Mechanical Properties of Twinned Copper Nanowires Under Uniaxial Compression

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Abstract—*Molecular dynamics (MD) Simulation has been employed to study the compression behaviour of twinned copper nanowires at fixed strain rate of 1 x 10^{10} s^{-1}. FCC structure of copper nanowires are subjected to uniaxial compression at 0.1K temperature. Copper nanowires of varying diameters have been chosen (2.88 nm and 5.76 nm). Embedded Atom Model (EAM) potentials have been used to calculate interatomic potentials among the atoms. The compressive properties and deformation modes have been observed and discussed. The dislocations criteria and change of atomic structures have also been analysed. Two types of twin boundaries have been inserted into the nanowires to investigate their effects. It has been found that nanowires with lower twin boundary spacing show higher yield strength and seemingly different deformation criteria.*

Keywords—*Twin boundary, nanowire, dislocations, aspect ratio*

I. INTRODUCTION

Metallic nanowires have become very significant in the realm of nanomaterial research. Recently, they are paying more attention because of some unique features. Metallic nanowires are being widely used in transistors, high efficiency photovoltaic devices, nanoprobes, nanoelectromechanical systems (NEMS) and biomedical fields [1, 2]. They are also very useful in different tribological applications such as-scanning tunneling microscope (STM) and atomic force microscope (AFM) for determining nanoscale surface textures [3]. The methodologies for the prediction of mechanical properties as well as the synthesis methods of these nanostructures include a wide range of varieties and hence more and more researchers and scientists are getting attracted to the unique mechanical and electrical properties of the nanowires. Some experimental data show that metallic nanowires can be stronger than their bulk materials. Marcel et al. has shown that the silver nanowires to have a higher yield strength than the bulk silver [4]. Wu et al [5] studied the tensile strength and failure of copper nanowires under uniaxial tension. From their study it can be concluded that bulk copper has much lower yield strength than copper nanowires. They also showed the cross-sectional area and strain rate dependent mechanical properties of nanowires. The yield strengths of gold whiskers have been reported over ten times stronger than the bulk [6].

The mechanical properties of the metallic nanowires are the main important factors for using it in real life applications. To make nanowires stronger, twin boundaries have been introduced in the nanowires [19, 20] which are expected to have very high mechanical properties relative to twin-free nanowires. It has been documented that metallic nanowires having twin boundaries exhibit very strong Hall-Petch effects as a function of Twin Boundary Spacing [21].

Park et al [7, 8] and Liang and Zhou [9] simulated the uniaxial tension of gold and copper nanowires and observed the shape memory effect and pseudo-elastic behaviour of the nanowires. Wang et al. [10] studied the temperature and strain rate dependent mechanical tensile properties of nickel nanowires whereas Koh et al [11] simulated the temperature and strain-rate dependent deformation characteristics and mechanical properties of the platinum nanowires under unidirectional uniform tension. They also stated 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. Park et al [12] used ⟨100⟩ and ⟨110⟩ crystal orientations to simulate axial tension and compression of copper, gold, and nickel nanowire. The main target was to find out mechanical deformation criteria of nanowires. Garcíamochales et al [13, 14] studied the influence of tensile force and temperature on Nickel nanowires and found that if the temperature is raised to 500K, the configuration enhanced but at very higher temperature the configuration declines. Zheng et al [15] and Lu et al [16, 17] studied the deformation and fracture mechanisms of gold nanowires below sub-20 nm range through experiments. Temperature and strain rate dependent mechanical properties of metallic nanowires have also been investigated [17].

As stated earlier, studying the metal nanowires in experimental approach is a gruesome task because of the current technological limitations. Analysis of the metallic nanowires, however, can be studied effectively using molecular dynamics method [18].

While the experimental work becomes relatively difficult, several atomistic simulation techniques have been utilized to model photon transport in nano structured materials [22]. Two prevailing methods are Monte Carlo (MC) simulation and Molecular Dynamics (MD) simulation. The MC method has been used to solve the Boltzmann Transport Equation (BTE) for phonon transport under the relaxation time approximation [22]. The distribution function obtained from Boltzmann's equation can be easily related to energy and therefore to temperature. The basic principle of the MC simulation is to track the phonon energy bundles as they drift and collide through the computational domain [22]. On the contrary Molecular Dynamics Simulation has been used to examine the thermal properties in nano structured materials where phonon-phonon scattering dominates heat transfer [23].

This method is now-a-days very popular method for calculating different transport properties. It is a very powerful toolbox in modern molecular modeling and enables us to follow and understand structure and dynamics with extreme detail-literally on scales where motion of individual atoms can be tracked. As nanowires have really small dimensions, MD simulation can act as a crucial numerical tool to study to the properties of these nanowires along with the deformation criteria. Many studies have been carried out to investigate the compressive properties of nanowires but very few of them involve the study of stress-strain behavior of metallic nanowire (copper). The main purpose of this paper is to investigate the stress-strain behavior of copper nanowire subjected to uniaxial compression and also to demonstrate the effects of twin boundaries on these nanowires. Using various twin boundary spacing this paper aims to discuss the dislocation criteria inside a copper nanowire uring uniaxial compression.

In the current study, mechanical properties of FCC copper nanowire have been investigated for one strain rate. To investigate the size effect of nanowire two different diameters (2.88 nm and 5.76 nm) have also been selected for a fixed temperature of 0.1K. To investigate the dislocations of the nanowires Dislocation Extraction Algorithm (DXA) has been used in this study.

II. Simulation Methodology

In the present study molecular dynamics simulations have been performed using the LAMMPS Molecular Dynamics Simulator [24]. LAMMPS use an interatomic potential to carry out these simulations. Here, embedded-atom-method potential for FCC copper has been used [25]. Ver few studies have been done to investigate the behavior of copper nanowire under compression. Using the compressive strain rate of 1 x 10^{10} s^{-1}, in this study, the effects of twin boundary on copper nanowire has been investigated. Nanowire models have been created using the lattice parameter 3.6 which supports the results from the previous studies. The aspect ratio (α) of these nanowires have been kept constant. Aspect ratio has been defined as-

$$\alpha = \frac{d}{l}$$

Where, d = diameter of the nanowire and l = length of the nanowire. In this case, α = 2. While α has been kept constant, the value of d and l have been varied to see the effect. Two types of nanowires have been created for the simulation purposes which have been shown in Fig. 1. At first, the diameter and length have been chosen as 2.88 nm and 5.76 nm respectively. This nanowire contained 3088 atoms. Later the diameter has been chosen as 5.76 nm and the length of the nanowire has been chosen as 11.52 nm, which consisted of 25376 atoms.

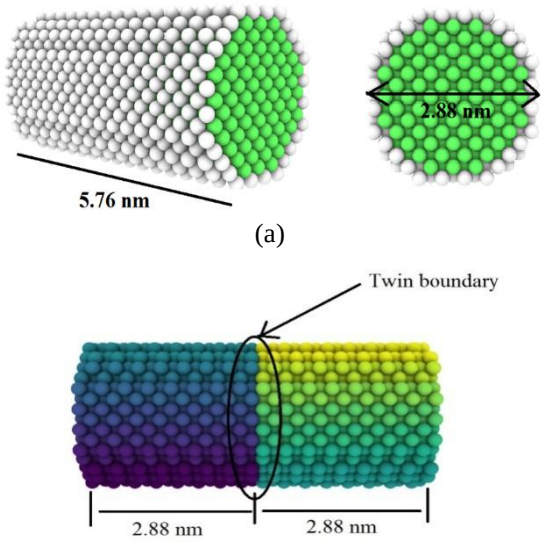


Fig. 1 Nanowire models (a) without twin boundary (b) with coherent twin boundary

The nanowires have been modeled in the [100] axial direction and the compression was also applied in the same direction. The simulation box has been taken as periodic in every directions. These simulations have been performed at the constant 0.1K temperature. Besides, the NPT ensemble has been used here with a time step of 0.001pico second. Before starting the simulation, all the nanowires were equilibrated for 30 ps. Uniaxial compression in the [100] direction has been applied. Besides centro-symmetry parameter has been used to colour the atoms along with the dislocations extraction algorithm. The reason behind using EAM potential is that the 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.

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

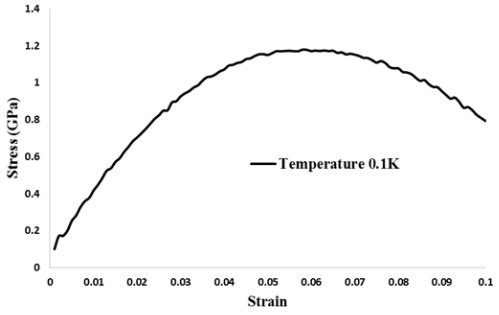
Where $\sum_i F_i(\rho)$ is embedded energy; $\phi_{ij}(r_{ij})$ is pair potential.

In this study, the effects of twin boundary has also been investigated. Two different nanowire models have been created with two types of twin boundary spacing. Here, coherent twin boundary has been created inside the nanowire. At first, the twin boundary spacing has been kept 2.88 nm and later this value has been taken as 1.44 nm. In the first case, one twin boundary has been created between the boundaries of the nanowire. In the second case, three twin boundaries have been inserted.

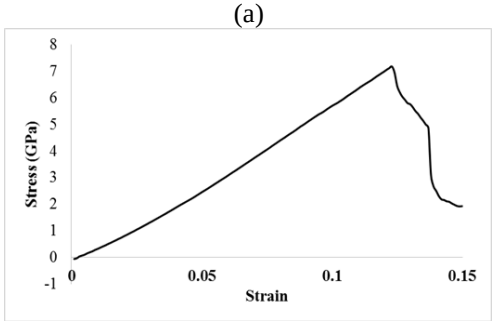
III. Results and Discussion

A. *Effect of uniaxial compression:*

In this study 1 x 1010 s-1 has been chosen as the strain rate which has been applied in the [100] direction at both ends of the nanowire.



(a)



(b)

Fig. 2 Stress-strain behaviour of copper nanowire at 0.1K temperature (a) compression (b) tension

From Fig. 2, the stress-strain relationship of the nanowire can be discussed. Unlike the tensile stress this value is much lower.Later in this study the effect of larger diameter has been shown. The compressive stress shows a smooth parabolic shape which rises to the maximum value of 1.2 GPa. Due to the large amount of compression, changes occur in the atomic level of the nanowire.

B. *Effect of aspect ratio:*

Here, the aspect ratio has been kept constant with a varying length and diameter. From Fig. 3 it is evident that the value of compressive stress is higher for larger diameter. In this particular case, the diameter is twice the initial diameter. The value of maximum stress is almost 2 GPa. This happens for the larger surface area of the cross-section of the nanowire. Due to a large cross-sectional area, the value of the yield strength increases.

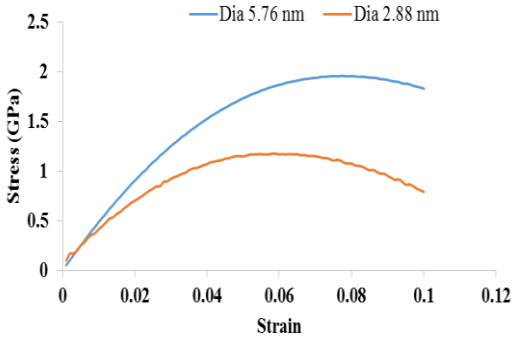


Fig. 3 Stress-strain behaviour of copper nanowire at 0.1K temperature for two different dimensions

C. *Effect of twin boundary:*

One of the main purposes of this paper is to investigate the effects of twin boundaries on copper nanowire. Using two distinguished twin boundary spacing, this simulation has been performed. As usual the nanowires have been equilibrated for 30 ps. Fig. 4 shows the twinned nanowire after energy minimization. The internal atomic structure of the nanowire changes due to compression which can be seen from the Fig. 5. It clearly demonstrates the surface morphology of twinned copper nanowire during compression. Up to 10% strain there is almost no change in the nanowire. But after the 15% strain rate there is drastic change in the nanowire morphology.

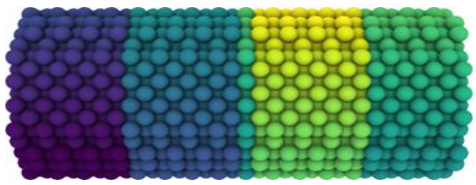
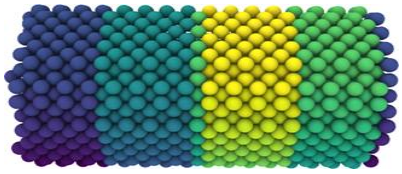


Fig. 4Equilibrated nanowire model of copper with three twin boundaries



5% strain

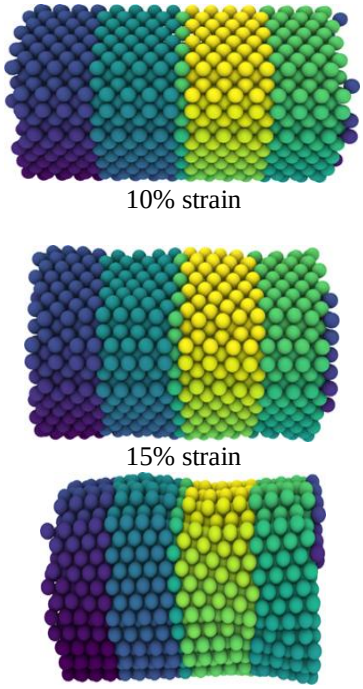


Fig. 5 Nanowires subjected to uniaxial compression at different strains

From Fig. 6, the deformation criteria can be discussed. Here, the defect mesh shows the deformation procedure at different strains. Rapid fracture occurs after 10% strain.

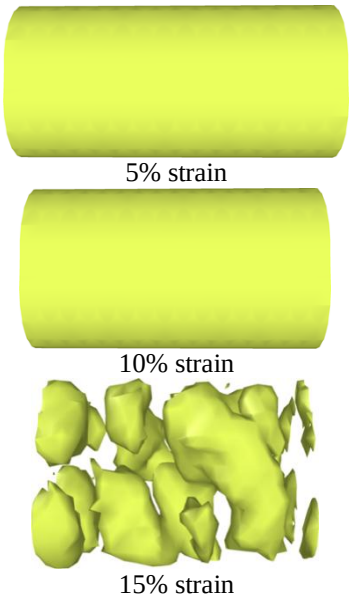


Fig. 6Equilibrated nanowire model of copper with three twin boundaries

At 15% strain, fracture becomes clearly visible which eventually initiates the occurrence of dislocation lines.

During this period dislocations lines get clearly visible. Partial and complete dislocations can be seen from Fig. 7. These dislocations lines have been shown using the DXA method. Here, these lines predict the deformation criteria of the nanowire. Most of the lines are partial dislocation lines. Different colors predict different atomic structures.

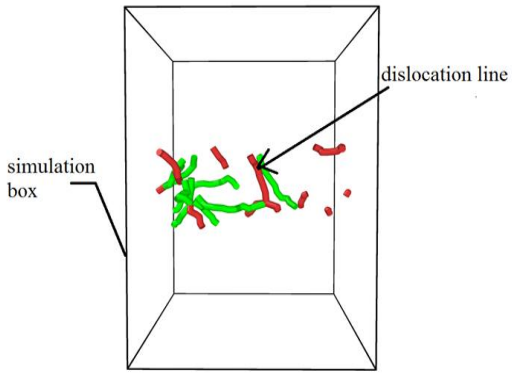


Fig. 7 Dislocations of copper nanowire during compression

Fig. 8 demonstrates the stress-strain behaviour of nanowires with and without twinning. Here, the nanowire with minimum twin boundary spacing shows the maximum yield strength. On the other hand, the nanowire without any kind of twinning shows lowest value of yield strength.

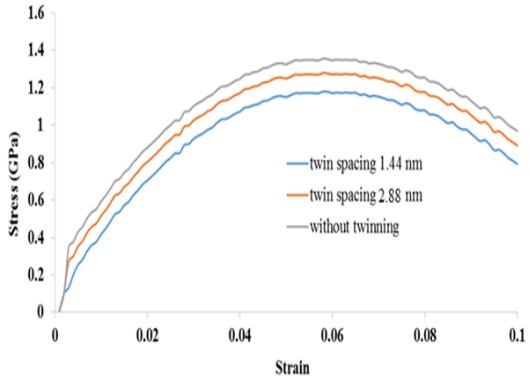
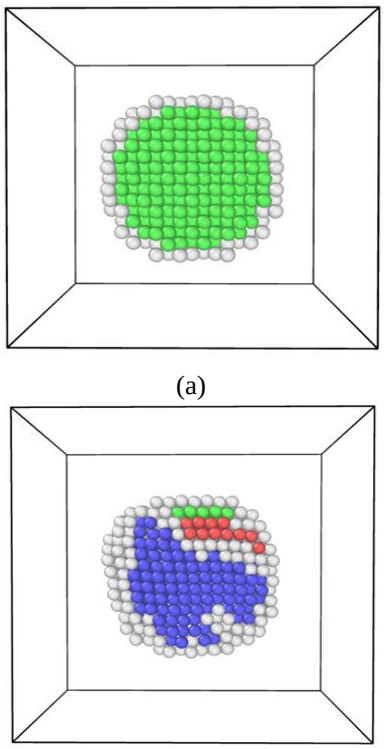


Fig. 8Comparison of mechanical behaviours of different copper nanowires

Besides, the change in atomic structure is also evident from Fig. 9. Here, the grey atoms indicate surface atoms. Due to compression the atomic structure of the initial configuration changes from FCC to others. The green atoms indicate FCC atoms. Again, it can be seen that because of compression, this FCC structure changes into BCC (blue atoms), hcp (red atoms) and other atomics structures.



(a)

(b)

Fig. 9 Change of atomic structures of copper nanowires during compression (a) before compression (b) after 20% strain

IV. CONCLUSIONS

The present study discusses the deformation criteria of twinned copper nanowire with the help of dislocations. The dislocation lines initiates fracture inside the nanowire and reduces the stress which have been discussed using the defect mesh. Besides, there is significant increase in stress with the lowering of twin boundary spacing. It has also been shown in this study how the atomic structures of copper nanowires change during uniaxial compression.

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REFERENCES

[1] Gleiter h. *Nanostructured materials: Basic concepts and microstructure*. Acta Mater, 2000, 48(1): 1−29.

[2] Lu L, Shen Y, Chen X, Qian L, Lu K. Ultrahigh strength and high electrical conductivity in copper. Science, 2004, 304(5669): 422−426.

[3] Zhang, H., & Huang, H. (2009). Do twin boundaries always strengthen metal nanowires? Nanoscale research letters, 34-38.

[4] Lucas, M., Leach, A. M., McDowell, M. T., Hunyadi, S. E., Gall, K., Murphy, C. J., &Riedo, E. Plastic deformation of pentagonal silver nanowires: Comparison between afmnano indentation and atomistic simulations. Physical Review B, 2008, 77(24).

[5] Wu H A, Soh A K, Wang X X, Sun Z H., Strength and fracture of single crystal metal nanowire. Key Engineering Materials, 2004, 261−263: 33−38.

[6] Wu, B., Heidelberg, A., & Boland, Mechanical properties of ultrahigh-strength gold nanowires. Nature Materials, 2005, 4(7), 525-529.

[7] Park H S, Gall K, Zimmerman J A., Shape memory and pseudo elasticity in metal nanowires. Physical Review Letters, 2005, 95(25): 255504.

[8] Park H S, Zimmerman J A., Stable nano bridge formation in (110) gold nanowire under tensile deformation. ScriptaMaterialia, 2006, 54(6): 1127−1132.

[9] Liang W, Zhou M., Atomistic simulations reveal shape memory of FCC metal nanowires. Physical Review, 2006, 73(11): 115409.

[10] Wang, Wei-dong, Cheng-long Yi, and Kang-qi Fan, Transactions of Nonferrous Metals, Society of China, 23 (2013), 3353-3361.

[11] Koh S J A, Lee H P, Lu C, Cheng Q H., Molecular dynamics simulation of a solid platinum nanowire under uniaxial tensile strain: Temperature and strain-rate effects [J]. Physical Review, 2005, 72(8): 5414.

[12] Park H S, Gall K, Zimmerman J A., Deformation of FCC nanowires by twinning and slip, Journal of the Mechanics and Physics of Solids, 2006, 54(9): 1862−1881.

[13] García-Mochales P, Paredes R, Peláez S, Serena P A., The formation of pentagonal Ni nanowires: Dependence on the stretching direction and the temperature. Physica Status Solidi A, 2008, 205(6): 1317−1323.

[14] García-Mochales P, Paredes R, Peláez S, Serena P A., Statistical analysis of Ni nanowires breaking processes: A numerical simulation study. Nanotechnology, 2008, 19(22): 225704.

[15] Zheng H, Cao A, Weinberger C R, Huang J Y, Du K,Wang J, Ma Y, Xia Y, Mao S X., Discrete plasticity in sub-10-nm-sized gold crystals. Nature Communications, 2010, 1(144): 1−8.

[16] Lu Y, Song J, Huang J Y, Lou J., Surface dislocation nucleation mediated deformation and ultrahigh strength in Sub-10-nm Gold nanowires. Nano Research, 2011, 4(12): 1261−1267.

[17] Alam, MdFerdous, Shahadat, Muhammad Rubayat Bin, "Temperature and Strain Rate Dependent Mechanical Properties of Ultrathin Metallic Nanowires: A Molecular Dynamics Study." 12th International Conference on Mechanical Engineering (ICME 2017)

[18] Lu Y, Song J, Huang J Y, Lou J, Fracture of Sub-20nm ultrathin gold nanowires. Advanced Functional Materials, 2011, 21(20): 3982−3989.

[19] Kang K, Cai W., Size and temperature effects on the fracture mechanisms of silicon nanowires: Molecular dynamics simulations. International Journal of Plasticity, 2010, 26(9): 1387−1401.

[20] Wu, B., Heidelberg, A., & Boland, J.E. Sader, X. Sun, Y. Li. Microstructure-hardened- silver nanowire, Nano Letter, 6(2006): 468-472.

[21] A. Cao, Y. Wei, Atomistic simulations of the mechanical behavior of fivefold twinned nanowires, Phys. Rev. B 74 (2006) 214108.

[22] H. Liu, J. Zhou, Plasticity in nano twinned polycrystalline Ni nanowires under uniaxial compression. Materials Letters 163 (2016): 179-182.

[23] ZHITING TIAN B.E., Tsinghua University, China, 2007; Nanoscale Heat Transfer In ARGON-Like Solids Via Molecular Dynamics Simulations

[24] M.R.B. Shahadat, A.S. Masnoon, S. Ahmed, AKM M Morshed, "Effect of the orientation of doped nanoparticles on thermal transportation of a solid: A molecular dynamics study" AIP Conference Proceedings 1851, 020084 (2017).

[25] S. J. Plimpton, J. Comp. Phys. 117, 1 (1995); http://lammps.sandia.gov/

[26] Daw M S, Baskes M I., Physical Review Letters, 50(17): 1285−1288 (1983).