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Analysis of Temperature and Strain Rate Effect on Mechanical Properties of Pure Gold Using Molecular Dynamics

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ABSTRACT

Material's mechanical properties are highly affected by the microstructural pattern of the materials, which is very critical for metals like pure gold, which is known for its exceptional ductility and conductivity at elevated temperatures and different strain rates. Understanding how temperature and strain rate affect the characteristics of the materials at the atomic level is highly important for applying this material in practical uses. Au (gold) has been studied for years because of its applications in different sectors like jewelry, aerospace, aviation, technology, electronics, etc. This research used classical molecular dynamics simulation to analyze the effects of temperatures and strain rates on the mechanical properties of the pure compound (Au). This pure element is very popular and useful because of its electrical conductivity, high corrosion resistance, and high mechanical properties. It has been observed that the highest strength was found at 15.293 GPa for pure gold at 400 K temperature at the highest strain rate (.025 ps^{-1}) and at 200 K temperature, 14.34 GPa was the lowest strength was found for Au while having the lowest strain rate (.00625 ps^{-1}). Here, pure gold shows ductile behavior in both high and low temperatures while having both high and low strain rates. The tensile property of pure gold (Au) is better at relatively higher temperatures than at lower temperatures along with the higher strain rate (.025 ps^{-1}) rather than the lower strain rate (.00625 ps^{-1}). This study demonstrated how temperature and strain rate influence tensile properties like elastic modulus and the ultimate strength of Au. The findings of this investigation might be helpful to understand the specific properties of this material in practical fields like electronics, mechanical, medical, and others.

Keywords: Molecular Dynamics, Strain Rates, Ultimate Tensile Strength, Young's Modulus.

1. Introduction

Researchers have shown a significant interest in 3d gold structures in recent years due to its remarkable mechanical, electrical, optical, and other unique properties. Among these materials, 3d gold stands out for its extensive application potential in developing nanoelectromechanical systems (NEMS) and in biomedical, optical, and electrical devices. The high surface-to-volume ratio of this imparts distinctive mechanical and structural properties, making them suitable for various applications such as interconnects in miniaturized electronics (nano-transistors), functional components in nano-sensors [1], nanoelectrodes which are very susceptible [2], and for atomic imaging [3] and also in AFM (atomic force microscopy) [4].

Understanding the mechanical properties of gold necessitates a thorough comprehension of their deformation mechanisms under varying loading conditions. For instance, Volkert [5] has experimentally investigated the effect of size in the deformation of gold nanocolumns, while Zhu et al [6] conducted fixed tensile tests on silver NWs with circumferences ranging from 34 to 130 nm using SEM machine (scanning electron microscopy). Their findings revealed that modulus of elasticity, elastic limit, and tensile strength increase as the circumference of the NW decreases, with the maximum elastic limit of silver NWs reaching 2.64 GPa. Lee et al. [7] analyzed the deformation mechanisms during uniaxial loading of [110]-oriented gold structures by employing a combination of transmission electron microscopy (TEM) and molecular dynamics (MD) simulations. Given the challenges associated with conducting experiments at the nanoscale, including the need for sophisticated instrumentation and the potential for measurement errors, computer simulations provide a cost-effective alternative. These simulations allow for extensive parameter experimentation, facilitating the observation of phenomena that are difficult to replicate experimentally.

In light of the existing literature, this investigation focuses on previously unexplored 3d gold structures at different loading rates and higher temperatures. The objective is to analyze important information about the deformation mechanism of gold under different loading conditions, utilizing the classical molecular dynamics simulator LAMMPS [8].

2. Methodology

The mechanical properties of Au are calculated using LAMMPS based on molecular dynamics. To describe the atomistic interactions concerning only Au−Au for pure gold atoms in the simulation. MEAM potential [9] has been utilized in the simulation [10]. This potential was developed to study the mechanical behavior of these specific materials over specific temperatures and pressures. The virial stress equation has been used to analyze the mechanical behavior of Au (3d structure) under uniaxial deformation mechanism which can be described as,

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$$\sigma_{\text{virial}}(r) = \frac{1}{\Omega}\sum_i[\{-m_i\dot{u}_i \otimes \dot{u}_i + \frac{1}{2}\sum_{j\neq i} r_{ij} \otimes f_{ij}\}]$$

where the total sum is taken for all the atoms in the volume, m_i indicates the mass of atom i, u_i denotes the time derivative of the interchange, r_{ij} means the location vector, and f_{ij} points to the interatomic force applied on atom i by atom j. To achieve a stable configuration, the conjugate gradient method is used for minimizing energy with stringent tolerances of 10^{-5} eV/Å and 10^{-8} for force and energy, respectively, and a maximum of 20 force/energy evaluations and 20,000 minimizer iterations. Following energy minimization, the system underwent equilibration simulations, first with a 3000 time-step NVT microcanonical ensemble and then a 30,000 time-step NPT ensemble, for the equilibration of the system pressure to one bar at a temperature of 300 K, ensuring convergence of energy and thermodynamic properties. The velocity Verlet integration technique is used for solving the motion equation with the time step of 1 fs, and a stable loading rate of 0.025 ps^{-1} is applied along the X axis, which, although higher than realistic rates, is suitable for atomistic calculations of material fracture behavior due to computational cost considerations [11] [12]. Finally, the open-source software OVITO is utilized for post-processing and visualization of the structure's calculated strain, stress, and trajectories, providing valuable insights into the material's behavior under various conditions [13].

3. Model of Analysis

Figure 1 illustrates the molecular dynamics simulation model of the pure gold structure, which was generated from a bulk face-centered cubic (fcc) Au single crystal with the lattice parameter of 4.08 Å.

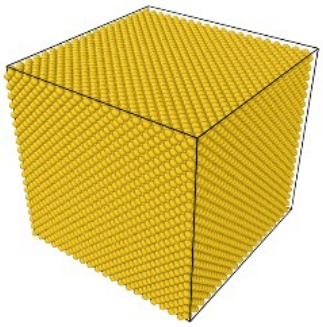

Fig 1: A 3d Structure of pure Au

The comprehensive simulation was conducted on a system comprising 32,000 atoms, spanning a 69.598592 nm^2 area with dimensions of 8.3425 nanometers (nm) in both the [100] and [010] directions, along with a substantial 15 Å vacuum space along the Z direction to prevent unwanted interactions and isolate the main body of the structure for calculation purposes.

Periodic boundary conditions were used in this research. Uniaxial tensile loading in the x direction is applied by adjusting the length of the simulation box in the loading direction at a fixed strain rate $\dot{\varepsilon} = v_x/L^0_x$, where v_x is the rate of change of the box length and L^0_x is the initial box length in the x direction after reaching the equilibrium.

Md. Riazul Islam et al. showed the strength of 3d high entropy alloy structures under different conditions in his research [14]. This research has followed the initial instructions and the conditions to get perfect results.

4. Result and Discussion

The operating temperatures of nano-transistors, nano-sensors, and nano-electrodes often vary under different environmental conditions. Therefore, it is very crucial to ensure the thermal and mechanical stability of this material across a wide range of temperatures and strains, enabling their effective performance in diverse applications [1].

4.1 Effect of temperature:

To understand how temperature affects the mechanical properties of a 3D gold (Au) structure in electrical systems and devices, researchers conducted a study where they exposed the structure to a range of temperatures, from low to high temperatures. Then researchers applied a controlled amount of tensile stress along the x-axis direction at different rates to see how the structure responded. This allowed them to investigate how temperature influences the structure's mechanical performance.

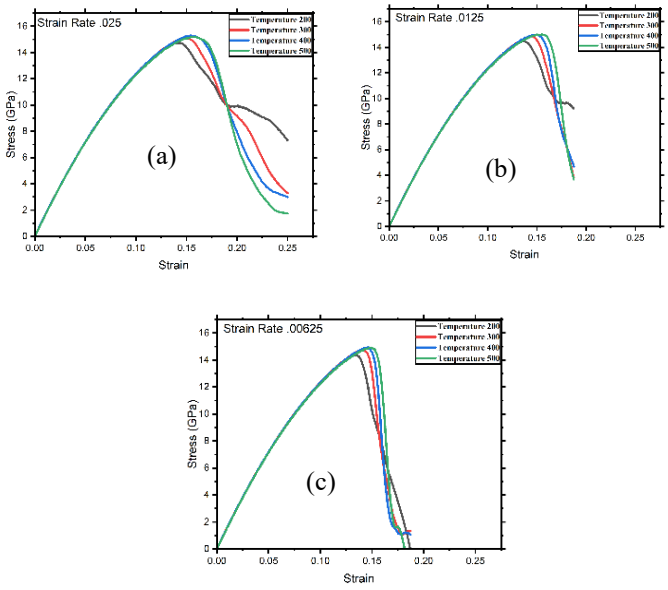

Fig 2: Stress-strain curve at different temperatures at the strain rate of (a) .025 ps^{-1} (b) .0125 ps^{-1} (c) .00625 ps^{-1}

It has been discovered that the modulus of elasticity and ultimate tensile strength of the 3D gold structure varied significantly with temperature. With increasing temperature from 200 K to 500 K, the tensile strength increased by 3.06%, which is unusual. Typically, most materials exhibit a decrease in tensile strength at high strain rates as temperature increases. However, in this case, the pure gold material showed an increase in tensile strength with temperature up to 400 K, and only then did it start to decrease. On the other hand, the yield strength decreased by 8.02% at the same loading rate of 0.025 ps^{-1}. This suggests that while the material becomes stronger in terms of tensile strength at higher temperatures, it also becomes more prone to deformation (i.e., it yields more easily). The overlapping linear section at the beginning of the curves indicates that the material's initial response to loading is not depending on temperature.

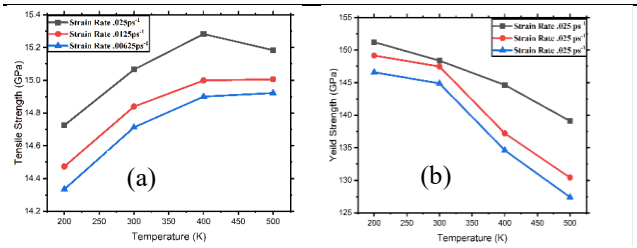

Fig 3: (a) Tensile strength, and (b) Elastic Modulus of Au at the strain rate of .025 ps^{-1} (b) .0125 ps^{-1} (c) .00625 ps^{-1}.

We observed that in the 3D Au structure, tensile strength increased with temperature at all strain rates, not just high strain rates. This means that whether the material was subjected to a high rate of deformation (0.025 ps^{-1}) or a lower rate of deformation (0.0125 ps^{-1} or 0.00625 ps^{-1}), its tensile strength still increased as the temperature rose. However, the yield strength, which is the stress at which the material begins to deform plastically, decreased linearly with increasing temperature at all strain rates. This suggests that while the material becomes stronger in terms of tensile strength at higher temperatures, it also becomes more prone to deformation. Another interesting observation is that the yield strength at lower temperatures (e.g., 200 K) is significantly higher than at room temperature. This implies that the material is more resistant to deformation at lower temperatures, but becomes softer and more prone to deformation as the temperature increases. These findings offer important insights into the mechanical behavior of 3D Au structures across various temperature ranges.

4.2 Effect of Strain Rate:

The study reveals the impact of different strain rates on the physical properties of gold (Au) structures. To achieve this, the researchers subjected bulk Au to different strain rates, ranging from 0.025 ps^{-1} to 0.00625 ps^{-1}, at distinct temperatures between 200 K and 500 K. The goal was to evaluate how the mechanical properties of Au change in response to different loading rates. The strain rate, which measures how rapidly a material is deformed, and can significantly influence the material's behavior under different loading conditions. The study's results are illustrated in Figure 1, which shows the stress-strain relationships for different strain rates. The stress-strain curve is a graphical depiction that illustrates the relationship between the stress exerted on a material and the corresponding strain it experiences.

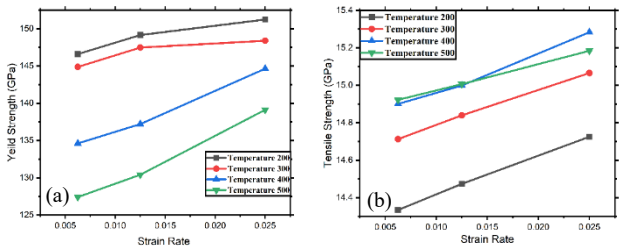

Fig 4: (a) Elastic Modulus, and (b) Tensile strength of Au at 200K, 300K, 400K, 500K temperatures.

Notably, the stress-strain curves for different strain rates exhibit similar shapes at a fixed temperature. This suggests that the loading rate has a minimal impact on the initial strength and elastic limit of the Au sample.

As the strain rate increases, the yield strength and tensile strength of Au both exhibit a significant increase at every temperature, with a notable enhancement of 3.06% and 2.66% respectively at 200 K, and similar trends are observed at other temperatures also.

5. Conclusions

The temperature and strain rate effect on the mechanical properties like ultimate tensile strength and the modulus of elasticity of Au including the stress-strain relationship using molecular dynamics was investigated in this work. By varying temperature and strain rate, different stress-strain curve was achieved and properties were calculated by using them. The outcome of this study can be summarized as follows:

(a) At 200 K temperature Au has an elastic modulus of 151.24 GPa, which is higher than others.

(b) The highest UTS which is 15.28 GPa at 400 K temperature.

(c) Temperature and strain rate strongly influence the mechanical properties of Au. At relatively higher temperatures, Au showed better properties than the lower temperatures. On the other hand, it showed better tensile properties at relatively higher strain rates.

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