Introduction
Nanoscale plastic deformation in metals is dominated by the nucleation and propagation of small defects in the crystal structure—dislocations. Understanding the mechanisms of dislocation nucleation and propagation is important for predicting the mechanical properties of nanoscale metallic materials. Nanoindentation is one way to analyze the mechanical properties of nanoscale metallic materials. Nanomechanical problems, such as nanoindentation, can be studied conveniently through atomistic simulations. There are generally two ways to perform atomistic simulations: molecular mechanics (MM) and molecular dynamics (MD). Many studies of nanoindentation have been done using the MM method, in which various dynamic parameters such as mass, loading velocity, and temperature are not taken into account. These variables may play an important role in how dislocations propagate through a material.

Method
In order to study the effect of the dynamic parameters, MD simulations should be performed. MD is performed by solving a system of differential equations based on Newton’s second law, so mass, velocity, and temperature are taken into account. Each variable will be isolated so its affects on dislocation propagation can be studied. The simulations are performed using LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator)[1]. The inter-atomic forces are modeled using the embedded atom method (EAM) which allows for the modeling of a large system of atoms[2]. The total energy of a system of atoms is given by the following:

\[ E_i = \sum_i r_i^0 + \frac{1}{\epsilon} \sum_{i<j} \phi_i (R_{ij}) \]

where \( r_i^0 \) is the embedding energy which is a function of the electron density \( \rho_i \), and \( \phi_i \) is the pair potential between atoms \( i \) and \( j \), which is a function of \( R_{ij} \), the distance between the atoms.

To render the atomistic configurations, the visualization software Atomeye is used [3]. Dislocations are located by evaluating each atom’s centrosymmetry parameter, which is defined as follows:

\[ P = \sum_i R_{1i} + R_{2i} \]

where \( R_1 \) and \( R_2 \) are vectors corresponding to the pairs of opposite nearest neighbors in the lattice [4]. Atoms in a perfect lattice structure will have a value of zero; atoms that are part of a defect will have a non-zero value for \( P \). Only atoms with \( P > 0.3 \) are displayed.

The computational domain for the simulations was approximately 170 x 60 x 170 Å with a nearly rigid spherical indenter of radius 40 Å. The lateral sides are fixed while the top and bottom sides are free.

Results
I. Effect of Mass
To study the effect of mass, it would not work to simulate a metallic bi-layer of different materials (Cu-Ni for example) because there would be other variables affecting dislocation propagation in addition to mass (namely, the interference of the interface on dislocation propagation). To isolate the effect of mass, a ‘virtual’ interface was created within a single material: copper, in this work. All of the atoms in the simulation are Cu, but the bottom half of the material was changed to have a greater mass than regular Cu. The above figure shows the initial configuration where the blue atoms are regular Cu and the red atoms are ‘greater mass’ Cu (2x and 10x). Three simulations were run: pure Cu (63.55 amu), two times mass difference (63.55 amu on top, 127.1 amu on bottom), and ten times mass difference (63.55 amu on top, 635.5 amu on bottom).

II. Effect of Temperature
To study the effect of temperature, simulations were run with no temperature controls and system temperatures kept at 10 and 300 degrees Kelvin. It should be noted that in the first case, the system is initially 0 Kelvin with no further temperature control.

III. Effect of Loading Velocity
To study the effect of loading velocity, simulations were run with three different indenter velocities: 0.5 m/s, 1 m/s, and 5 m/s.

Conclusion
It was found that the dynamic parameters did affect the propagation of dislocations. Dislocation propagation was slowed down when going from a smaller to a larger atomic mass. High temperature facilitated the nucleation of dislocations but inhibited further propagation. Higher loading velocities, when compared to lower velocities at the same indentation depth, propagated dislocations a shorter distance.

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References