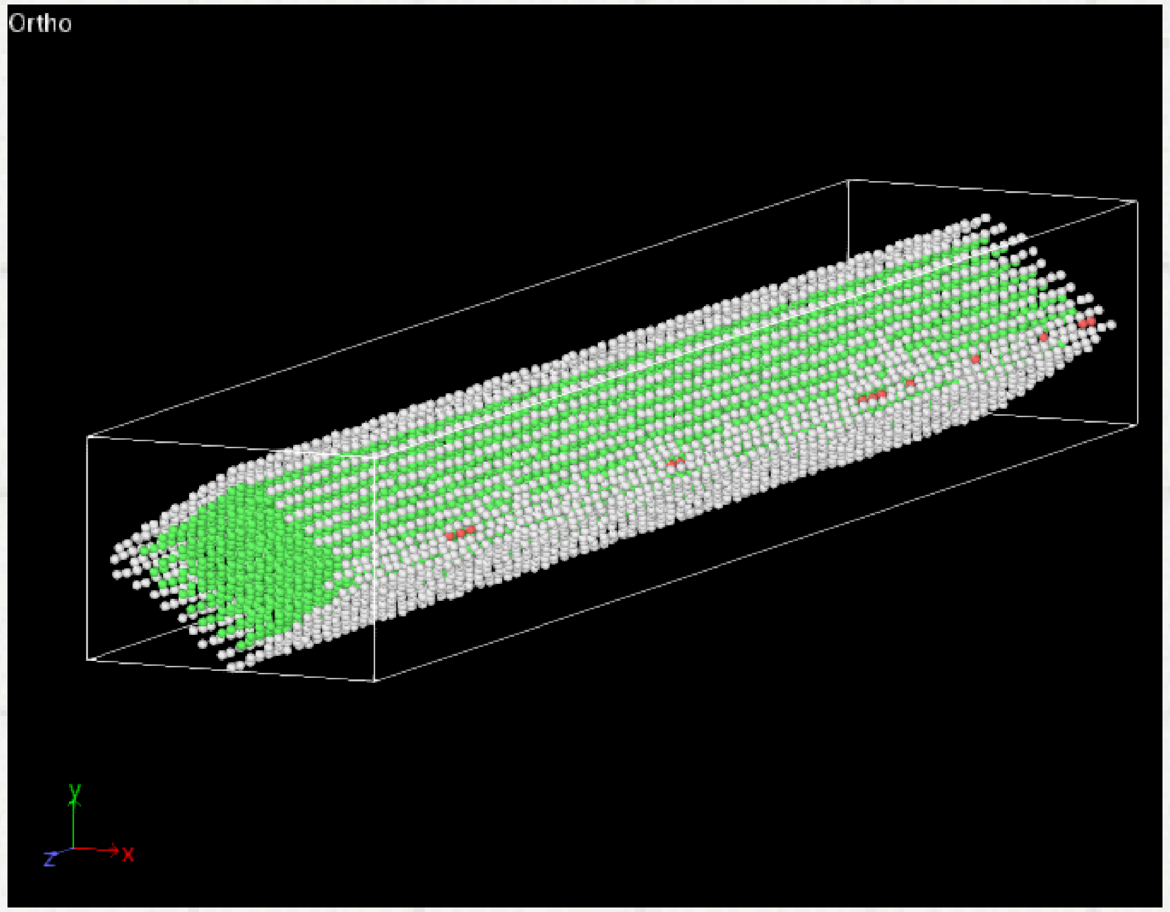
- Using MD simulations with the LAMMPS software to examine the influence of strain rate and temperature on the deformation characteristics of Au nanowires.
- Apply Embedded Atom method(EAM) pair wise potential to investigate nanoscale deformation mechanisms
- The embedding energies for all atoms and their pairwise interactions are summed to determine the system's total energy.
- Au nanowire is constructed in the simulation with a specified crystallographic structure and dimensions. So, The EAM potential calculates the forces acting on each atom due to its interactions with neighboring atoms.

Methodologies

This study employs classical molecular dynamics simulations via the LAMMPS software package to explain the deformation behavior of rhombohedral gold (Au) nanowires.

- The Embedded Atom Method (EAM) potential is used to accurately model pairwise interactions within the Au nanowire.
- Periodic boundary conditions are applied along the loading direction (z-axis) to simulate an infinitely long nanowire.
- Simulations are conducted under a canonical (NVT) ensemble, maintaining a constant number of atoms, volume, and temperature at 300 K.
- The strain rate used in the simulations will need to be converted into real-world units (e.g.2.5x10^9 s^-1)
- Stress and strain data are collected throughout the simulation to find yield strength and elastic modulus are extracted.
- The OVITO visualization software is employed to analyze atomic-level deformation mechanisms.

Specification of Au Wire



- Lattice with a lattice parameter = FCC 4.07 nm
- Origin(0 0 0), and Orientation (orient z 1 1 0 orient x 0 0 -1 orient y -1 1 0)
- Number of Atoms = 8000
- Size of rhombohedral box = (34.41734, 25.59622346, 208.76024)
- **Initial Condition:** Temperature=300K, Strain rate=0.0025ps, Number of running step=50000

LAMMPS Overview

LAMMPS is a classical molecular dynamics (MD) code that models ensembles of particles in a liquid, solid, or gaseous state. It can model atomic, polymeric, biological, solid-state (metals, ceramics, oxides), granular, coarse-grained, or macroscopic systems using a variety of interatomic potentials (force fields) and boundary conditions.

```
# Structure generation #
units           metal
atom_style      atomic
boundary        m m p
```

```
fix             1 all nvt temp 300.0 300.0 10.0
fix             2 all deform 200 z erate 0.0025
```

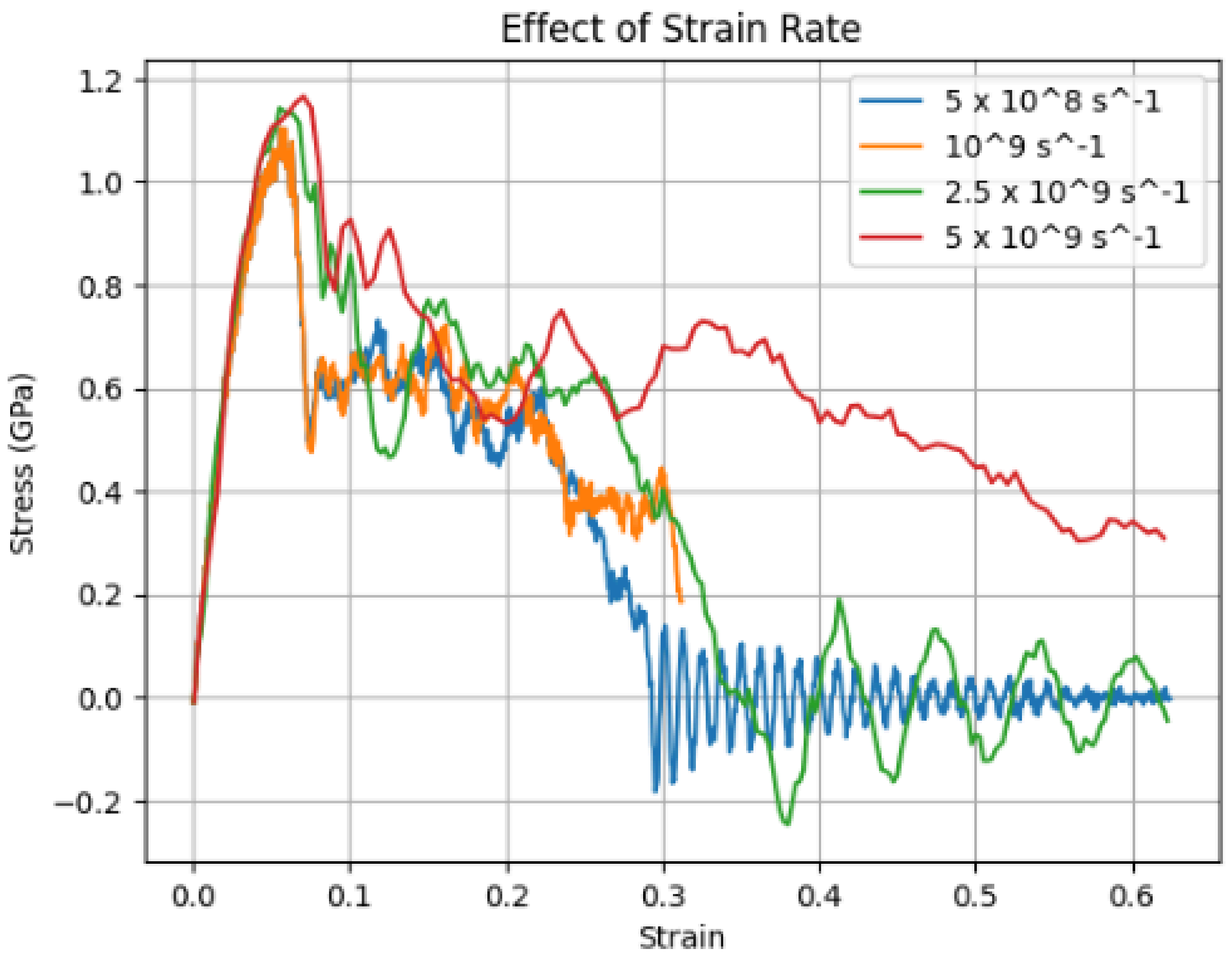
```
dump            1 all atom 2000 initial_equilibrium.dump
fix             1 all npt temp 300.0 300.0 10.0 z 0.0 0.0 10.0 drag 1.0
run             5000
unfix           1
undump          1
```

Result and Discussion

- Effect Of strain Rate and Temperature On Deformation
- Calculation of Yield strength, Yield Strain Rate and Modulus
- Visualization of deformation on OVITO

Effect of Strain Rates on Deformation of Au

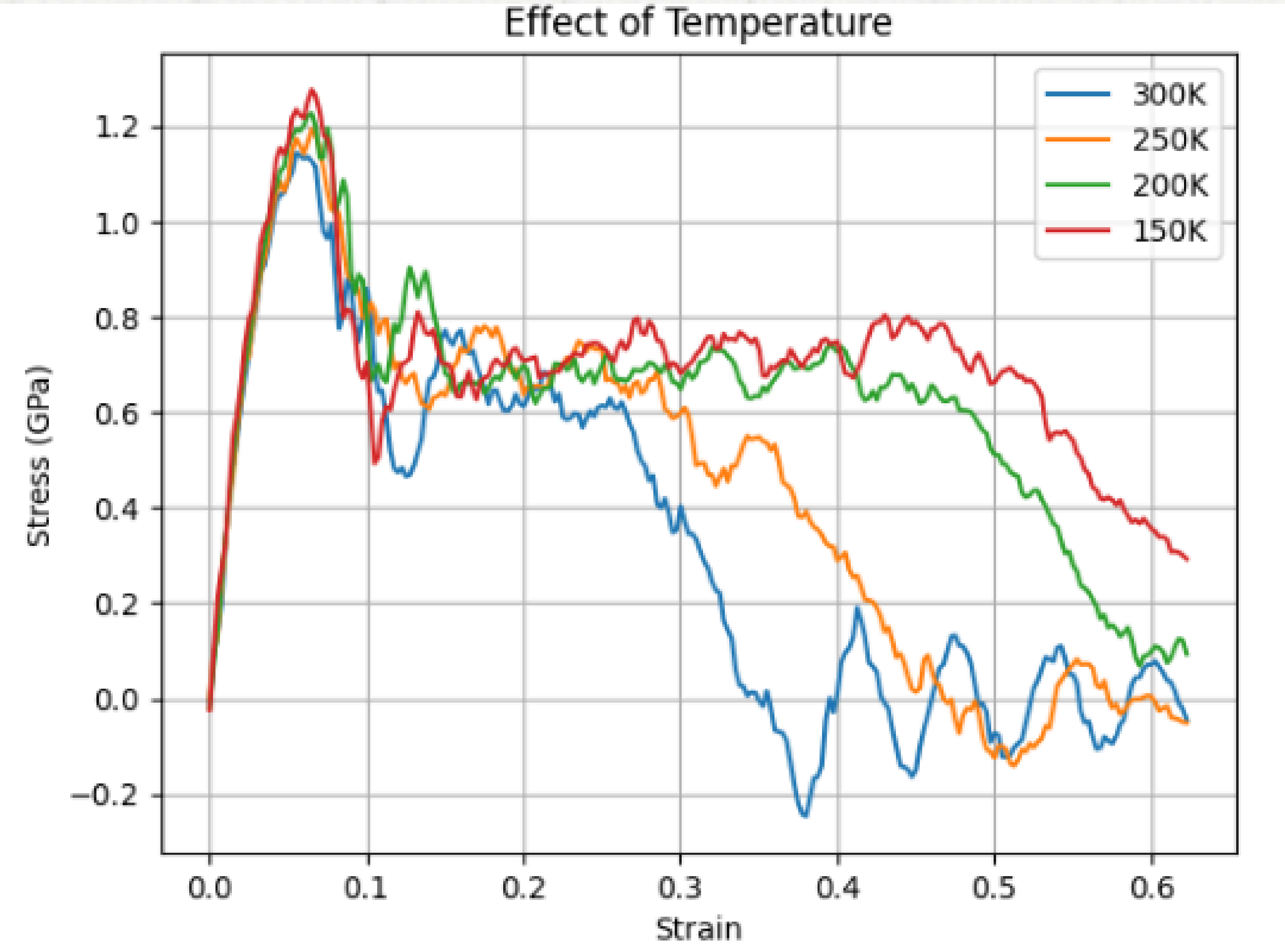
- The stress required to achieve a strain level increases as the strain rate increases.
- At higher strain rates, atoms have less time to rearrange and accommodate the deformation, so higher stress is required.
- We see that the elastic part remains unaffected by varying strain rates.
- The nonlinear part shows the plastic behaviour of the material after fracture.



Note: Run steps are adjusted at different strain rates to show similar strain on each stress and Temperature is constant (300K).

Effect of Temperature on Deformation of Au

- Overall, the graphs say that deforming the Au nanowire is easier at higher temperatures. The yield stress decreases as the temperature is higher.
- Likely due to increased atomic mobility at higher temperatures, allowing for easier atomic rearrangement and dislocation activity to accommodate the deformation.
- The material appears to soften more readily at higher temperatures. It can be seen in the steeper slopes at 250K and 300K curves.



Note: The strain rate and no. of run steps are kept fixed Strain rate = 0.0025/ps Run steps = 50000

Calculating Stress-strain response, yield strength, modulus

Steps For calculating yield strength and Yield strain:

- Calculating the slope of the stress-strain curve under elastic conditions by doing a linear fit
- That slope is called youngs modulus (hook's Law)
- Take 0.2% of strain and draw a line parallel to the modulus line
- The intersection of the stress-strain curve and 0.2% strain line gives the value of yield strength.
- **Young Modulus = 18.514 GPa**

Note : value of modulus is constant because it depends upon material

Tables:

This calculation is done at temp = 300K

Strain Rate (nm^-1)	Yield Strain(%)	Yield Strength
0.5	5.66	1.01
1	5.81	1.04
2.5	6.23	1.12
5	6.75	1.12

This calculation is done at strain rate = 0.0025/ ps

Temperature (k)	Yield Strain%	Yield Strength (GPa)
150	6.98	1.25
200	6.73	1.21
250	6.73	1.21
300	6.23	1.12

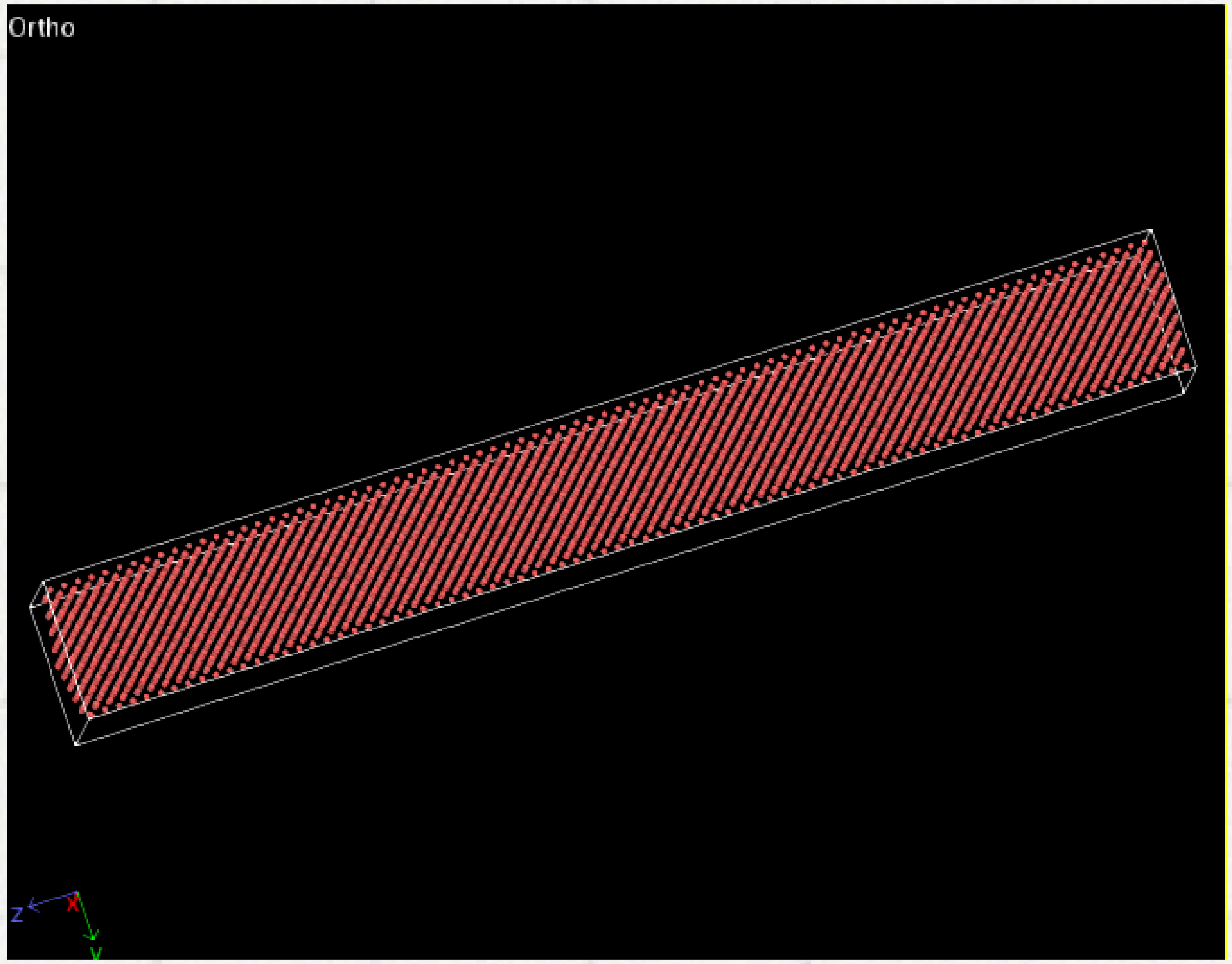
Strain Rate:

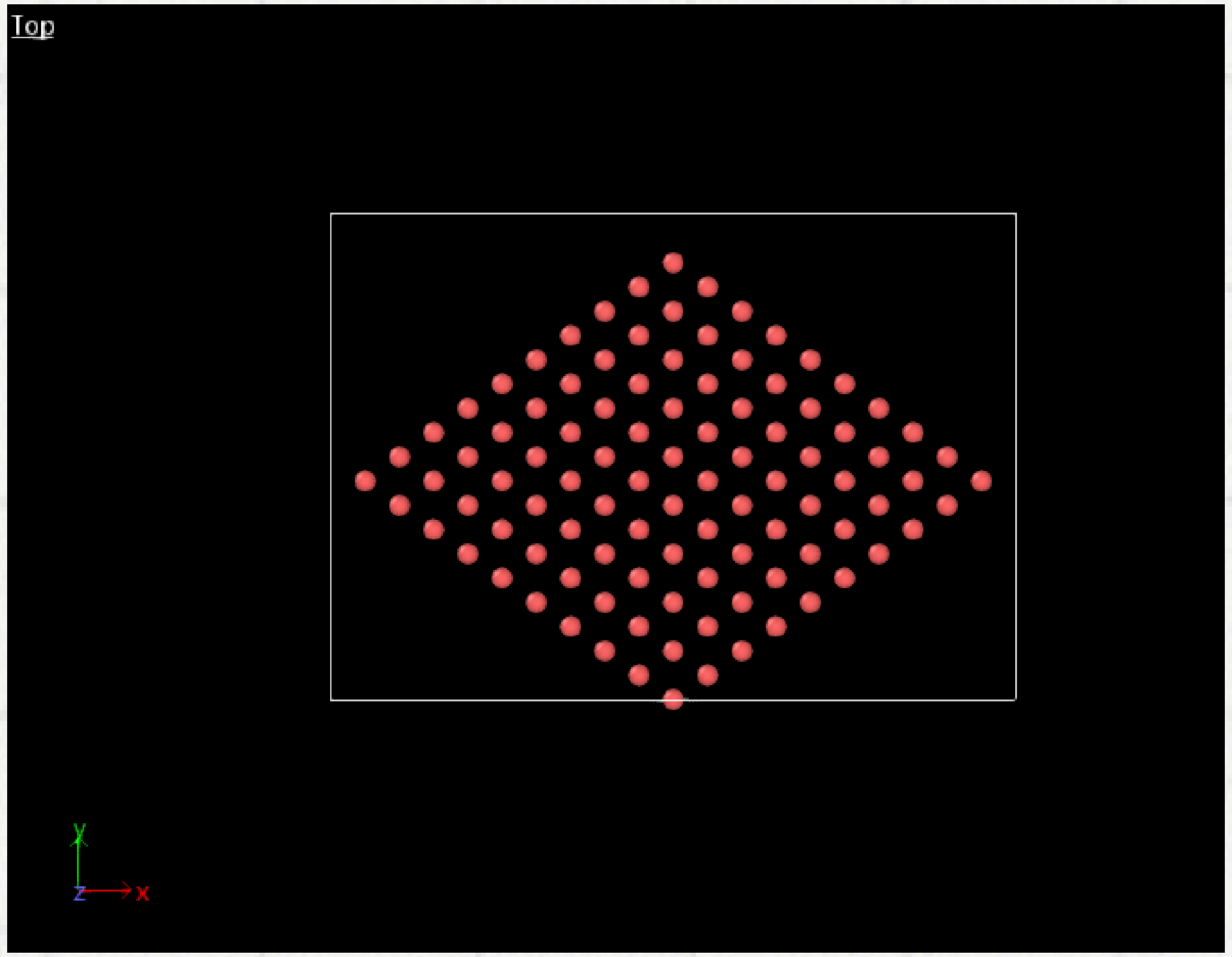
- Increasing strain rate leads to higher yield strength and yield strain.
- Materials become stronger and tolerate more deformation before yielding under faster loading.

Temperature:

- Increasing temperature reduces yield strength and yield strain.
- Materials become softer and yield more easily at higher temperatures.
- This trend may not apply to all materials at extreme temperatures.

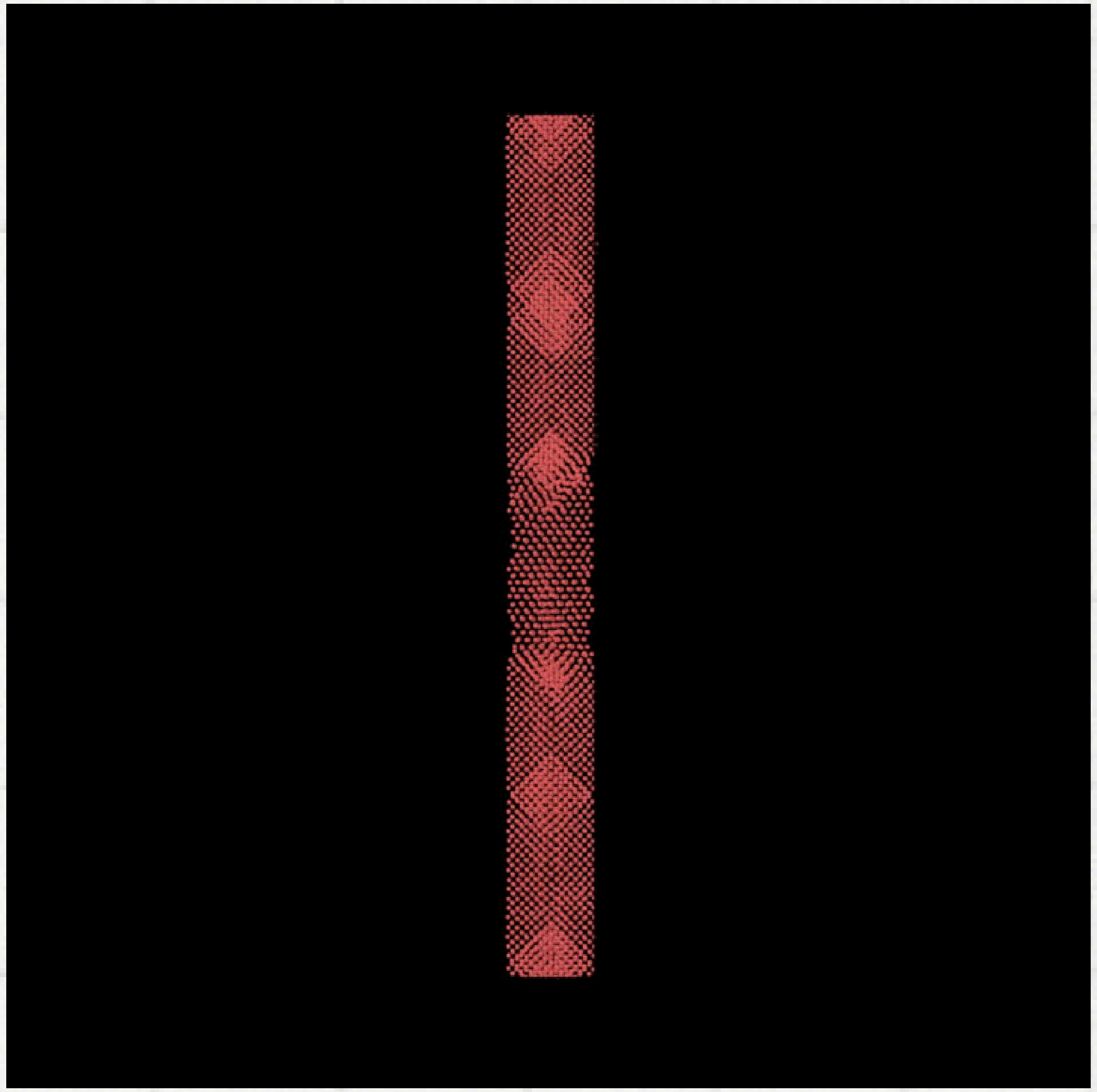
OVITO Visualization





Fracture Simulation

- The nanowire starts elastic deformation initially, which we can observe as the wire gets elongated along the z-axis, and the cross-section area shrinks without any deformation.
- The wire starts to plastically deform as we can observe non-uniform stretching of the wire.
- The wire starts forming a neck structure after the point of Ultimate Tensile Strength.
- The material finally fractures, with the wire breaking into two parts.



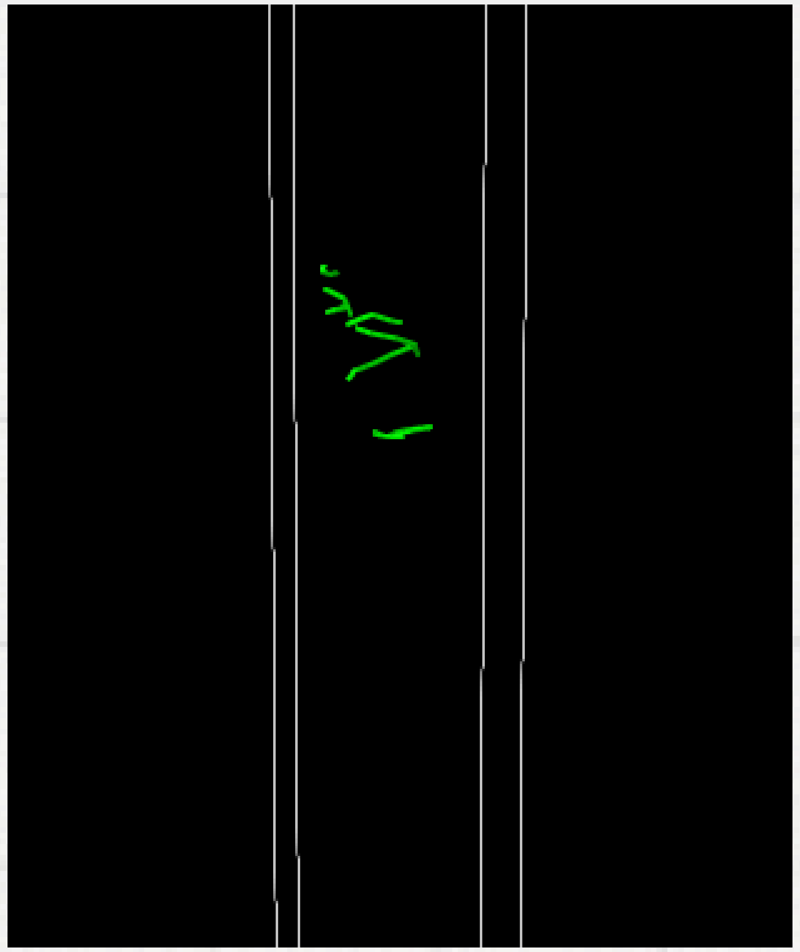
Dislocation Analysis

- Ovito has a modifier which works on the construction of burgers circuits and identifying different types of dislocations.

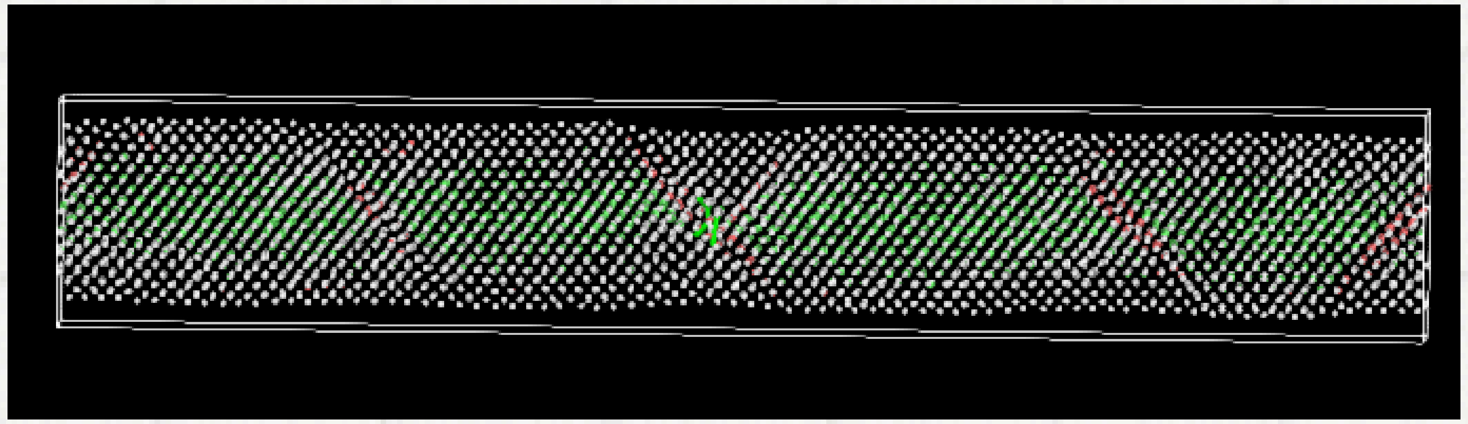
- The analysis reported multiple instances of Shockley partial dislocations.

Dislocation analysis results:

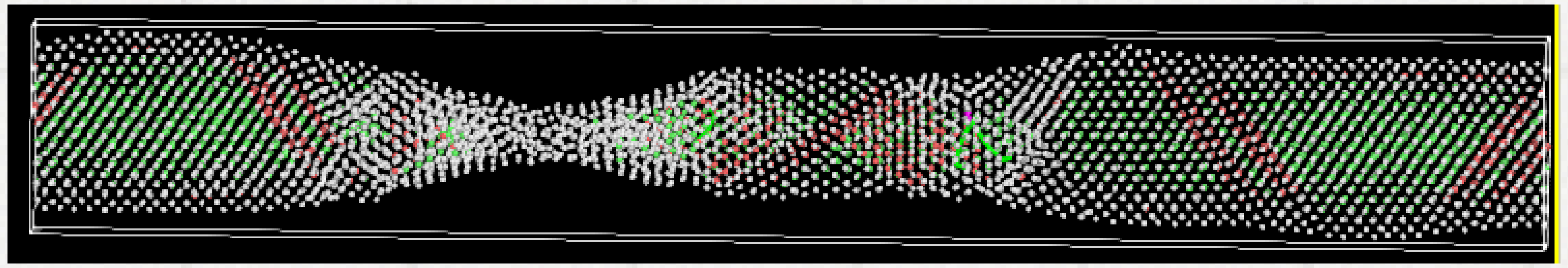
Dislocation type	Segs	Length
Other	0	0
1/2<110> (Perfect)	0	0
1/6<112> (Shockley)	8	101.996
1/6<110> (Stair-rod)	0	0
1/3<100> (Hirth)	0	0



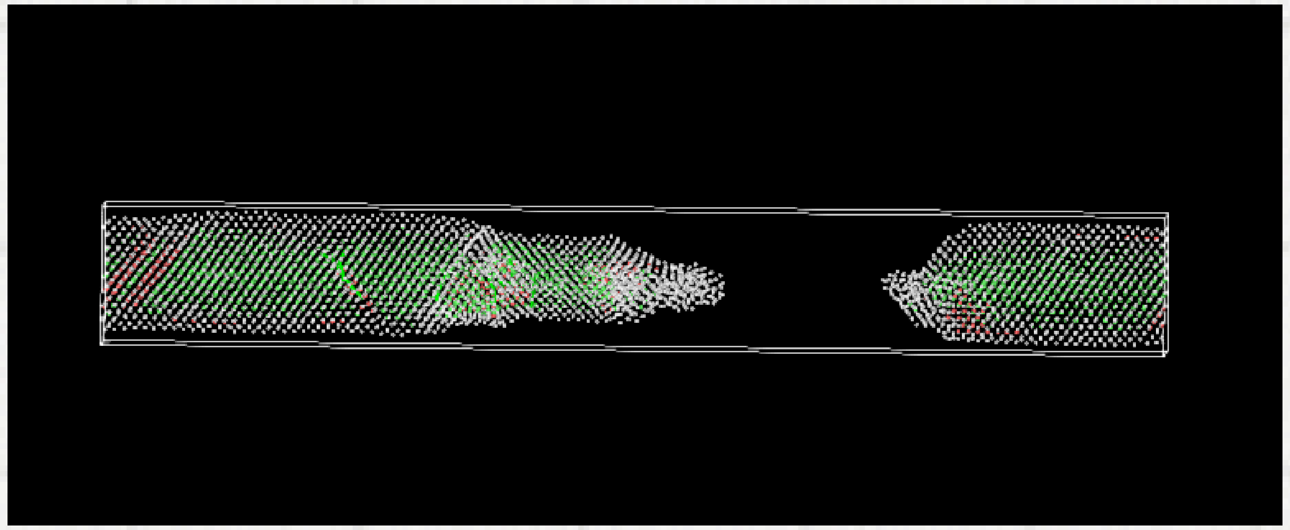
Dislocations at Stages



	Dislocation type	Segs	Length
	1/2<110> (Perfect)	0	0
	1/6<112> (Shockley)	2	18.3596
	1/6<110> (Stair-rod)	0	0
	1/3<100> (Hirth)	0	0
	1/3<111> (Frank)	0	0



	Dislocation type	Segs	Length
	1/2<110> (Perfect)	0	0
	1/6<112> (Shockley)	3	33.8848
	1/6<110> (Stair-rod)	1	2.85635
	1/3<100> (Hirth)	0	0
	1/3<111> (Frank)	0	0



	Dislocation type	Segs	Length
	Other	0	0
	1/2<110> (Perfect)	0	0
	1/6<112> (Shockley)	6	99.2495
	1/6<110> (Stair-rod)	0	0
	1/3<100> (Hirth)	0	0

Conclusion

- Observed the deformation of Au nanowires using MD simulations using LAMMPS and concepts based on EAM. The simulation shows gold nanowire deforms under uniaxial tension along the z-axis.

- As the temperature decreases from 300K to 150K with a stepsize of 50K, the material fractures slower than at higher temperatures. At 150K, the material does not fracture at all.

- As the strain rate varies, the material is strained slowly, which means that the material will take time to fully elastically deform and start plastic deformation, which will lead to fracture. At higher strain rates, the material deforms faster.

Thank you