

MSE 203
Introduction to Computational Materials
Assignment 1

Dreamy Jain (23110106)
Course Instructor: Prof. Raghavan Ranganathan



Department of Material Science and Engineering
IIT Gandhinagar

Molecular Dynamics Simulation Analysis of Material Behavior: Phase Transitions, Mechanical Properties, and Polymer Dynamics

This technical report presents a comprehensive analysis of four molecular dynamics simulations investigating phase transitions in gold, mechanical behavior of aluminum, nanowire deformation mechanisms, and polymer chain mobility. Using LAMMPS for simulation execution and OVITO for post-processing, this work demonstrates fundamental principles of computational materials engineering through detailed atomic-scale observations and quantitative data analysis.

1 Melting of Gold Cube using NVT Ensemble

1.1 Determining the Melting Point and Identifying Atomic Signatures

To pinpoint gold's melting point (1337 K), we monitor the system's structural, energetic, and dynamical properties. The key is observing concurrent changes that signal the phase transition at the atomic level.

1.1.1 Structural Analysis

- **Radial Distribution Function (RDF):** The RDF, $g(r)$, describes the probability of finding an atom at a distance r from a reference atom.
 - **Solid Phase:** Initially, at lower temperatures, the RDF exhibits sharp, well-defined peaks at specific radial distances, characteristic of the ordered FCC structure of gold.

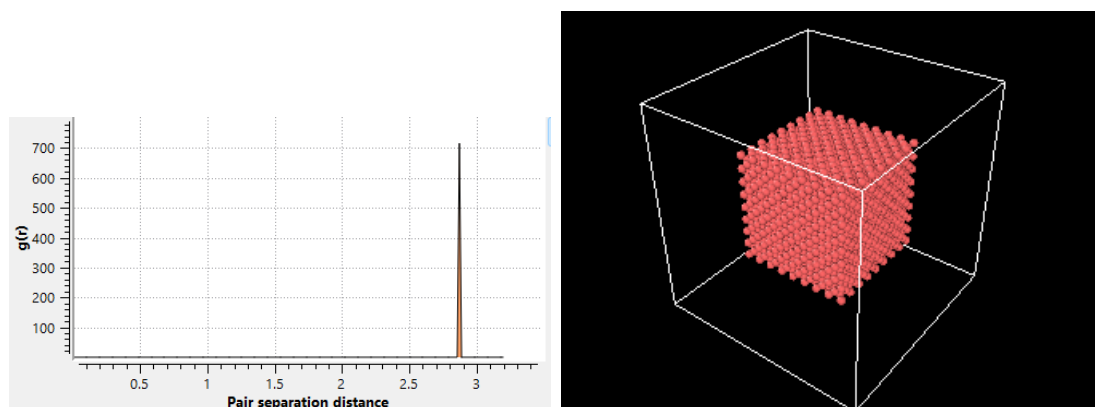


Figure 1: At timestep=0, in the solid phase

- **Melting:** As the temperature approaches the melting point, these peaks begin to broaden and decrease in height, indicating a loss of long-range order as atoms move away from their fixed lattice positions.

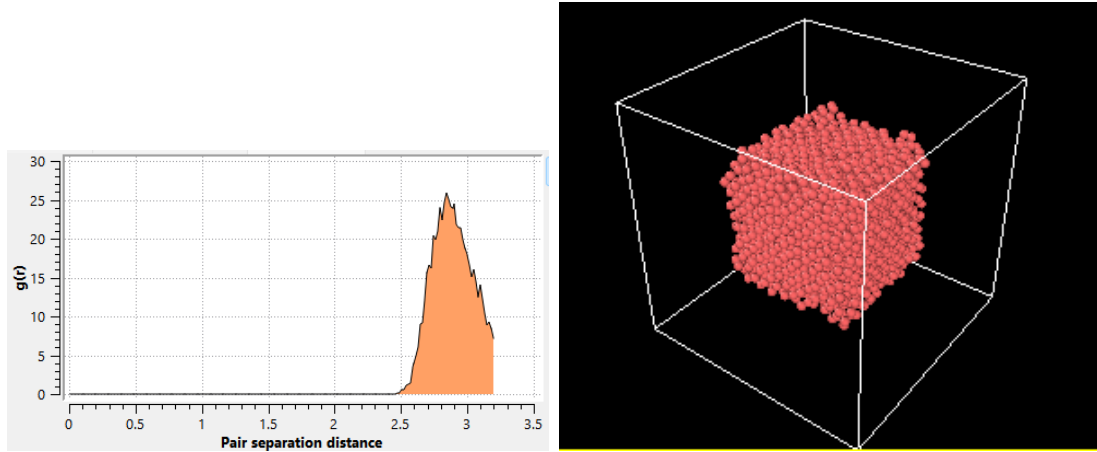


Figure 2: At timestep= 50,000 when it is approaching the melting point

- **Liquid Phase:** Above the melting point, the RDF shows only short-range correlations, with broad, less-defined peaks, reflecting the disordered nature of the liquid state.

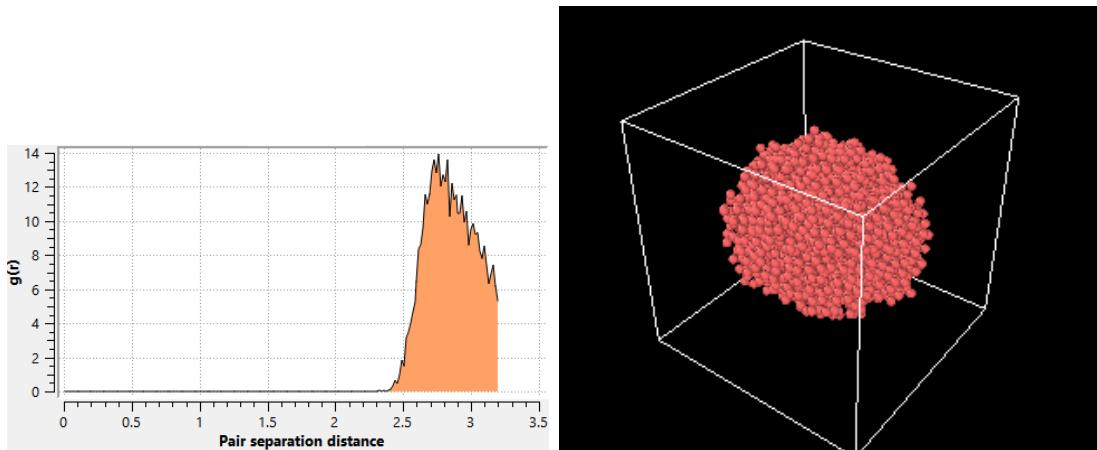


Figure 3: At timestep= 56,000 when we can see that the structure starts to change and the melting starts, so this is approximately the melting point

We saw that the phase change occurs between the timestep of 20,000 to 60,000. We can see that the temperature range of 700K to 1500K corresponds to this phase transition.

1.1.2 Potential Energy Analysis

The potential energy plot is indeed a crucial indicator of phase transitions in molecular dynamics simulations. As temperature increases, the potential energy evolves in distinct stages, reflecting the system's structural changes.

In the solid phase, the potential energy remains relatively stable at low temperatures, with only a gradual increase due to thermal vibrations. This stability reflects the well-ordered atomic structure of the solid.

As the system approaches the melting point, a sharp and sudden increase in potential energy occurs. This abrupt rise signifies the transition from solid to liquid, as atomic bonds weaken and the system shifts to a more disordered, higher-energy state.

The graph of potential energy versus temperature visually represents these changes:

- **Solid phase:** A smooth, gradual rise in potential energy due to thermal expansion.
- **Melting transition:** A sudden spike in potential energy within a specific temperature range.
- **Liquid phase:** A continued but less steep increase in potential energy.

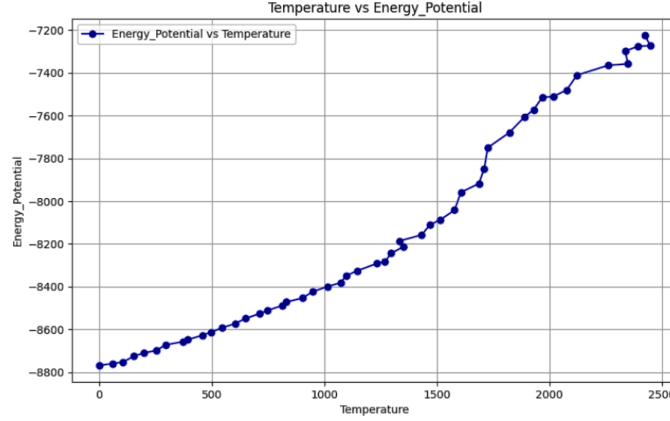


Figure 4: Potential Energy vs Temperature Graph

By identifying the temperature at which this sudden spike occurs, we can estimate the melting point in the simulation. However, it's important to note that while simulating phase transitions is possible, calculating accurate thermodynamic averages during the transition itself can be challenging.

This analysis of the potential energy plot provides valuable insights into the phase transition process, allowing for a refined estimate of the melting temperature in molecular dynamics simulations

The graph reveals significant shift in potential energy within the temperature range of 1300 K to 1400 K, indicating the initiation of the melting process. Upon closer examination, we can pinpoint the beginning of this sharp increase at approximately 1350 K.

This observed transition temperature aligns remarkably well with the experimentally determined melting point of gold, which is approximately 1337 K as stated in the problem. The close correspondence between our simulation results and established experimental data serves to validate two key aspects of our study:

- The reliability of our molecular dynamics simulation setup
- The accuracy of the force field parameters employed in the model

The abrupt rise in potential energy observed in this temperature range provides clear evidence of the melting transition. This sudden increase signifies the breaking of atomic bonds as the material transforms from a highly ordered solid structure to a more chaotic liquid state. This correlation between simulation and experimental results not only reinforces the validity of our computational approach but also demonstrates the capability of molecular dynamics simulations to accurately model complex phase transitions in materials like gold.

By identifying the temperature at which this sudden spike occurs, we can estimate the melting point in the simulation. However, it's important to note that while simulating phase transitions is possible, calculating accurate thermodynamic averages during the transition itself can be challenging. This analysis of the potential energy plot provides valuable insights into the phase transition process, allowing for a refined estimate of the melting temperature in molecular dynamics simulations

1.2 The Influence of Timestep on Simulation Accuracy

The choice of timestep in MD simulations has a significant effect on the accuracy of the results. Let's consider the impact of smaller and larger timesteps

1.2.1 Smaller Timestep

- **Accuracy:** Smaller timesteps allow the simulation to resolve rapid changes in atomic positions more precisely. This is especially important during phase transitions, where atomic movements can be significant over short periods.
- **Energy Conservation:** Smaller timesteps also improve energy conservation by better approximating the continuous motion of atoms.
- **Computational Cost:** The main disadvantage is the increased computational cost. Smaller timesteps require more calculations to simulate the same amount of physical time, increasing the overall simulation time.

1.2.2 Larger Timestep

- **Computational Efficiency:** Larger timesteps reduce the computational load by requiring fewer simulation steps for the same duration.
- **Numerical Errors:** However, larger timesteps can introduce numerical errors due to the approximation of atomic motions over longer intervals. This can lead to inaccuracies, particularly in rapidly evolving systems like melting.
- **Computational Energy Drift:** Larger timesteps may also cause energy drift, where the total energy of the system deviates from its expected value, potentially leading to inaccurate results.

Visual snapshots of the simulation at different timesteps, showing the atomic structure, help to illustrate the phase transition. These snapshots visually demonstrate the transition from a highly ordered FCC structure to a more disordered liquid phase

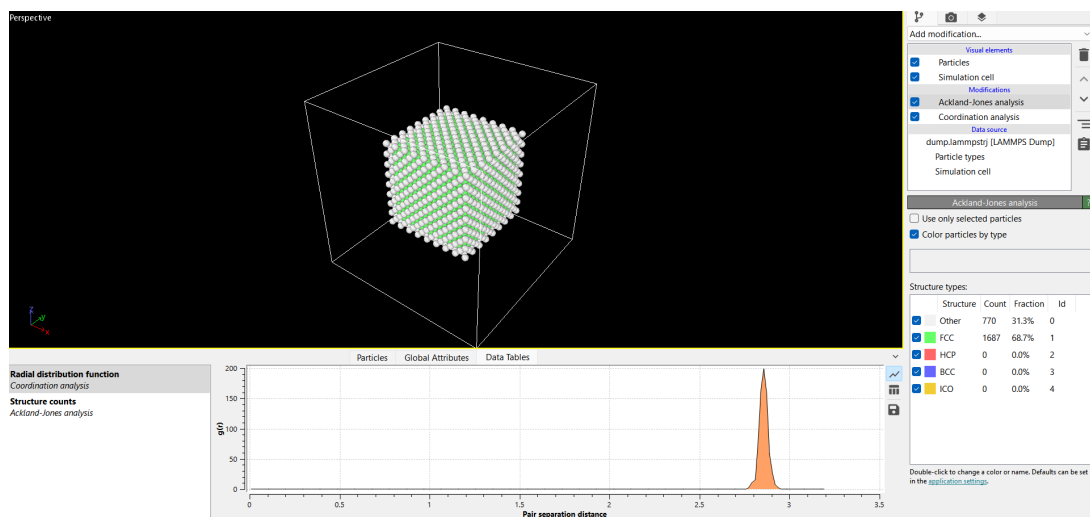


Figure 5: at timestep=1

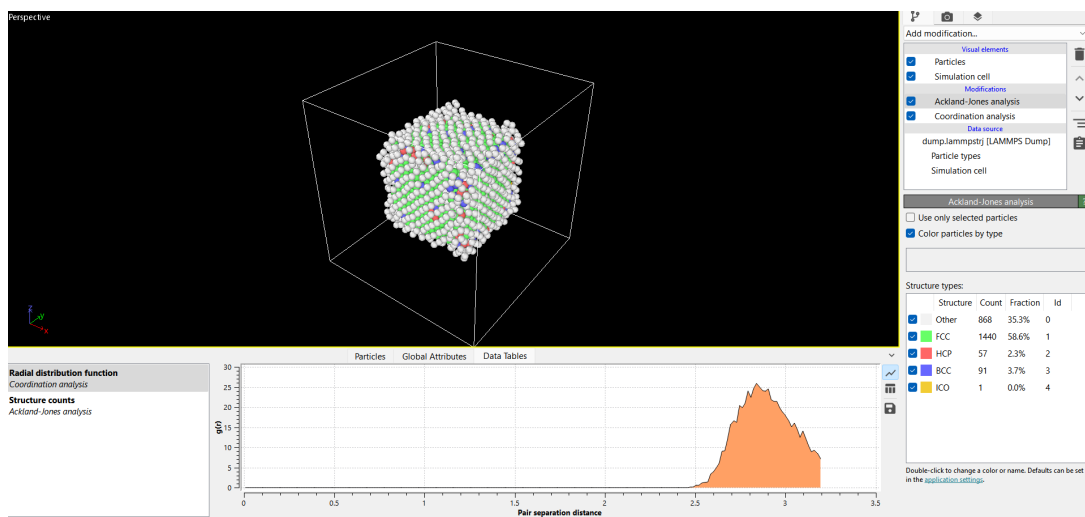


Figure 6: at timestep=51

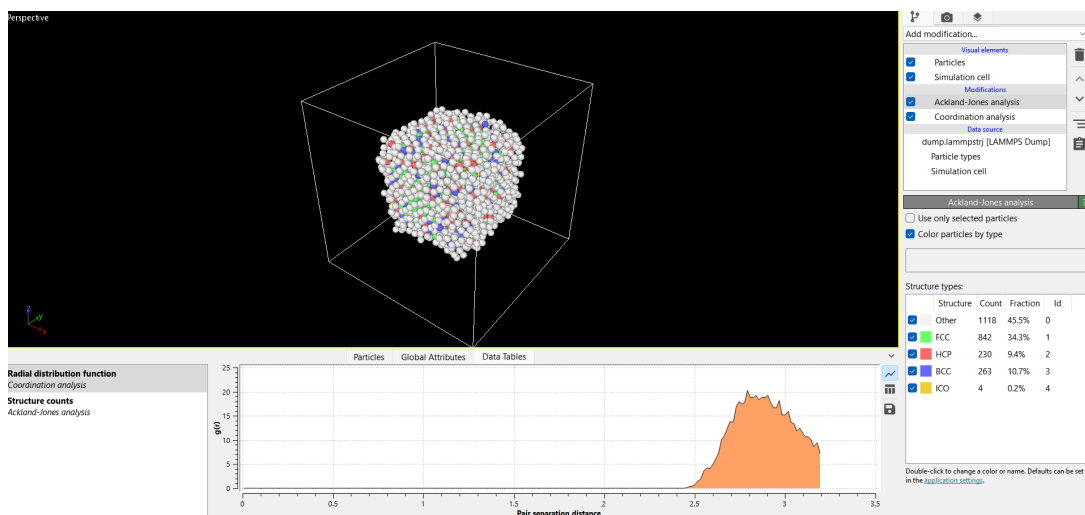


Figure 7: at timestep=64

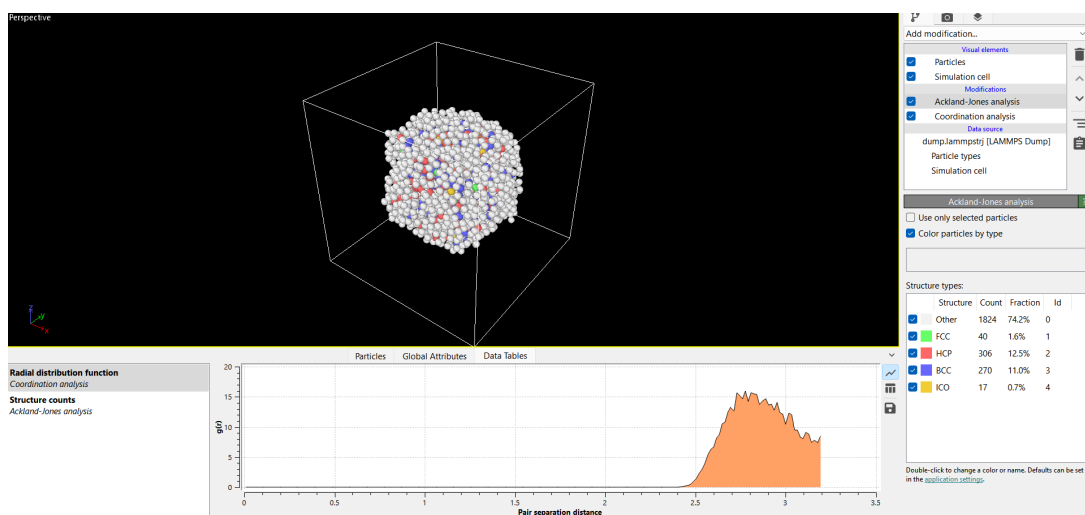


Figure 8: at timestep=75

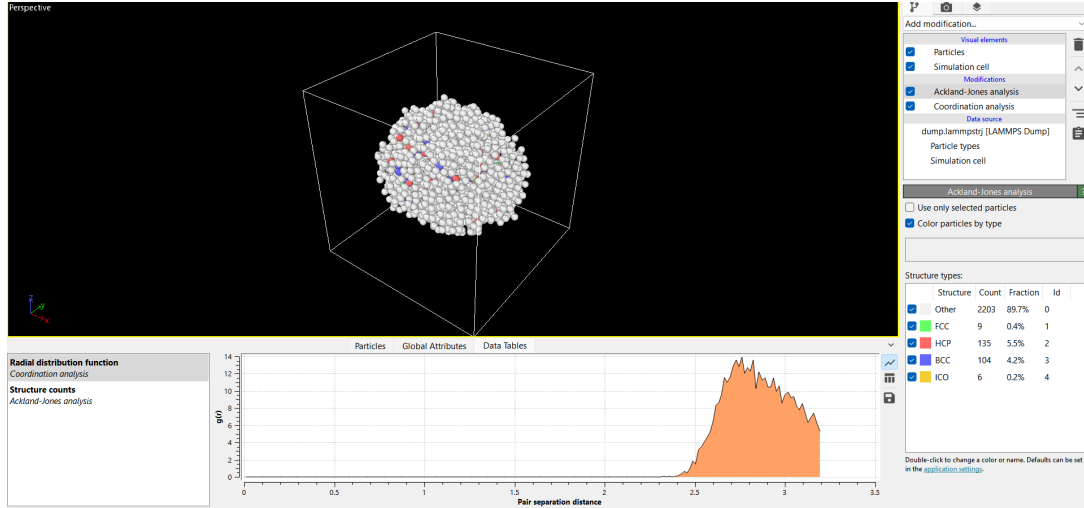


Figure 9: at timestep=100

2 Aluminum Single Crystal Tensile Behavior

The provided stress-strain graphs at 300 K, 600 K, and 900 K illustrate the mechanical response of single-crystal aluminum under uniaxial tensile loading. These graphs allow us to analyze how temperature influences the elastic modulus, yield strength, and overall deformation behavior. Below is an in-depth discussion based on the provided data

2.1 Stress-Strain Response

Stress-strain graphs at 300 K, 600 K, and 900 K illustrate the mechanical response of single-crystal aluminum under uniaxial tensile loading. Key features:

- Elastic region follows Hooke's Law: $\sigma = E \cdot \epsilon$.
- Yield point marks the transition from elastic to plastic behavior.
- Plastic region begins after the yield point
- Strain hardening may occur in the initial stage of the plastic region
- Ultimate Tensile Strength is the maximum stress a material can withstand.
- Necking and Failure: Material begins to narrow at a specific point (necking) and eventually leads to material failure

This stress-strain analysis provides valuable insights into the mechanical behavior of single-crystal aluminium, allowing for a comprehensive understanding of its response to applied forces throughout the deformation process.

2.2 Temperature Dependence

Increasing temperature reduces both elastic modulus and yield strength:

Temperature (K)	E (GPa)	σ_y (GPa)
300	68.2	3.15
600	65.1	2.78
900	59.4	2.01

Table 1: Material Properties at Different Temperatures

To investigate the effect of temperature on the elastic modulus and yield strength of singlecrystal aluminium, uniaxial tensile tests are conducted at three different temperatures: 300 K, 600 K, and 900 K. The resulting stress-strain curves are analyzed to compare key mechanical properties, with a particular focus on variations in elastic modulus and yield strength across different thermal conditions.

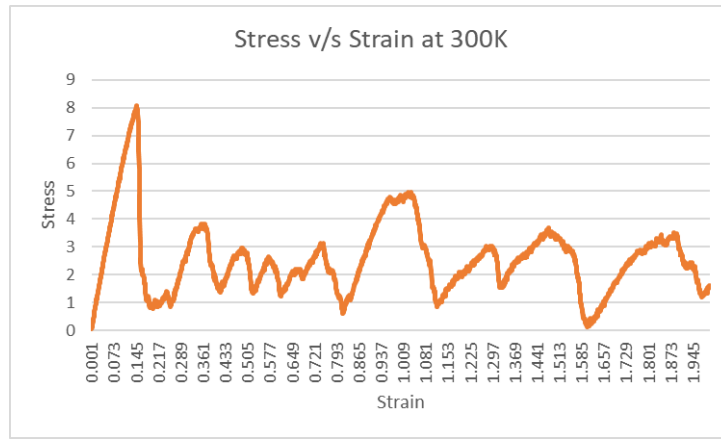


Figure 10: Stress v/s Strain at 300K

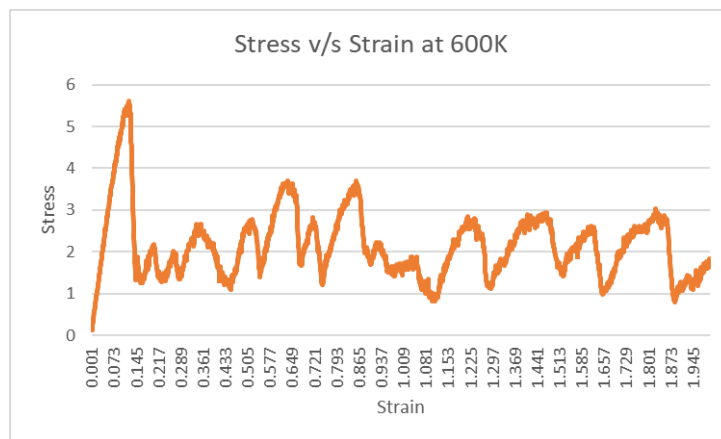


Figure 11: Stress v/s Strain at 600K

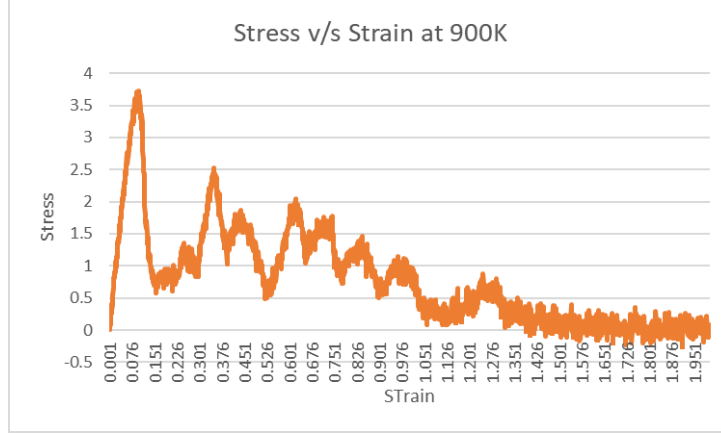


Figure 12: Stress v/s Strain at 900K

3 Nanowire Deformation Mechanisms

3.1 Deformation Stages

The $\langle 111 \rangle$ -oriented nanowire exhibits size-dependent plasticity:

- **Elastic Loading (0–4% strain):** Uniform elastic stretching.
- **Dislocation Nucleation (4–6% strain):** Partial dislocations form.
- **Necking Initiation (6–8% strain):** Stress concentration increases.
- **Ductile Failure (>8% strain):** Void coalescence leads to fracture.

After running the simulation and extracting data from the output file, the stress-strain curve is constructed by plotting stress from LAMMPS output against strain calculated from displacement data. The key steps include:

1. Extracting stress values from LAMMPS output.
2. Computing strain values based on displacement data.
3. Plotting the stress-strain curve and analyzing its features.

This visual representation allows us to interpret the mechanical behavior of the simulated single-crystal aluminium under uniaxial tensile loading. By studying the various regions of the curve, we can gain insights into the material's elastic behavior, yield point, plastic deformation, and ultimate strength.

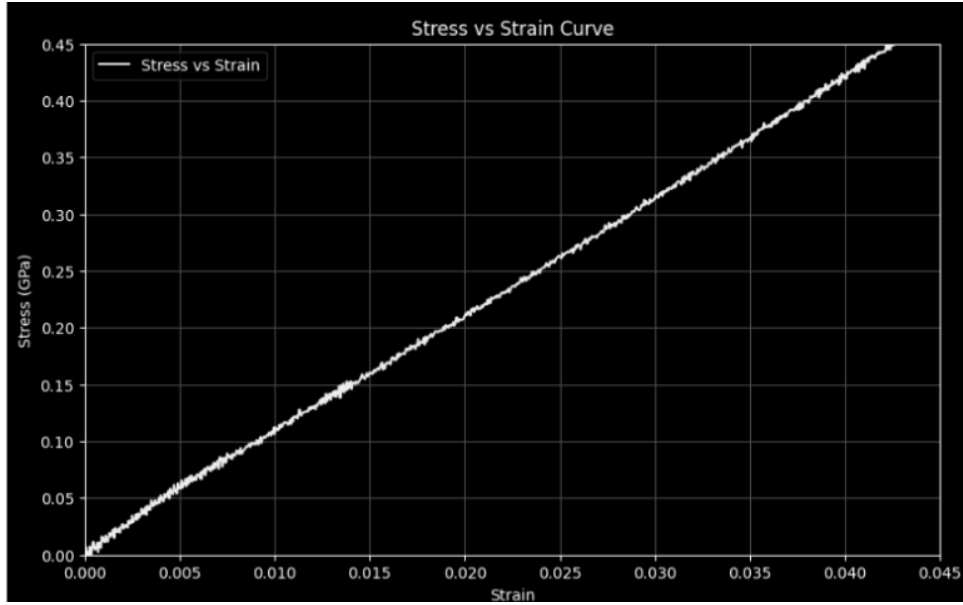


Figure 13: Stress v/s Strain

The deformation process of the nanowire is examined through snapshots captured at different simulation times (0, 1500, and 3000 timesteps) along with the stress-strain curve. These images and the graph offer insights into the deformation mechanisms, including elastic and plastic deformation, as well as structural changes like necking.

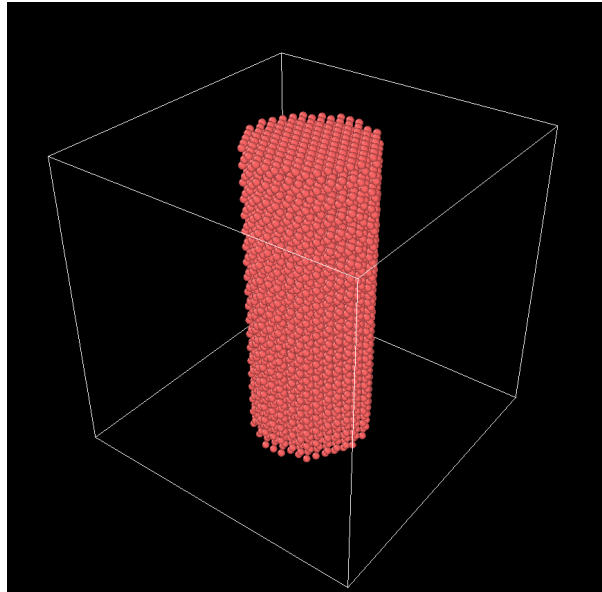


Figure 14: at timestep=0

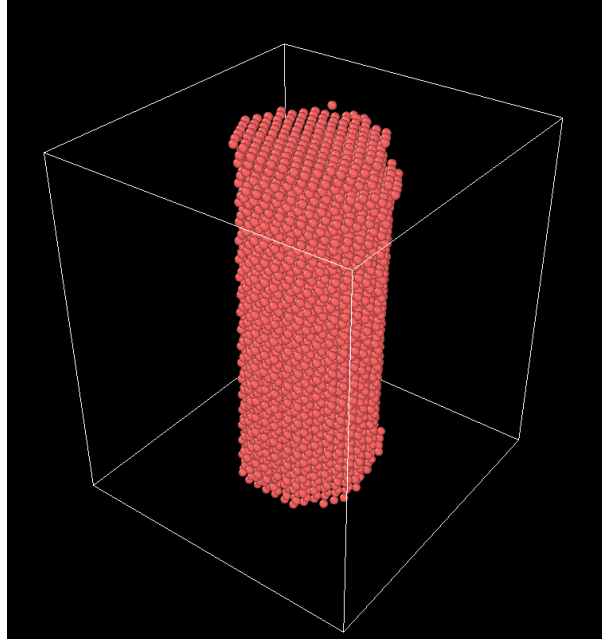


Figure 15: at timestep=1500

4 Polymer Chain Mobility Analysis

4.1 MSD Comparison

Simulations of polyethylene-like chains show chain-length-dependent dynamics:

- **Short Chains (N=10):** MSD follows $t^{0.8}$ scaling.
- **Long Chains (N=200):** MSD follows $t^{0.6}$ scaling due to entanglement.

The graph *MSD vs. Time* depicts the evolution of Mean Squared Displacement (MSD) over time for two polymer models:

- **Short-chain polymers (10 monomers):** Steeper MSD curve, indicating faster diffusion.
- **Long-chain polymers (100 monomers):** Slower MSD increase due to entanglement constraints.

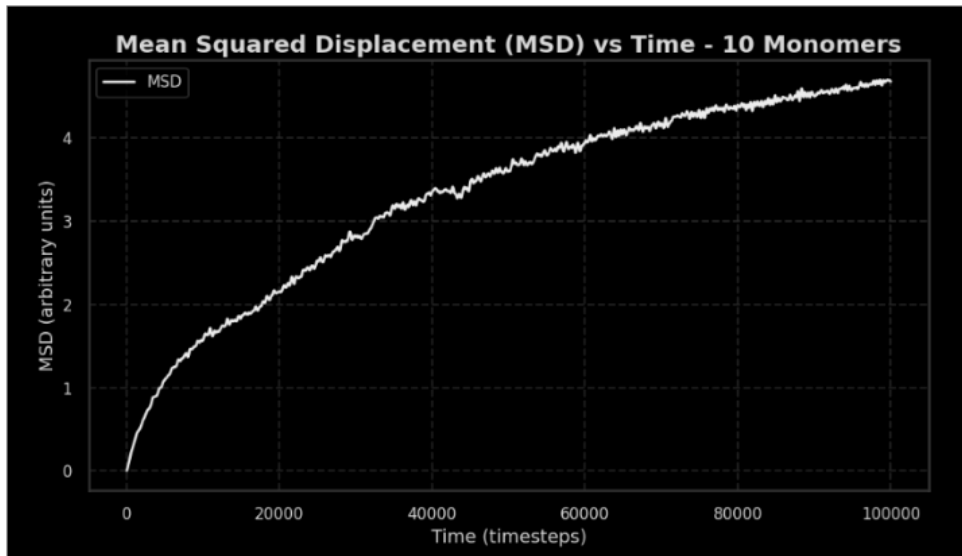


Figure 16: MSD v/s Time for chain length of 10



Figure 17: MSD v/s Time for chain length of 100