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Research Article

Molecular Dynamics Simulations of Deformation Behaviour of Gold Nanowires

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Metallic nanowires show great potential for applications in miniaturization of electronic devices due to their extraordinary mechanical strength and electrical properties. Experimental investigations of these properties are difficult due to their size and complications in performing experiments at such length scales. Computational techniques based on classical molecular dynamics simulations (using LAMMPS) provide an effective mean to understand the mechanical deformation behaviour of such nanowires with considerable accuracy and predictability. In the present investigation, we have discussed the deformation behaviour of Au nanowires due to tensile loading using classical molecular dynamics simulations (LAMMPS). The effect of strain rate and temperature on the yield strength of the nanowire has been studied in detail. The deformation mechanisms have also been discussed.

1. Introduction

In recent years, nanomaterials have drawn considerable attention due to their unique mechanical, electrical, optical, and other properties. Being one of the typical nanomaterials, metallic nanowires (NWs) have broad application prospects in making nanoelectromechanical systems (NEMS) and biomedical, optical, and electrical devices. Due to their high surface-to-volume ratio, nanowires offer unique mechanical and structural properties which find applications in several domains of interest such as interconnects in miniaturization of electronics (nanotransistors), functional components in nanosensors, high sensitivity nanoelectrodes, tips of scanning tunneling, and atomic force microscopies [1–4]. To understand the mechanical properties of nanowires, it is important to understand their deformation mechanism under different loading conditions. Volkert and Lilleodden experimentally studied the size effects in the deformation of submicron gold columns [5]. Zhu et al. [6] performed in situ tensile testing of Ag NWs with diameters between 34 and 130 nm using a scanning electron microscope (SEM). Young's modulus, yield strength, and ultimate tensile strength were observed to increase as the NW diameter decreased. The maximum yield strength of Ag NWs was found to be 2.64 GPa. Lee et al. [7] performed a combined TEM and MD simulation study to analyse the conditions under which a particular deformation mechanism takes place during the uniaxial loading of [110]-oriented Au nanowires. Since performing experiments at the length scale of a nanowire requires sophisticated instrumentation and results are always prone to errors, computer simulations may instead be used which will be both cost-effective and there will be freedom to experiment with the parameters to observe the phenomena under investigation, which will otherwise be very difficult with experiments.

Attempts to theoretically understand the behaviour of metallic NWs started after the pioneering work of Landman et al. [8]. They used computer simulations to show that the contact of a thin metal STM tip on a flat metal surface produces, upon stretching, a series of successive stages of elastic deformation with atomic rearrangements that eventually led to the formation of atomically thin NWs. Park et al. [9] used MD simulation to show that the indentation of a Ni STM tip on a gold surface produced very thin NWs. Wu

et al. [10] studied the tensile behaviour of Cu nanowires and found the strength of the Cu nanowire more as compared to bulk copper metal. Liang and Zhou [11] studied response of Cu nanowires in dynamic tensile deformation using LAMMPS. They found that the yield stress decreases with the specimen size and increases with the loading rate. Yuhang et al. [12] studied the deformation and melting behaviour of Si nanowires with the help of MD simulations. Branício and Rino [13] and Wen et al. [14] studied the deformation behaviour in Ni nanowires, using MD simulation. They found that surface effects allow the larger cross-sectional nanowires to support greater stress for any given strain than the smaller ones. Wang et al. [15] studied the temperature and tensile rate dependence of the deformation behaviour. Koh et al. [16] studied the deformation behaviour of Pt nanowires and its dependence on temperature and strain rate. Dou and Derby [17] studied the deformation mechanism in Au nanowires and nanoporous gold. They compared the scale dependence of the strength of Au micropillars/nanowires and nanoporous gold [18] and have shown that, for both sets of samples, the correlation between yield strength and length scale shows considerable similarity. Pu et al. [19] studied the applicability of various semiempirical potentials for the MD study of the deformation of the Au nanowires. Park and Zimmerman [20] also proposed the formation of a stable nanobridge, during the deformation of Au nanowires by tensile stress. Gall et al. [21] discussed the yield strength asymmetry in the Au nanowires with MD simulations.

As has been mentioned in the above literature review, several researchers have investigated various aspects of deformation behaviour of Au nanowires having different aspect ratios. In the present investigation, we have chosen only those combinations of diameter and length (aspect ratio) of the Au nanowire which have not been considered before. The motive behind this choice was to contribute some useful information to the already existing knowledge on deformation behaviour of Au nanowires. We have used classical molecular dynamics simulator LAMMPS to simulate Au nanowires under different loading conditions such as strain rate and temperature. Section 2 explains the basic methodology of simulations, followed by Section 3 on simulation results. The last section discusses the conclusions of the current work.

2. Simulation Methodology

In the present work, the deformation behaviour of cylindrical Au nanowires of aspect ratio (length/diameter) 6 has been studied using classical molecular dynamics simulator LAMMPS. The pairwise interactions have been modelled using EAM potential function in LAMMPS. Periodic boundary conditions have been applied along the direction in which strain is applied (y direction). All the simulations have been performed using NVT ensemble at 100 K temperature.

3. Results

The simulation parameters have been displayed in Table 1. Simulations are mostly performed at 100 K. Before applying strain to the wire, the system is equilibrated for approximately 75 ps. After the wire is equilibrated, a longitudinal strain rate of $10^9\,s^{-1}$ is applied along y direction, and the resulting longitudinal stress has been calculated.

Table 1: Simulation parameters for Au nanowire deformation.

Parameter	Value
Length	24 nm
Diameter	4 nm
Temperature	100 K
Strain rate	$10^9\,s^{-1}$
Time step	0.005 ps

The snapshots showing the deformation of the Au nanowire at different times have been given in Figure 1. This figure has been prepared to show the evolution of stress in the nanowire as a function of strain. From the stress-strain graph placed with the snapshots in Figure 1, we see that the deformation region is very small, which corroborates the finding that nanocrystalline materials have low ductility as compared to coarse-grained materials [22]. The yield stress is found to be 1.08 GPa at the strain of 7.8%. After straining the nanowire further, the stress falls down abruptly to a smaller value (but not zero) signaling the initiation of plastic deformation and consequent loss in the strength of the nanowire. Since the nanowire is not fractured yet, a small increase in the stress (as compared to the yield stress) again with strain is obvious which is expected to continue further with strain before fracture. Several studies have pointed that the deformation mechanism in the nanowire may be either due to deformation twining or dislocation slip, depending on the material, strain rate, and temperature, but a concrete understanding of this is still a matter of debate. Usually, deformation twinning is prominent at low temperatures, and high strain rate and dislocation slip happen at comparatively high temperatures.

3.1. Effect of Strain Rate. When the strain rate is comparatively higher, the rate of dislocation generation is faster than the rate of dislocation annihilation. This leads to material hardening which causes the nanowire strength to increase. Figure 2 depicts the effect of strain rate on the strength of the Au nanowire. We see that as strain rate is increased, the yield stress is also increased concomitantly. We also see that as strain rate is increased, the fracture strain is also increased.

Table 2 summarizes the values of yield stress and yield strain corresponding to Figure 2.

3.2. Effect of Temperature. The effect of temperature on yield stress and strain has been shown in Figure 3. We see that as temperature increases, the yield stress decreases. The yield strain does not seem to depend significantly on temperature. The reason behind decrease in the yield stress with increase in temperature might be due to the dependence of dislocation motion on temperature. During the deformation of the nanowire, the dynamic hardening of the material as a result of nucleation of dislocations and recovery due to climb of dislocations might be occurring simultaneously. Table 3

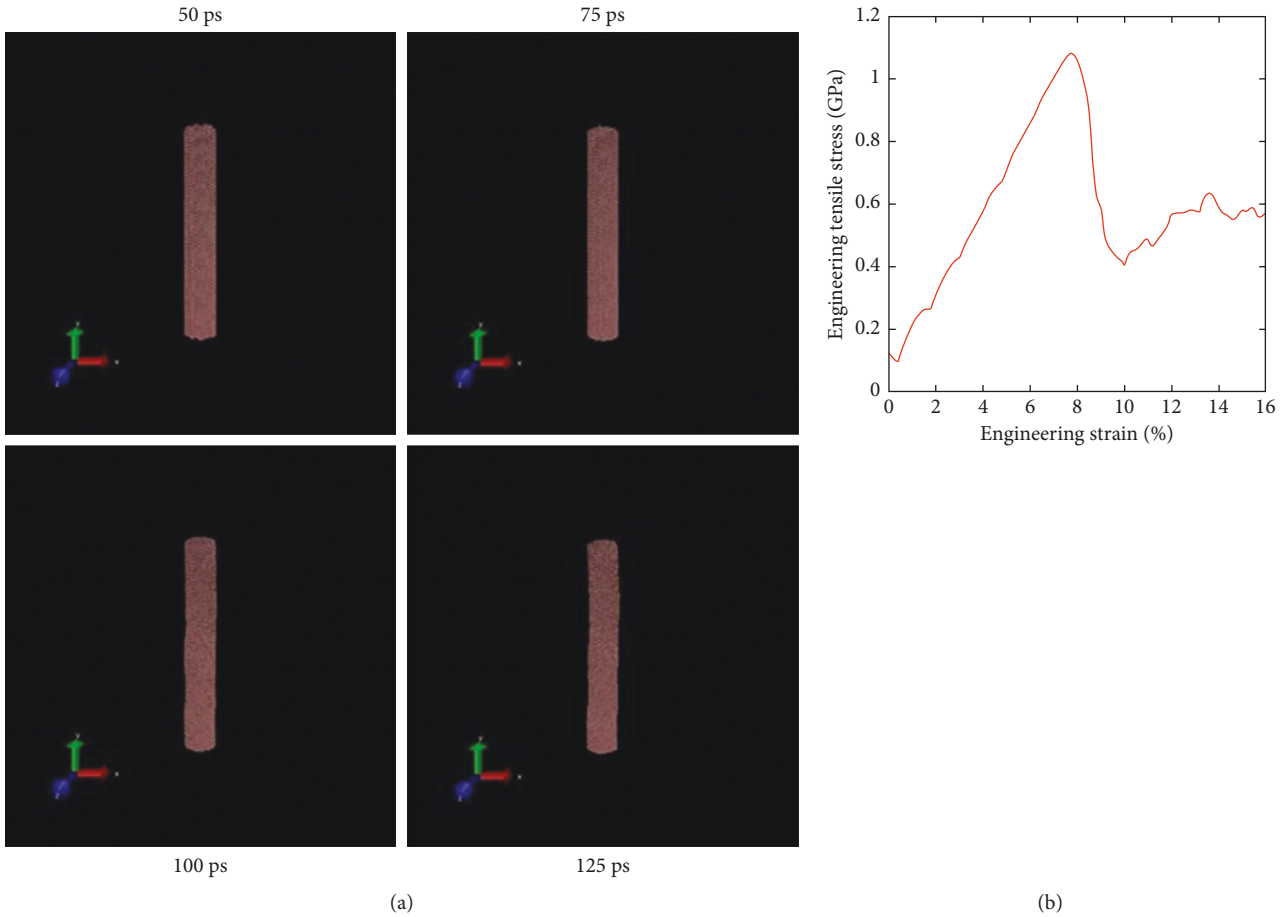

Figure 1: The snapshots showing the deformation of Au nanowire with time. The simulation parameters are given in Table 1. The stress-strain curve has been shown in the right.

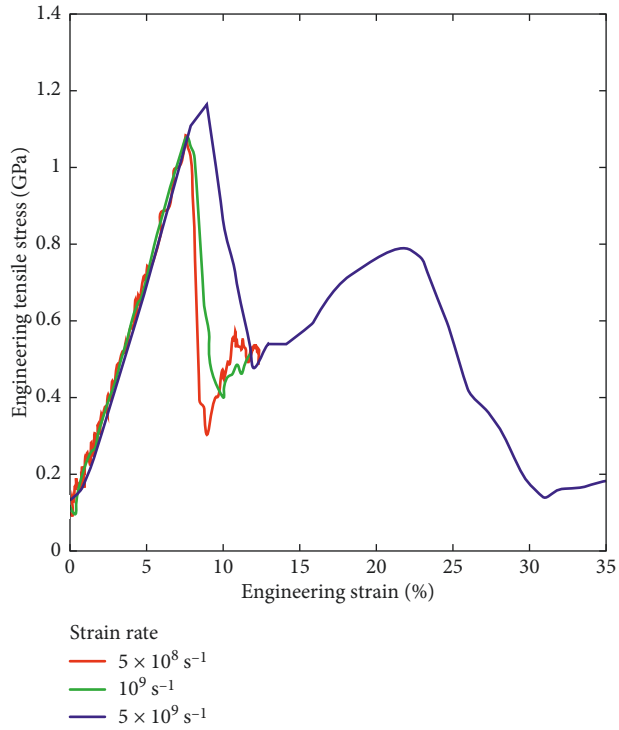

Figure 2: The effect of strain rate on strength of Au nanowire. The simulation parameters are same as those in Table 1.

Table 2: The yield stress and strain as a function of strain rate.

Strain rate (s^{-1})	Yield stress (GPa)	Yield strain (%)
5×10^{8}	1.072	7.6
1×10^{9}	1.082	7.8
5×10^{9}	1.160	9.0

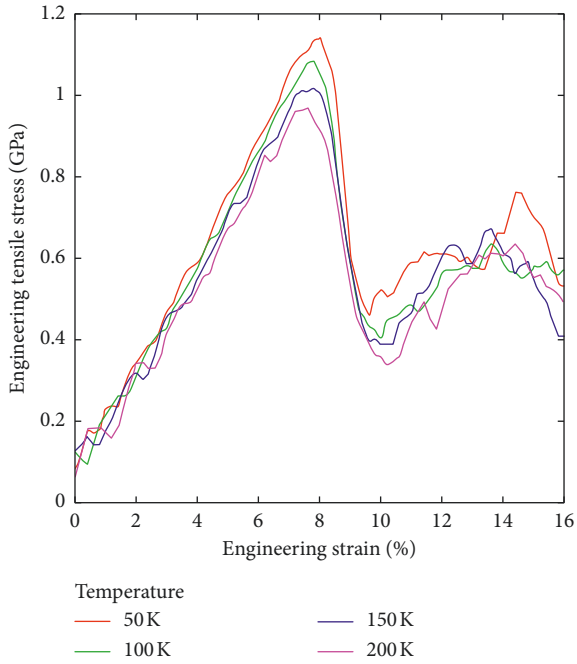

Figure 3: The dependence of yield stress and strain on temperature. The simulation parameters are same as in Table 1.

Table 3: The yield stress and strain as a function of temperature.

Temperature (K)	Yield stress (GPa)	Yield strain (%)
50	1.14	8.0
100	1.08	7.8
150	1.01	7.8
200	0.97	7.6

summarizes the values of yield stress and strain as a function of temperature.

4. Conclusions

Deformation behaviour of Au nanowires has been studied using classical molecular dynamics simulator LAMMPS. The interactions between Au atoms have been modelled using EAM potential. The nanowire is deformed by applying uniform uniaxial strain along y direction, and corresponding stress developed in the nanowire has been calculated. The loss of ductility in the nanowire (as compared to coarse-grained Au) has been observed, which has also been reported by Koch [22]. When strain rate is increased, the yield stress and strain of the nanowire increase possibly due to the phenomenon of strain hardening. Increase in the simulation temperature at the same strain rate decreases the yield stress of the nanowire, without significantly affecting the yield strain. Loss in the strength of the nanowire at higher temperature might be due to faster recovery of the material over the rate of dislocation nucleation. In the present study, the effect of surface energy on the deformation behaviour of the Au nanowires has not been considered because of a previous study [23] in which the authors observed that a diameter of 10 nm acts as the threshold, below which the surface energy decreases with decrease in the diameter. The role of surface energy would have been significant if we would have studied the melting behaviour of the nanowire because of its dependence on the surface atoms and surface energy more than the atoms in the bulk. Surface energy is actually the surface elastic energy which is connected with the surface relaxations, which are induced by the ambient temperature. This is the reason why the surface energy affects the melting behaviour more than the deformation behaviour.

Data Availability

The data used to support the findings of this study are available from the corresponding author upon request.

Conflicts of Interest

The authors declare no conflicts of interest exist.

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