Fracture Mechanism of Single and Polycrystal Silver Nanowire: Computational Study

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Abstract— *Molecular Dynamics Simulation has been used as the computational tool to investigate the mechanical properties and fracture mechanism of silver nanowire. Two types of nanowires have been chosen in this study- single crystal and polycrystal. Using two different strain rates (1 x 10^9 s^{-1} and 1 x 10^{10} s^{-1}) the stress-strain behaviour has been shown for these nanowires. To study the temperature effect, the simulations have been performed under four different temperatures (0.01K, 300K, 600K, 900K). Embedded Atom Method (EAM) potentials have been used as the interatomic potential to perform the MD simulations. It has been found that the maximum value of stress reduces with the increase in temperature. The yield strength of the polycrystalline nanowire is lower than the single crystal nanowire but at the same time the polycrystalline nanowire shows significant amount of ductility.*

Keywords — *Nanowire, polycrystal, Molecular dynamics, strain rate, plasticity*

I. Introduction

1D structures of nanomaterials have been a major research topics in the recent years. These structures are popular due to their fascinating electronic, photonic, thermal, electro-chemical and mechanical properties. These nanowires are extensively used in electronics, sensors, photonics, thermo-electrics, photovoltaics, photoelectrochemical systems, batteries, mechanical systems, and biological systems [1, 2]. The mechanical behaviour of metals with the body-centered cubic (bcc) and face-centered cubic (fcc) structures has been primarily studied due to their high strengths and high melting temperatures, which make them attractive for structural applications [3-6]. Recently, a lot of studies have been conducted on the compression and tension of submicron cylindrical samples prepared by the focused ion beam (FIB) technique which have made it possible to investigate the effect of sample size on the mechanical behaviour of various metals and their alloys [7-10]. In addition to the mechanical properties, there are also a number of studies on the structural changes of nanomaterials [11-13]. The yield strengths of gold whiskers have been reported over ten times stronger than the bulk [14].

Because the size of nanowires is very small, it is difficult to manipulate and control the deformation mechanism of nanowires by experimental ways, such as scanning tunneling microscopy (STM) and other techniques [15]. However, computational tools can play crucial role in this regard. Molecular dynamics (MD) simulation is an effective method to study the deformation and fracture properties of metallic nanowires. MD simulation solves Newton's equations of motion for a collection of interacting particle over a number of time steps. Some significant research works have been carried out to study nanowires. Diao et al [16] analysed the strength of gold nanowires with the method of molecular dynamics simulation. Park et al [17] and Liang and Zhou [18] simulated the uniaxial tension of gold and copper nanowires, and observed the shape memory effect and pseudo-elastic behaviour of the nanowires.

The temperature dependence and strain-rate dependence of the deformation characteristics and mechanical properties of the platinum nanowires under unidirectional uniform tensile have been investigated by Koh et al [19]. They pointed out that under the conditions of low temperature and low strain rate, the stress-strain curves of platinum nanowires show a stepped cycle distribution, and the nanowire maintains ordered and stable crystal structure at this time. Wang et al [20] studied the temperature and strain rate dependences of mechanical tensile properties of ultrathin nickel nanowires. The fracture mechanism and dislocation criteria of nickel, silver, platinum and gold nanowires have also been studied using MD simulation [21]. However, it is not clear which factor will dominate the deformation and fracture mechanism of nanowires [22]. Besides, most of the studies have been carried out using single crystal nanowires. Hence, the fracture mechanism and mechanical properties of polycrystalline metallic nanowires should be extensively studied.

The aim of this paper is to compare the single and polycrystalline nanowires and get a comprehensive idea of their mechanical properties. Here, silver nanowire has been studied to find out the effects. Polycrystalline

nanowires have been created using the voronoi tessellation. The effect of temperature on the mechanical properties has also been studied.

II. Computational Procedure

In the present study silver nanowire has been chosen with a distinct diameter of 1.5 nm. The perfect single-crystal silver nanowires are in the form of face centered cubic (FCC) lattice structure. Molecular Dynamics (MD) simulation has been used to investigate the mechanical properties of these silver nanowires. Uniaxial tension has been applied to these nanowires in the [100] crystallographic orientation. Although some studies used nanowhiskers to carry out similar investigations, in this simulation were of cylindrical shape with circular cross-sectional area. Circular cross-sections were chosen as studies suggest that circular cross-sections present the most stable and natural cross-sectional configuration [23-25]. Here the lattice parameters of the corresponding bulk structures have been used. The value of lattice parameter (α) of silver has been chosen as 4.09 A0. The length (l) and diameter (d) of the nanowires were modelled using the lattice parameter so that we can establish a non-dimensional size analysis. Other effects that are dependent on nanowire length-to-diameter ratio were eliminated in this way. The length of each nanowire was 25 times the lattice parameter while the diameter was almost seven times. The dimension of the nanowire was taken as d = 3.0 nm and l = 10.225 nm. The simulation box in the other two directions ([010] and [001]) has been taken as twice the diameter.

Two types of nanowires have been created with the same dimension– single and polycrystalline nanowires. The single crystalline nanowire contained 4425 atoms while the polycrystalline nanowire contained 4255 atoms. Polycrystalline nanowire was constructed using voronoi tessellation which generated polycrystals with grains at random positions and orientations. In this study 10 grains were created in this manner. To perform the simulation Large-scale atomic/molecular massively parallel simulator (LAMMPS) [26] code has been used. The axial direction of silver nanowires model is the ⟨100⟩ crystallographic orientation of FCC lattices. For this purpose, periodic boundary conditions were applied in all three ⟨100⟩ ⟨010⟩ ⟨001⟩ crystallographic directions. To get a better result, in the present study embedded atom method (EAM) potential [27, 28] has been used to describe the interactions between the atoms to carry out the molecular dynamics simulation. From the previous studies it is evident that EAM potential provides the best result for these types of simulations. EAM potential is a kind of N-body potential that reflects the interactions between atoms as well as the corresponding anisotropic. The total potential energy of the crystal is divided into two parts: one part of the energy is pair potential between the atoms in the crystal lattice; the other is the embedded energy of atoms embedded in the electron cloud background, and it represents the many-body interactions. The pair potential and embedded potential that form the EAM potential are selected in accordance with the experience. For the EAM potential, the total potential energy of the crystal can be expressed as-

$$U = \sum_{i} F_i(\rho) + \frac{1}{2}\sum_{j \neq i} \phi_{ij}(r_{ij})$$

Where $\sum_{i} F_i(\rho)$ is embedded energy; $\sum_{j \neq i} \phi_{ij}(r_{ij})$ is pair potential, which can be selected according to the needs of the different forms; ρ is the summation of electron cloud density generated by all other atoms extranuclear except the i-the atom in the position of i-th atom, which can be expressed as-

$$\rho = \sum_{j \neq i} f_i(r_{ij})$$

Where, $f_i(r_{ij})$ is the charge density that the j-th atom extranuclear contribute in the position of the i-th atom; r_{ij} is the distance between the i-th atom and the j-th atoms. Energy minimization has been done before the simulation was actually conducted. The nanowire were relaxed for 50 picoseconds. Here, time step was chosen as .001 ps and the NPT ensemble has been used. Four different temperatures have been used to carry out this study 0.01K, 300K, 600K, 900K.

III. Results And Discussions

The process of the tensile deformation of the nanowire is evident from figure 1. The morphology of the nanowires can be detected and described during deformation. In this study, two distinct strain rates have been used: $1x10^{10}$ s^{-1} and $1x10^{9}$ s^{-1}. To keep the computational cost low, higher strain rates have been chosen. After being fully relaxed, the system reached a minimum energy state which has been shown in Fig. 1. When the nanowire has been sufficiently relaxed, some atoms of the nanowires are rearranged, incorporating some local lattice defects. In this simulation, the nanowire models relaxed for at least 50 ps to ensure sufficient relaxation time.

In this simulation the deformation mechanism can be divided into several states: elastic deformation yielding state of deformation, plastic deformation and fracture of nanowires. From the figure it is evident that, the nanowire is stretched almost linearly before the yielding state. After that the yield state of the nanowire can be observed due to the maximum stress. The maximum value of stress occurs because of the lattice defects inside

the nanowires during the tensile test. The strain still keeps increasing, as a result of which plastic or permanent deformation occurs to the nanowires. At this point the stress drastically decreases and it continues until fracture of the nanowires happen.

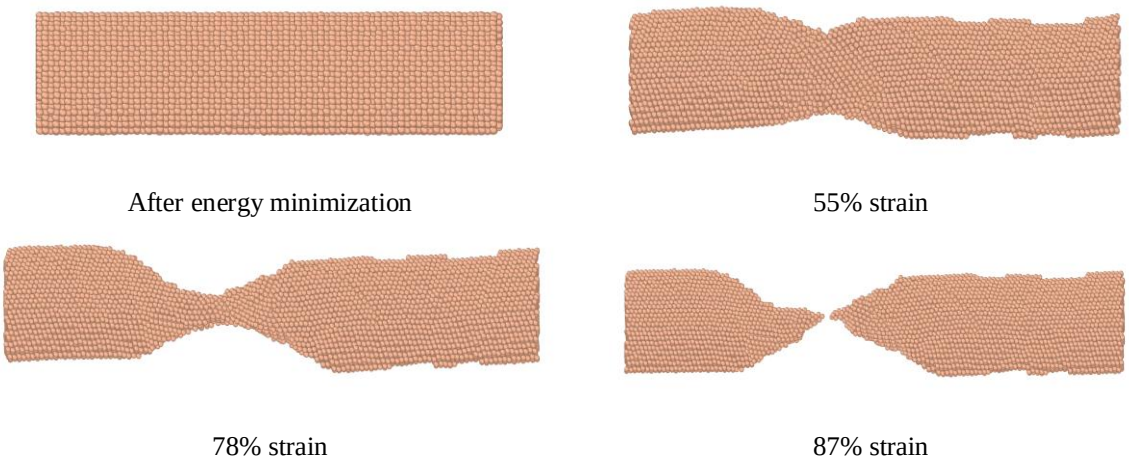

Fig. 1 Fracture mechanism of single crystal Silver nanowires (strain rate 1 x 10^9)

The polycrystalline nanowires show better ductility which can be shown from figure 2. Unlike the single crystal nanowire it stretches for a longer period of time before fracture.

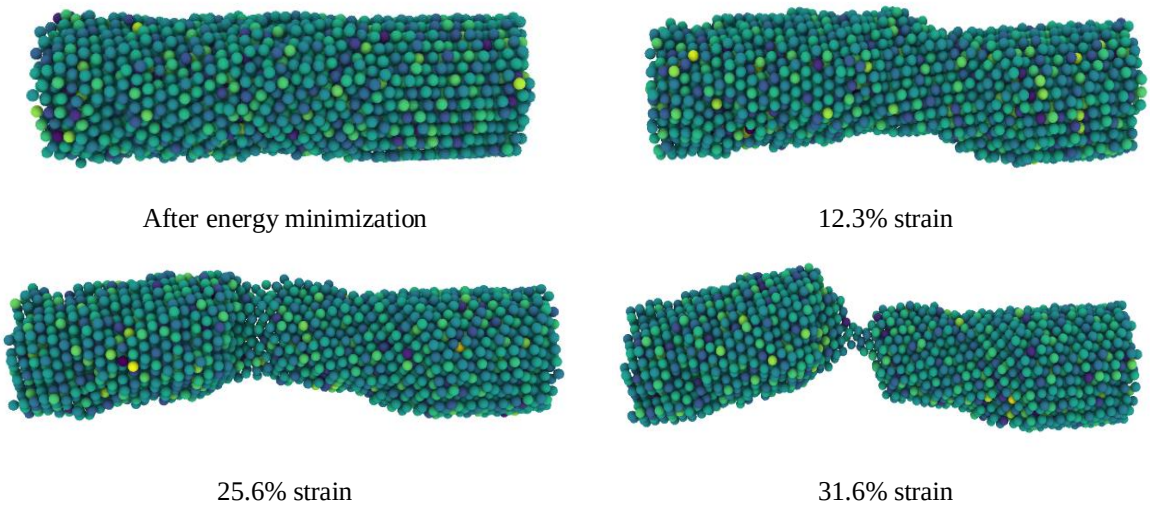

Fig. 2 Fracture mechanism of polycrystal Silver nanowires (strain rate 1 x 10^9)

A. Effect of Temperature:

Figure 3 explains the stress-strain behaviour of silver nanowire at different temperatures. In Fig. 3 stress-strain curve of Ag nanowires have been presented for four different temperatures. The maximum value of stress occurs for temperature 0.01K. With the increase in temperature the value of stress gradually decreases. Here, stress has been calculated in GPa. From Fig. 3, it can be found that the elastic modulus and yield strength of nanowires decrease with the increasing of temperature. According to the theory of thermodynamics, the total kinetic energy of all the atoms of the system generally satisfies the following equation-

$$E_k = \sum_{i=1}^{N} \frac{1}{2} m v_i^2 = \frac{3}{2} N k_B T$$

Where E_k is the total kinetic energy of the system; N is the total number of atoms; k_B is the Boltzmann constant and T is the thermodynamic temperature.

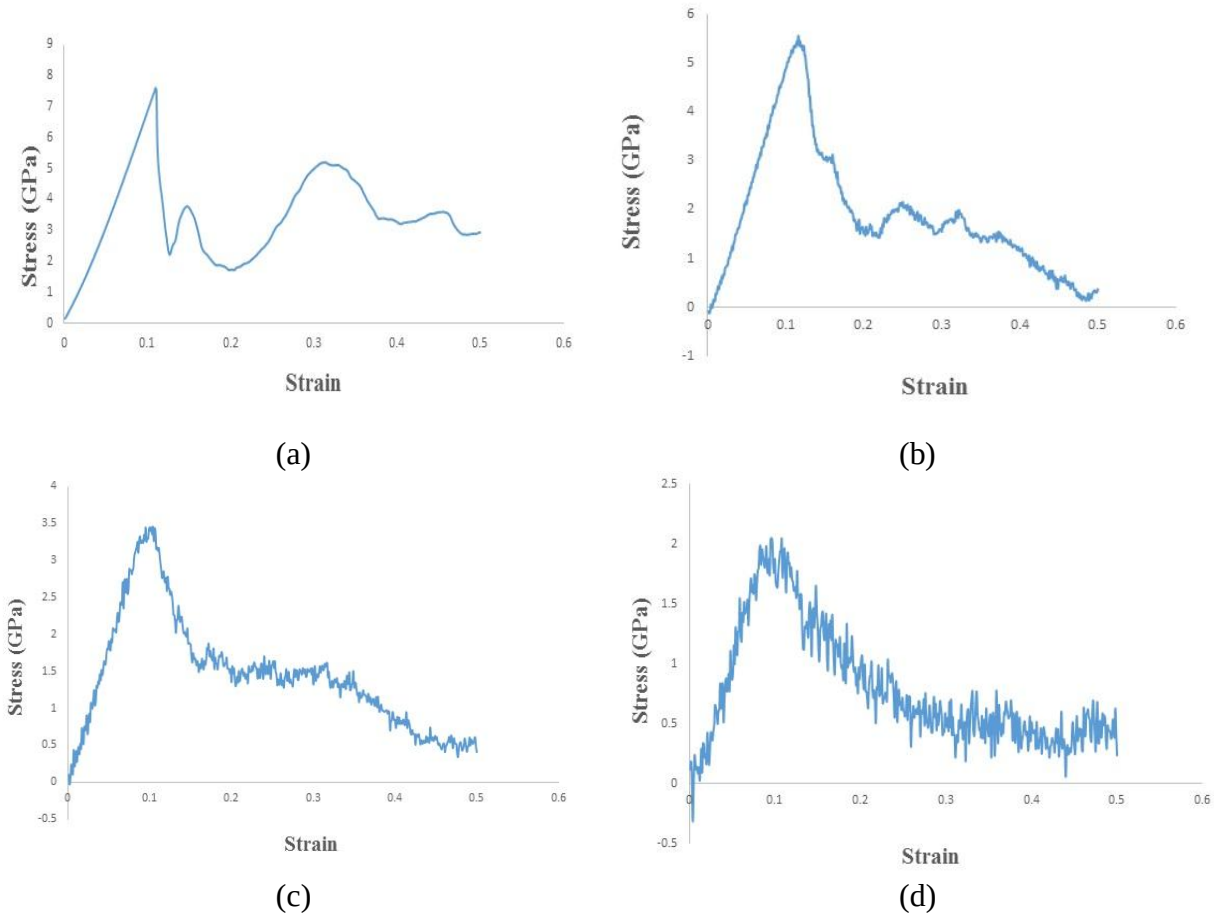

Fig. 3 Stress-strain behaviour of silver nanowire using strain rate 1 x 10^{10} (a) T= 0.1K (b) T= 300K (c) T= 600K (d) T= 900K

B. Effect of strain rate:

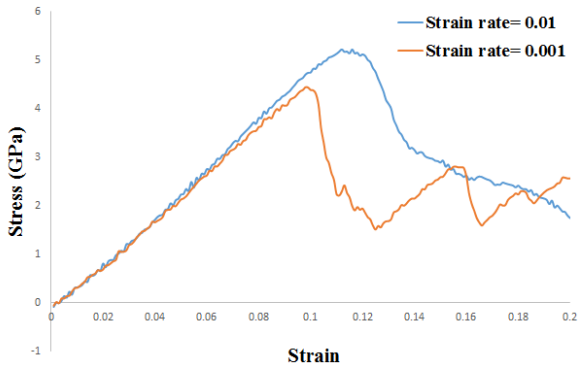

Fig. 4 Stress-strain behaviour of silver nanowire using strain rate 1 x 10^{10} and 1 x 10^{9}

From figure 3 it is clear that the stress-strain behaviour is almost identical for two different strain rates. But for the higher strain rate slightly lower value of maximum stress can be observed. It might be due to the rapid tension of the nanowire. Because of the higher strain rate, the nanowire is subjected to rapid dislocations of crystals and hence producing lower stress.

C. Effect of grains:

Here, polycrystal nanowire with 10 grains has been created. Then using the strain rate of 1 x 10^{9} s^{-1}, the molecular dynamics simulation has been performed. Meanwhile the temperature was kept fixed at 0.01K. The grains had immense effect on the plasticity of the nanowire. There was no sharp fall in stress when compared to the single crystal nanowire. As a result the elasticity of the nanowire was increased to a great extent. For single crystal nanowire the maximum value of the stress was 7.8 GPa while for polycrystal nanowire it was 2.9 GPa (Figure 5).

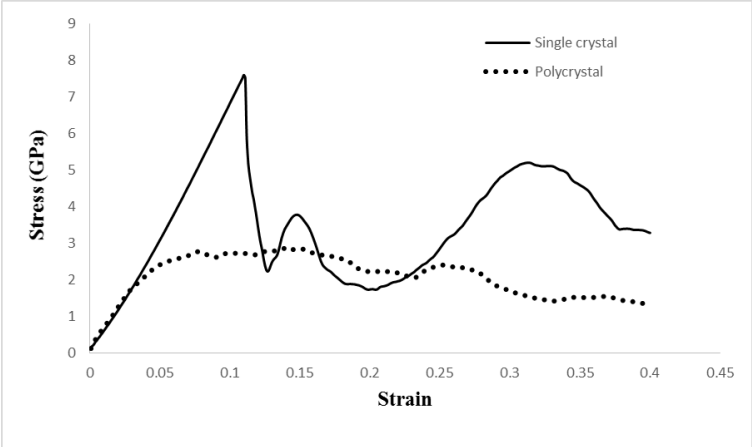

Fig. 5 Stress-strain behaviour of silver nanowire using strain rate 1 x 10^9 s^{-1} at 0.01K

The yield strength of the nanowires have been calculated by using slope upto the maximum stress point. From figure 6 it can be shown that the yield strength of single crystal silver nanowire at 300K temperature is 69.411 GPa. Also from Table I the change of yield strength of single crystal nanowires for various temperatures can be easily shown.

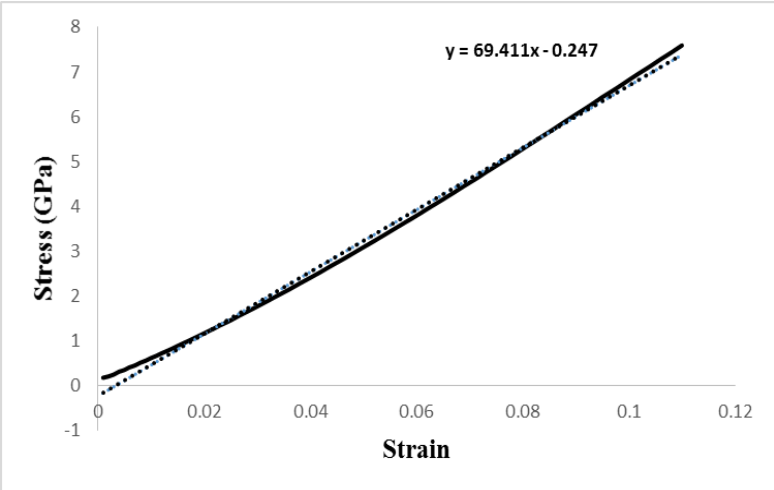

Fig. 6 Stress-strain behaviour of silver nanowire using strain rate 1 x 10^9 s^{-1} at 0.01K

TABLE I

Yield Strength of Silver Nanowires for Different Temperatures at .01 strain rate

Temperature (K)	Yield strength (GPa)
0.01	69.411
300	51.183
600	35.45
900	20.793

IV. CONCLUSIONS

In this present study, the temperature and strain rate dependent fracture mechanism of silver nanowire has been studied. Due to the extensive applications of FCC metallic nanowires, this study has shed light on several important mechanical characteristics of such nanowires. The stress-strain behavior has shown different variations for single and polycrystalline nanowires. For polycrystalline nanowires, the yield strength reduces with significant increase in ductility. Besides, with the increase in temperature the maximum value of the stress also reduced to a large extent. The effect of strain rate has also been shown in this study as well.

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