

Modeling a shear test in the micro canonical ensemble:

Introduction:

Steps

1. Creation of FCC crystal
2. Random generation of velocity
3. Calculation of interatomic forces.
4. Integration scheme to update the position.

While calculating the energy for the system the energy remains constant. Velocity verlet and verlet has the similar trend while leap frog has a different trend. The three graphs for the velocity verlet algorithm are mentioned below:





