Molecular Dynamics Simulation of Mechanical Properties of Cu Nanowire with Grain Boundaries

A report submitted in partial fulfillment of the requirement for the degree of

BACHELOR OF SCIENCE IN MECHANICAL ENGINEERING

Submitted by

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ABSTRACT

Molecular dynamics (MD) is a computer simulation method for analyzing the physical movements of atoms and molecules. The atoms and molecules are allowed to interact for a fixed period of time, giving a view of the dynamic "evolution" of the system. Material has inherent faults in the real life. Based on the molecular dynamics (MD) method, the single-crystalline copper nanowire with different surface defects is investigated through tension simulation. For comparison, the MD tension simulations of perfect nanowire are firstly carried. It has concluded that the surface-volume ratio significantly affects the mechanical properties of nanowire. It is found that the Young's modulus is sensitive to surface defects. And the yield strength and yield point show a significant decrease due to the different defects. Different defects are observed to serve as a dislocation source.it is difficult to obtain lattice structure in real life. So defect in material structure persists among which grain boundary is prominent. In this thesis, we have conducted an MD simulation on copper with grain boundary to see its effect on mechanical properties. This study has provided a comprehensive and deep investigation into the mechanical properties of Cu NWs which can be helpful in determining the feasibility of practical applications of Copper in components of electrical devices compared to currently used materials such as Indium Tin Oxide. It has been exhibited by this study as well as the ones before it that MD simulation is an effective tool not only for the characterization of the properties of NWs, but also for the prediction of novel and unexpected properties.

Keywords: Nanowire, Copper, Defect, Molecular Dynamics, Tension, Surface.

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CHAPTER 1
INTRODUCTION

1.1 Introduction

Nanocrystalline copper (Cu) is considered to be one of the best interconnected material in Integration Circuit (IC) industry, because of its ultra-low resistivity and high mechanical stability. Mechanical properties of nanocrystalline Cu are completely different from those of bulk monocrystalline Cu. These properties are of high importance in the assessment of the thermo-mechanical reliability of the interconnected IC structure. To investigate the effects of the grain sizes and temperature on the mechanical properties of nanocrystalline Cu, Molecular Dynamics simulations of uniaxial tensile test are performed in this study. The results show that the elastic modulus of nanocrystalline Cu with grain sizes of 4.65–12.41 nm gradually increases with the increase of the mean grain sizes, the corresponding flow stress concurrently increases, and the flow stress is proportional to the square-root of the grain size, which satisfies the Inverse- Hall–Petch relation. Furthermore, the elastic modulus linearly decreases with increase of temperature. Meanwhile, the deformation activation energy of nanocrystalline copper for various grain sizes were obtained. All of the tensile simulation tests confirmed that the mechanism of plastic deformation for nanocrystalline Cu with 4.65–12.41 nm grain sizes is mainly specific to the grain boundary sliding and grain rotation. The dislocation nucleation and migration, which is usually the deformation mechanism of plasticity for macroscopic materials, is no longer the dominant factor for nanocrystalline Cu.

1.2 Objectives:

- To evaluate Mechanical properties of Copper
- To study the Copper structure with grain boundaries at Nano level
- To evaluate the Young's Modulus for Pristine Cu & different temperature
- To study how the grain sizes affect mechanical properties of Cu NW

1.3 Organization of Book

This project book consists of six chapters. The first chapter contains the statement of the introduction, the objectives of the study, and the project organization. Chapter two contains a literature review in detail. Chapter three describes the project's molecular dynamics simulation. Chapter four deals with the Methodology. In the fifth chapter deals with Parametric Study, we have done the conclusion and future work of the project and also about some aspects we had to overcome while doing the project lastly, we gave the conclusion of the book.

CHAPTER 2

LITERATURE REVIEW

2.1 LITERATURE REVIEW

As electronic technology goes for thinner and lighter components, Integration Circuit (IC) chips continue to increase integration density and reduce feature size in accordance with Moore's Law. Electroplated Cu has been applied to not only interconnections in printed wiring boards, but also thin film interconnections and Through Silicon Via (TSV) in semi- conductor devices because of its low electric resistivity, high thermal conductivity, low electromigration rate and good compatibility with the multilayered interconnecting process. The use of electroplated Cu as a metal connection in IC chips can reduce the loss of electrical energy and increase the speed of ICs [1]. The electroplating process usually adopts the electroplating solution of the sulfate system and follows the Faraday's law of electrolysis, then the grains of polycrystalline Cu are formed after electroplating and annealing processes. The length scale of Cu grain in TSV-Cu and other IC interconnected structure is less than a micrometer, therefore, the crystalline of Cu are mainly composed of nano-size crystallites with mechanical properties, such as Young's modulus and yield strength completely different from the conventional bulk Cu [2]. Nanocrystalline metal usually refers to a polycrystalline material with grain size of 1–100 nm, which is characterized by fine grain size, high defect density, and a large percentage of grain boundary. At the grain boundary, the atomic arrangement is disordered, the lattice distortion is large, and the property of grain boundary is different from the interior grain. Grain boundaries have a major impact on the mechanical properties of nanocrystalline metallic materials [3]. Furthermore, the grain size is an important factor affecting the mechanical properties of traditional coarse-grained metals. It is known from the Hall–Petch relation that the strength of the polycrystalline metal material increases with decreasing of the grain sizes. However, the continued decrease of the grain size causes the softening of the nanocrystalline material, which is described by the Inverse-Hall–Petch relation [4–6]. Con- sidering the deformation behavior under stress, fine grain size and high grain boundary to volume ratio may lead to distinctive deformation mechanism. Meanwhile, the temperature is one of the most important factors for the mechanical reliability of the interconnected structure [7–9], which is worth to investigate. The method of Molecular Dynamics (MD) simulations is suitable to

investigate the mechanical properties and deformation mechanism of nanocrystalline metals [10]. The mechanical properties and deformation mechanisms of nanocrystalline materials have been primarily studied with a focus on the impact of grain size [11–13], strain rate [14–16] and temperature [17–21]. Zhou et al [13] claimed tensile modulus and flow stress increases with increase of grain sizes when then mean grain size is in the range of 2.6–53.1 nm in detail. Zhang et al [15] investigated the strain rate effect on mechanical properties. The results also showed a transition of deformation mechanism from grain-boundary based mechanisms to dislocation mediated mechanism at the grain size about of 10 nm, which is insensitive to the strain rate. Xiang et al [16] proved that the tensile modulus and flow stress increase with increase of grain sizes. The mechanical properties of metallic nanowires at different temperatures were studied by MD simulations, and the results showed that the elastic modulus and the yield strengths are gradually decreasing with the increase of temperature [17–19]. Gan et al [20] also confirmed the temperature softening effect on strength and Young's modulus of gold nanofilms. Li et al [21] focused on the temperature and pressure dependences of the elastic properties of Tantalum single crystals by atomic simulation, and concluded that the elastic modulus linearly decreases with increase of temperature. However, despite the numerous aforementioned investigations, there has not been a systematic atomic simulation study on the temperature and grain size dependences of nanocrystalline Cu under tensile loading. From this point of view, it is necessary to establish an atomic simulation method to compute the effect of the temperature and grain size on mechanical properties. In this paper, a series of large-scale MD simulations of uniaxial tensile tests were performed to investigate the mechanical properties of nanocrystalline Cu, considering the effects of strain rates, grain sizes and temperature.

CHAPTER 3

MOLECULAR DYNAMICS SIMULATION

3.1 Molecular dynamics :

Molecular dynamics (MD) is a computer simulation method for analyzing the physical movements of atoms and molecules. The atoms and molecules are allowed to interact for a fixed period of time, giving a view of the dynamic "evolution" of the system. In the most common version, the trajectories of atoms and molecules are determined by numerically solving Newton's equations of motion for a system of interacting particles, where forces between the particles and their potential energies are often calculated using interatomic potentials or molecular mechanical force fields. The method is applied mostly in chemical physics, materials science, and biophysics.

3.2 Microcanonical Ensemble:

In the microcanonical ensemble, the system is isolated from changes in moles (N), volume (V), and energy (E). It corresponds to an adiabatic process with no heat exchange. A microcanonical molecular dynamics trajectory may be seen as an exchange of potential and kinetic energy, with total energy being conserved. For a system of N particles with coordinates X and velocities V, this pair of first order differential equations may be written in Newton's notation as,

$$F(X) = -\nabla U(X) = M\dot{V}(t)$$
$$V(t) = \dot{X}(t).$$

The potential energy function U(X) of the system is a function of the particle coordinates X. It is referred to simply as the potential in physics, or the force field in chemistry. The first equation comes from Newton's laws of motion; the force F acting on each particle in the system can be calculated as the negative gradient of U(X). For every time step, each particle's position X and velocity V may be integrated with a symplectic integrator method such as Verlet integration. The time evolution of X and V is called a trajectory. Given the initial positions (e.g., from theoretical knowledge) and velocities (e.g., randomized Gaussian), we can calculate all future (or past) positions and velocities.

3.3 Canonical Ensemble:

In the canonical ensemble, amount of substance (N), volume (V) and temperature (T) are conserved. It is also sometimes called constant temperature molecular dynamics (CTMD). In NVT, the energy of endothermic and exothermic processes is exchanged with a thermostat. A variety of thermostat algorithms are available to add and remove energy from the boundaries of an MD simulation in a more or less realistic way, approximating the canonical ensemble. Popular methods to control temperature include velocity rescaling, the Nosé–Hoover thermostat, Nosé–Hoover chains, the Berendsen thermostat, the Andersen thermostat and Langevin dynamics. The Berendsen thermostat might introduce the flying ice cube effect, which leads to unphysical translations and rotations of the simulated system. It is not trivial to obtain a canonical ensemble distribution of conformations and velocities using these algorithms. How this depends on system size, thermostat choice, thermostat parameters, time step and integrator is the subject of many articles in the field (Wikipedia).

3.4 Potentials in MD simulations:

A molecular dynamics simulation requires the definition of a potential function, or a description of the terms by which the particles in the simulation will interact. In chemistry and biology this is usually referred to as a force field and in materials physics as an interatomic potential. Potentials may be defined at many levels of physical accuracy; those most commonly used in chemistry are based on molecular mechanics and embody a classical mechanics treatment of particle-particle interactions that can reproduce structural and conformational changes but usually cannot reproduce chemical reactions. The reduction from a fully quantum description to a classical potential entails two main approximations. The first one is the Born–Oppenheimer approximation, which states that the dynamics of electrons are so fast that they can be considered to react instantaneously to the motion of their nuclei. As a consequence, they may be treated separately. The second one treats the nuclei, which are much heavier than electrons, as point particles that follow classical Newtonian dynamics. In classical molecular dynamics, the effect of the electrons is approximated as one potential energy surface, usually representing the ground state. When finer levels of detail are needed, potentials based on quantum mechanics are used; some methods attempt to create hybrid classical/quantum potentials where the bulk

of the system is treated classically but a small region is treated as a quantum system, usually undergoing a chemical transformation. (Wikipedia)

3.5 Pair potentials versus many-body potentials:

The potential functions representing the non-bonded energy are formulated as a sum over interactions between the particles of the system. The simplest choice, employed in many popular force fields, is the "pair potential", in which the total potential energy can be calculated from the sum of energy contributions between pairs of atoms. Therefore, these force fields are also called "additive force fields". An example of such a pair potential is the non-bonded Lennard–Jones potential (also termed the 6–12 potential), used for calculating van der Waals forces.

$$U(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

Another example is the born (ionic) model of the ionic lattice. The first term in the next equation is Coulomb's law for a pair of ions, the second term is the short-range repulsion explained by Pauli's exclusion principle and the final term is the dispersion interaction term. Usually, a simulation only includes the dipolar term, although sometimes the quadrupolar term is also included. When nl = 6, this potential is also called the Coulomb–Buckingham potential.

In many-body potentials, the potential energy includes the effects of three or more particles interacting with each other. In simulations with pairwise potentials, global interactions in the system also exist, but they occur only through pairwise terms. In many-body potentials, the potential energy cannot be found by a sum over pairs of atoms, as these interactions are calculated explicitly as a combination of higher-order terms. In the statistical view, the dependency between the variables cannot in general be expressed using only pairwise products of the degrees of freedom. For example, the Tersoff potential, which was originally used to simulate carbon, silicon, and germanium, and has since been used for a wide range of other materials, involves a sum over groups of three atoms, with the angles between the atoms being an important factor in the potential. Other examples are the embedded-atom method (EAM), the EDIP, and the Tight-Binding Second Moment Approximation (TBSMA) potentials, where

the electron density of states in the region of an atom is calculated from a sum of contributions from surrounding atoms, and the potential energy contribution is then a function of this sum.

CHAPTER 4

METHODOLOGY

Our molecular dynamics MD simulations employed copper NW with a square cross-section and grain boundary. We choose the X- direction as the tensile loading direction for grain boundary Copper NW. The NW can be set either with periodic or non-periodic BCs along the longitudinal direction. Especially, for the non-periodic BCs, a constant strain rate is often applied by fixing one end of the NW, then applying a constant velocity to the free end. We have used LAMMPS as a simulator for this research purpose. We have employed the P-S-S boundary condition for this model. Here, the style P means the box is periodic so that particles interact across the boundary, and they can exit one end of the box and re-enter the other end. The style S, shrink-wrapped, means the box is non-periodic so that particles do not interact across the boundary and do not move from one side of the box to the other. For style S, the position of the face is set to encompass the atoms in that dimension (shrink-wrapping), no matter how far they move. Note that when the difference between the current box dimensions and the shrink-wrap box dimensions is large, this can lead to lost atoms at the beginning of a run when running in parallel. This is due to the large change in the (global) box dimensions also causing significant changes in the individual sub-domain sizes. If these changes are farther than the communication cutoff, atoms will be lost. For this boundary case, a constant strain rate is imposed on the NW after the relaxation process. We used conjugate minimization to have the minimized model. For the initial purpose, we have kept a temperature of 0.01k for the model. After ramping up the temperature, we imposed a constant strain rate of 10^9 1/s on both sides of the x-axis, which has periodic boundary conditions. This strain rate was selected after testing various strain rates, which would be discussed in the following sections. Several approaches have been developed to extract the mechanical properties of NWs (e.g., Young’s modulus) from MD simulation results, such as the virial stress method and energy method for the derivation of Young’s modulus as proposed by Diao et al. In the present research, Young’s modulus will be determined directly from the stress-strain curve using linear regression, which is the traditional approach. According to the definition of yield strength in continuum mechanics and the atomic configurations during simulation, yield strength is referred to as the stress when plastic deformation first appears, i.e., partial dislocations first emitted, and the corresponding strain is taken as yield strain. The engineering strain is used in this work, which is defined as:

$$\epsilon = (l_o - l)/l_o$$

Here l is the instantaneous length and lo is the initial length of the NW after the energy minimization.

CHAPTER 5

PARAMETRIC STUDY

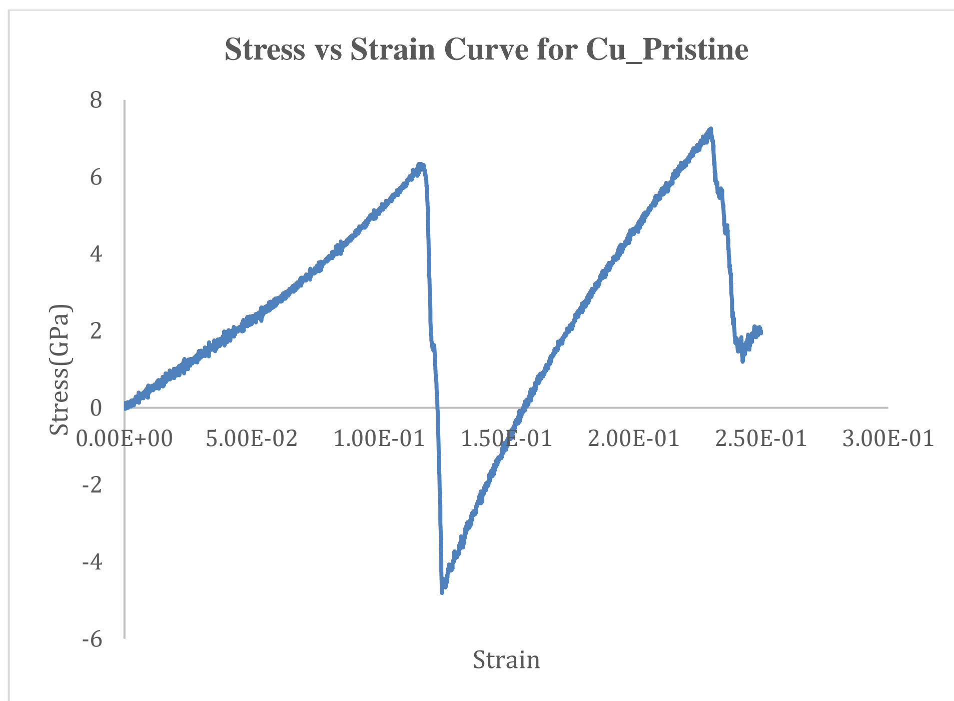
5.1 Mechanical Properties of Pristine Cu:

Copper is a tough, ductile and malleable material. These properties make copper extremely suitable for tube forming, wire drawing, spinning and deep drawing. The other key properties exhibited by copper and its alloys include:

- Excellent heat conductivity
- Excellent electrical conductivity
- Good corrosion resistance
- Good biofouling resistance
- Good machinability
- Retention of mechanical and electrical properties at cryogenic temperatures
- Non-magnetic

Material	Copper
Density, kg/m^3	8960
Heat capacity, J/kg·K	383
Thermal conductivity, W/m·K	386
Young's modulus, GPa	124
Poisson's ratio	0.34
A, MPa	90
B, MPa	292
N	0.31
C	0.025
M	1.09
T_m, K	1356
T_0, K	298
Reference strain rate, s^{-1}	1

5.2 Comparison of mechanical properties between Cu pristine and grain boundary:



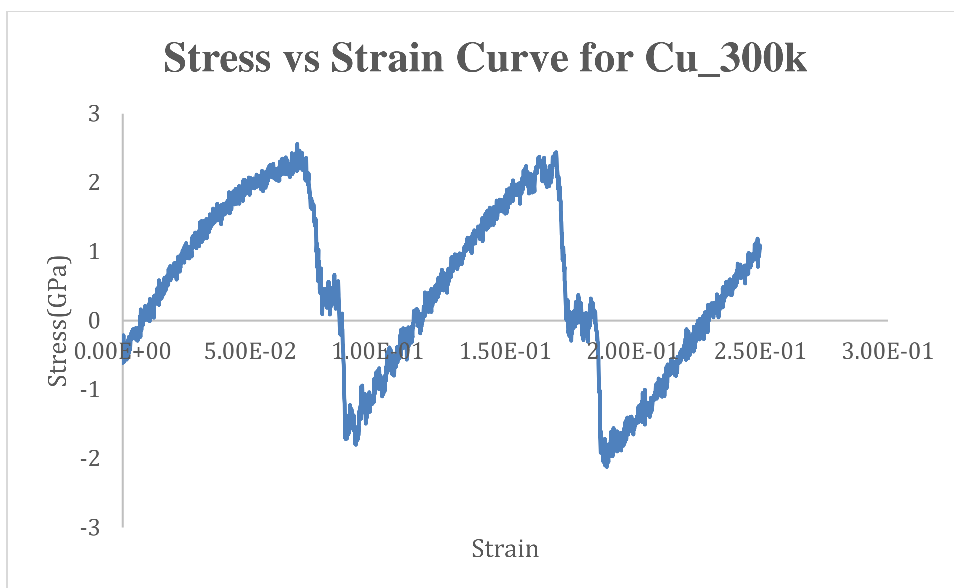


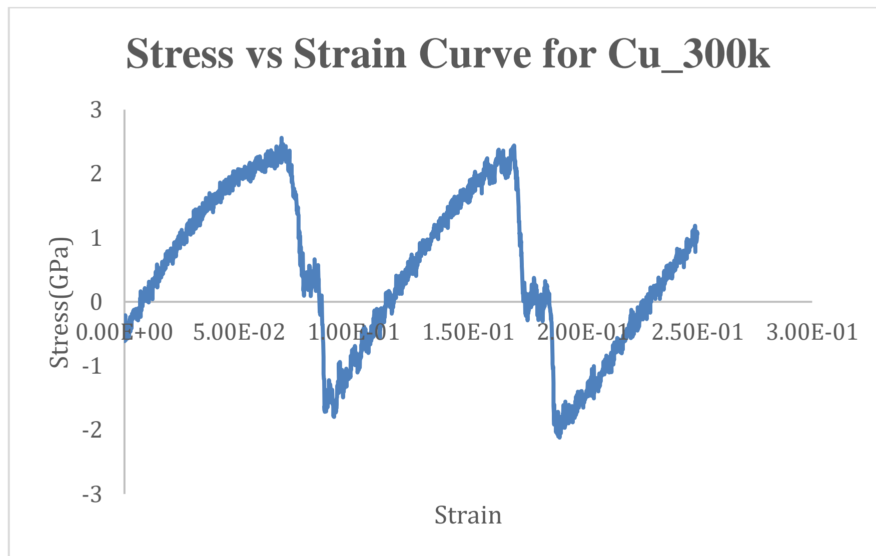
Table for both Pristine & Grain Boundary Young's modulus (E) value

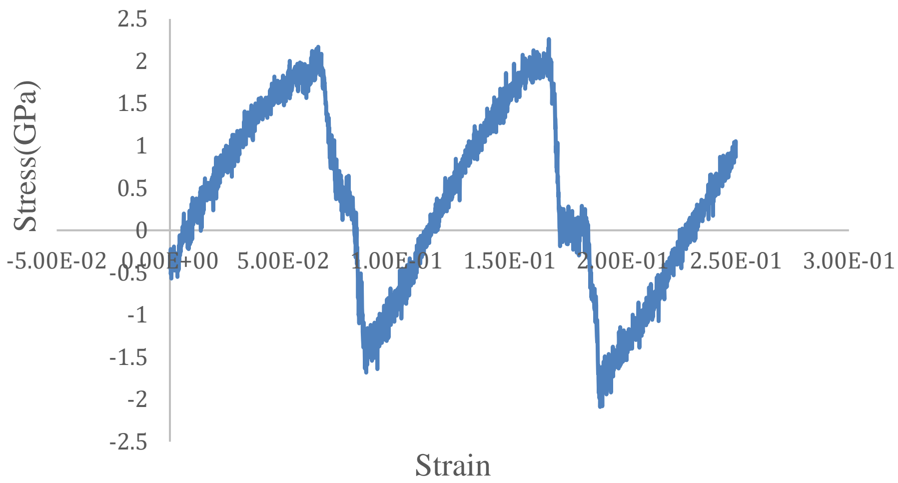
Name	Young's modulus (E) value, GPa
Cu_Pristine	E=60
Grain Boundary(GB)	E= 43

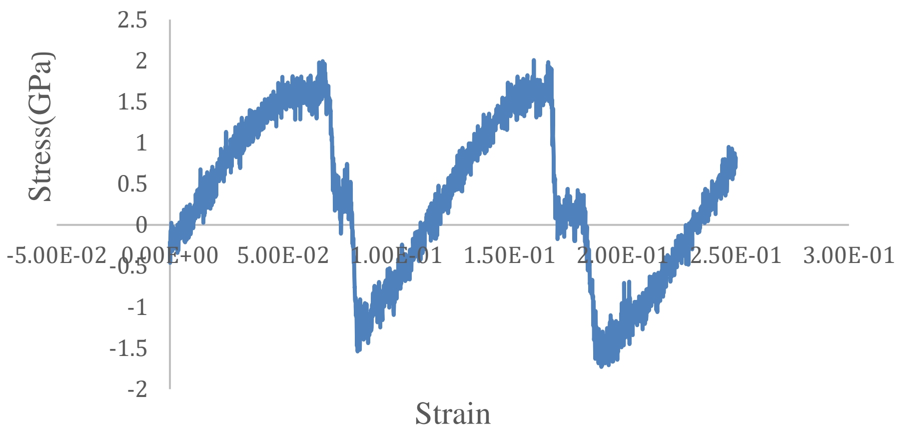
Table The mechanical properties of nanocrystalline copper

	References	Grain size (nm)	Temperature (K)	Strain rate (s^{-1})	Elastic modulus (GPa)	Flow stress (GPa)	Transition zone[a] (nm)
Current results	—	4.65–12.41	1–500	5×10^8	54–92	1.2–2.5	—
MD studies	Zhou [14]	2.6–53.1	300	1×10^8	25–75	0.84–1.25–0.9	8–20
	wang y[21]	9.0–24	300	10^8	55–83	2.2–4.0	16–20
	Zhang [21]	3.8–27.3	300	1×10^7	—	0.5–2.5	17.2
				1×10^{10}			11.5

Effect of temperature variation in mechanical properties:




Stress vs Strain Curve for Cu_450k
Stress(GPa)
2.5
2
1.5
1
0.5
0
-0.5
-1
-1.5
-2
-2.5
-5.00E-02
0.00E+00
5.00E-02
1.00E-01
1.50E-01
2.00E-01
2.50E-01
3.00E-01
Strain


Stress vs Strain Curve for Cu_600k
Stress(GPa)
2.5
2
1.5
1
0.5
0
-0.5
-1
-1.5
-2
-5.00E-02
0.00E+00
5.00E-02
1.00E-01
1.50E-01
2.00E-01
2.50E-01
3.00E-01
Strain

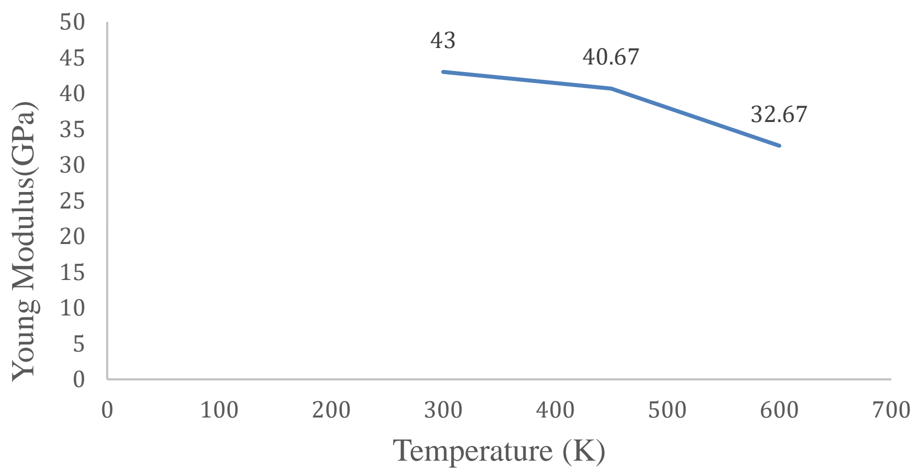

Temperature Effect
Young Modulus(GPa)
50
45
40
35
30
25
20
15
10
5
0
43
40.67
32.67
0
100
200
300
400
500
600
700
Temperature (K)

Table for different temperature Young's modulus (E) value:

300K	450K	600k
E= 43	E= 40.67	E= 32.67

Continuation of study on the same testing sample, this time taking different temperatures, is conducted. “Temperature vs young’s modulus graph” shows the stress-strain curves at different temperatures from 300k to 600k. It is generally found that the stress-strain curve exhibits larger fluctuations for higher temperatures. Particularly, all stress-strain curves appear linear before yielding and become saw-tooth-shaped after yielding, with the stress reducing dramatically. The following table is showing young’s modulus for grain boundary Copper NW at a different temperature: - Table showing temperature and young’s modulus values The change in young’s modulus due to temperature variation is also shown in “Temperature vs young’s modulus graph”. Apparently, Young’s modulus is decreased when the simulation temperature increases, the same as reported by Yuan et al. Small molecule regulators of autophagy
identified by an image-based high-throughput screen. Proceedings of the National Academy of Sciences, 104(48), 19023-19028.), e.g., Young’s modulus at 300K is found to be about 20% higher
than those at 600 K. Hence, it is concluded that temperature exerts significant influence on mechanical properties of NWs.

CHAPTER 6

CONCLUSION

6.1 Conclusion:

Mechanical properties of copper were studied using Molecular Dynamics method. At various temperature the elastic constants were found to be in agreement with experimental values. The strength in terms of maximum tensile stress of the system was also found to be in agreement with experimental findings. Based on this high level of agreement with experimental data we conclude that molecular-dynamics simulations can serve as reliable and realistic tool for studying such complicated mechanical processes in metals as fracture in a sample containing grain boundaries. it is concluded that temperature exerts significant influence on mechanical properties of NWs. In future studies these issues will be addressed.

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