LAMMPS: aluminum (Al) molecular modeling simulation

Description:

How does the atomic-scale structure and mechanical response of single-crystal aluminum evolve under uniaxial tensile deformation, and how do thermal fluctuations and simulation size affect the stress-strain behavior and energy convergence of the system?

Tools:

To answer this question, we employed classical molecular dynamics (MD) simulations using the LAMMPS engine with an embedded atom method (EAM) potential for aluminum. This approach is particularly suited to capture the many-body interactions governing metallic bonding and plasticity in Al. Simulations were conducted under various system sizes and time steps to study convergence, while energy autocorrelation analysis was used to estimate decorrelation times, ensuring statistically independent sampling of thermodynamic properties. Stress-strain curves were obtained under controlled deformation protocols, enabling the extraction of elastic and plastic regimes. This methodology provides atomistic resolution of dislocation nucleation, strain localization, and defect evolution—phenomena that are challenging to isolate experimentally at the nanoscale. Thus, MD modeling with EAM potentials and post-processing with autocorrelation and energy analysis is a well-justified approach for exploring mechanical reliability and thermal behavior in nanoscale aluminum systems.

2.0 Software Environment Setup

The simulations were executed using LAMMPS (Mar 2020+), a widely-used classical molecular dynamics engine.
Python (NumPy, Matplotlib) was used for post-processing and autocorrelation analysis.
All simulations were conducted on a CPU-based cluster using a SLURM scheduler.

2.1 System Initialization Protocols

The system consists of FCC aluminum initialized with a lattice constant of 4.0 A,
replicated 15 x 15 x 15 times to form a cubic simulation box containing 13,500 atoms.
Periodic boundary conditions were applied in all directions.
The lattice was oriented along the x[100], y[010], and z[001] crystallographic directions.

2.2 Interatomic Potential

The EAM (Embedded Atom Method) potential file 'Al99.eam.alloy' was used to simulate Al-Al interactions.
This potential captures many-body metallic bonding effects and has been validated extensively for structural and mechanical properties.

2.3 Equilibration & Energy Decorrelation

Energy minimization was performed using the conjugate gradient method with box relaxation.
Subsequently, the system was equilibrated using an NVT ensemble at 273 K over 1000 steps with a timestep of 0.0025 ps.
Autocorrelation analysis of the potential energy yielded a decorrelation time (tau) of approximately 60-80 steps,
indicating reliable sampling of thermodynamic properties.

2.4 System Size Justification

A system size of 15 x 15 x 15 unit cells was selected to ensure bulk-like behavior while remaining computationally efficient. This setup (13,500 atoms) aligns with literature (e.g., Tschopp et al., Acta Mater. 2007) which showed size convergence for cohesive energy and elastic constants in FCC aluminum for N >= 1000 atoms.

- **FCC lattice constant** a=4.0 A˚=4.0×10−10m
- **Unit cell type**: FCC (4 atoms per unit cell)
- **Total atoms**: 13,500
- **Number of unit cells**:

$$\text{unit cells} = \frac{13{,}500\,\text{atoms}}{4\,\text{atoms/unit cell}} = 3{,}375\,\text{unit cells}$$

Volume of One FCC Unit Cell:

$$V_{\text{unit cell}} = a^3 = (4.0\,\text{Å})^3 = 64\,\text{Å}^3$$

Total Volume:

$$V_{\text{total}} = 3{,}375 \times 64\,\text{Å}^3 = 216{,}000\,\text{Å}^3$$

I have organized the project into separate input files, each designed to generate a specific output when run individually. Additionally, a Python script is included to analyze the mechanical properties of aluminum from the LAMMPS simulation results.

Simulation Sequence:

1. **# Aluminum Atomic structure from LAMMPS**

- Input file: Input file: **in_lattice.nvt**
- SLURM Submission Script: **submitlattice-job.sh**
- Output files: **al.data-lattice.out**

2. **# Energy convergence during minimization:**

- Input file: Input file: **in_autocorrelation.nvt**
- SLURM Submission Script: **submitenergycon-job.sh**
- Output files: **al.data-lattice.out, energy_convergence.log**

3. **# Autocorrelation of energy components:**

- Input file: Input file: **in_autocorrelation.nvt**
- SLURM Submission Script: **submitenergycon-job.sh**
- Output files: **al.data-lattice.out, energy_time_series.log**

4. **# Stress – Strain Response of Aluminum:**

- Input file: Input file: **in_tensile.nvt**
- SLURM Submission Script: **submittensile-job.sh**
- Output files: **al.tensiledata.out, alAl_tens_100.def1.txt**

Conclusion

Using energy minimization and NVT equilibration on a sufficiently large FCC Al system (13,500 atoms), we identified the minimum energy configuration and computed the cohesive energy.

The observed decorrelation time (tau ~ 60-80 steps) confirms thermodynamic stability.

These results validate that the chosen methods and system size are appropriate for investigating equilibrium thermodynamics and preparing structures for subsequent deformation studies.