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Molecular dynamics simulation to evaluate flexural properties of Cu nanowires under different loading conditions

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Abstract: An extensive study of mechanical properties on the Copper nanowire is conducted in this paper. A three-point bending method, based on AFM bending experiment, has employed in order to obtain mechanical properties of Cu NWs. Tensile test by means of strain rate is a well-known method to evaluate mechanical properties in Molecular Dynamics (MD) simulations. A comparisional analysis between young's modulus gain through tensile test and bending test, employed in this paper, has shown that mechanical strength is slightly more in axial loading than lateral loading direction. Also, study on different loading rate is done here to evaluate which loading rate should be indicated as impact load rather than bending load. For any nanomaterial, their superior mechanical properties are evident due to their large surface-to-volume ratio. In this paper to evaluate this phenomenon, a study of bending effect on various Cu NWs depth has shown that with the decrement of depth of the material, and so by increasing surface-to-volume ratio, mechanical properties of the material increases. Additionally, an effect of various indenter size is studied to gain insight on its effect on mechanical properties of Cu NWs.

Keywards: Cu Nanowire, AFM Bending Method, Young's Modulus, Impact Load.

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Introduction

The physical properties of nanowires and nanomaterials have been dragged wide attentions with both experimental and numerical study recently. In particular, the mechanical properties as well as structure of metallic nanowire have undergone considerable investigation. These nanowires are attracting due to the increase in diverse areas including nanocomposites strengtheners, the active components of NEMS [1], force and pressure sensing [2], ultra-high resolution mass sensing [3], and other devices [4].

According to literature review in situ bending experiments, carried out in nano-scale, are widely used in characterization of mechanical NWs [5]. Based on bending testing, researchers have investigated and tested different kinds of NWs. A number of molecular dynamics study also have been dedicated to studying the bending behaviors of NWs. These

studies mainly focus on the dynamic deformation rather than the mechanical properties [6]. It is noted that, a complete description of the bending deformation of NWs, including the elastic and plastic deformation as well as failure, is still lacking [7].

Recently, a method has been developed which utilizes an AFM in contact mode to apply a bending force to a single nanowire or nanotube in a single or double-clamped configuration [8]. The force–deflection response obtained from the AFM experiments is then analyzed with continuum elastic bending theory to extract the elastic modulus of the nanowires [9]. Specific results obtained by Wu et al [8] for silver and gold nanowires show that young's modulus is comparable to the bulk modulus and that it is essentially independent of nanowire diameter, while in other AFM bending investigations, young's modulus of silver nanowires was found to increase with decreasing diameter [10].

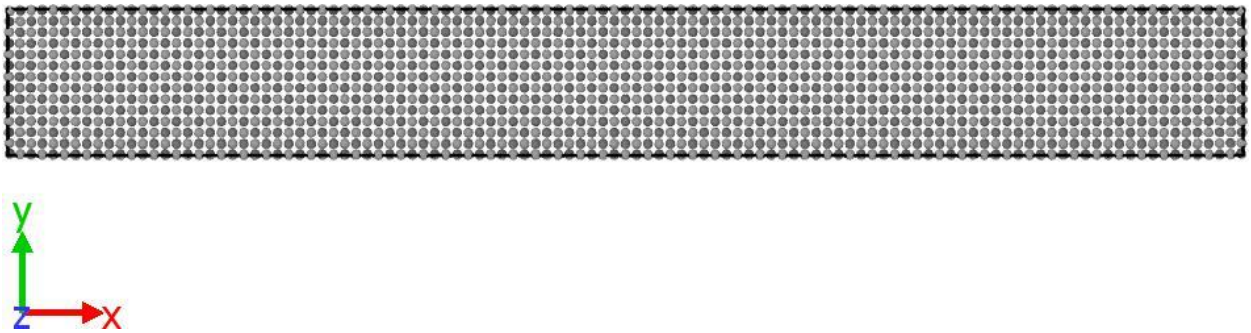
Therefore, in this paper, a comprehensive study of the mechanical properties of copper NW under bending will be conducted on pristine NW. Beginning of this paper will consist of brief explanation of theoretical and modeling basic. After that different beam theories will be introduced and the selection of the best theory, with or without modification, will be discussed. Following this an extensive parametric study for the pristine copper NW will be presented to validate the bending model and derive the optimized settings.

Theoretical and Modeling Basic

According to AFM bending method, the fig:1 is a representation of a three-point bending model for a doubly clamped NW. Previous works have been seen to utilize forces or displacement directly. To mimic the real AFM bending situation, we have used a virtual nano-indenter to apply the load. For all simulations, the nanowires were created with atoms in positions corresponding to a bulk FCC crystal lattice. Periodic boundary conditions were not imposed in any direction. Cu NW of a square cross-section, and the initial atomic configuration positioned at the perfect FCC lattice site, i.e., the x, y and z coordinate axes represent the lattice direction of [100], [010], [001] respectively is employed in this work. During the simulation, the tip is set rigid.

The NW is divided into two regions, mobile and boundary region. Atoms at both end of the boundary regions were constrained with a zero-force boundary condition, these atoms remained fixed in their positions during the entire incremental loading process. The temperature was maintained at 0.01k.

Before application of bending deformation, the NW underwent energy minimization using the conjugate gradient method; this energy minimization causes atoms near free surfaces to contract. MD simulations in this work were performed using the EAM potential [11] [12]. In this model of atomic interaction, the total energy U of a system of N atoms is a summation over two terms, a classical pair interaction and a many-body, embedding energy term. This scheme has been utilized extensively in NW simulations because of its accuracy in capturing electron density variation at free surfaces.



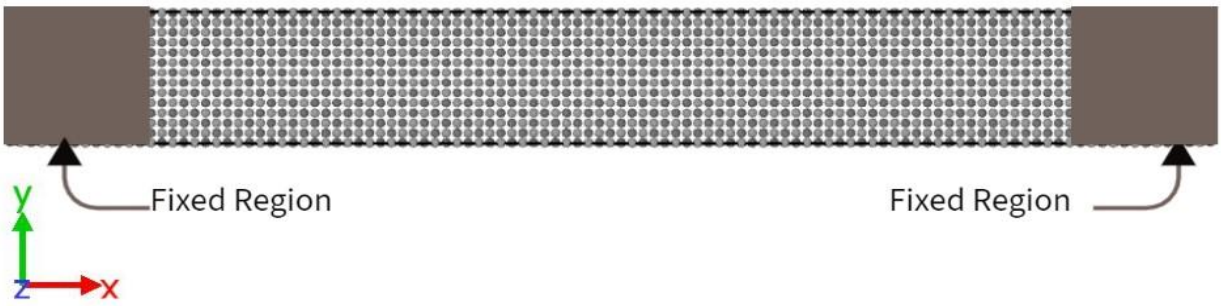


Fig. 1: Three Point Bending Model of Cu NW for MD simulation

Following these the loading process started and generated force-deflection curve is used to evaluate different mechanical parameters. All the simulations were done using Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) [13].

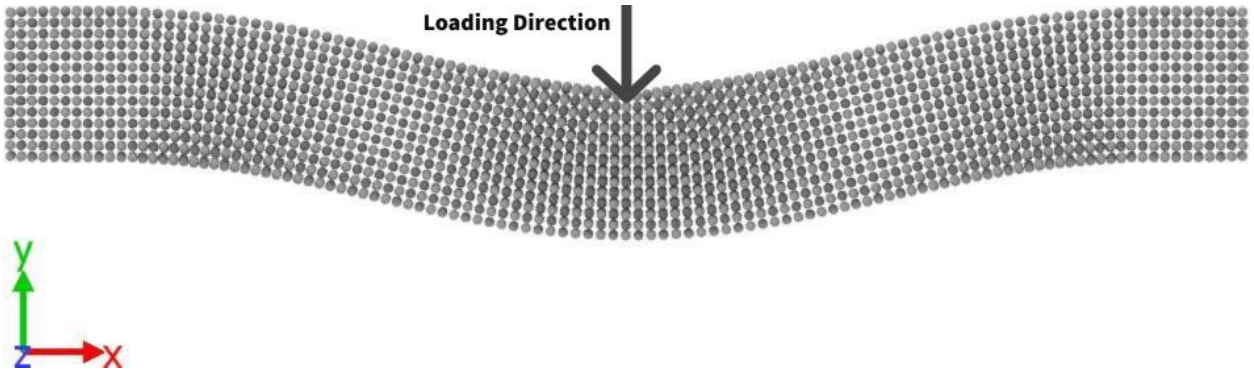


Fig. 2: Beam Bending under Uniaxial Central Load

Different Beam Theories

A beam deforms and stresses develop inside it when a transverse load is applied to it. In the quasi-static case, the amount of bending deflection and the stresses that develop are assumed not to change over time. In a horizontal beam supported at both ends and loaded downwards in the middle, the material at the over-side of the beam is compressed while the material on the underside is stretched. The effective young's modulus of the nanowires from the bending simulations can be calculated by using a method derived from continuum beam theory. For small deflections caused by a concentrated load, the strain energy δU in a beam is given by,

$$\delta U = \int_0^L \frac{EI}{2} \left(\frac{d^2 v}{dx^2}\right)^2 dx \tag{1}$$

where L is the length, E is young's modulus, I is the moment of inertia, ν is the beam deflection and x is the coordinate along the axial direction [13]. only the effects of the bending moment on the strain energy are considered; since, if a beam is sufficiently long (L/t >8, where t is thickness), then the energy due to shear deformation may be neglected [14].

From continuum theory, the deflection ν of a doubly clamped beam with a concentrated load P at the middle is given by,

$$v = -\frac{Fx}{12EI}\left(\frac{3L^2}{4} - x^2\right) = -\frac{48\delta x}{12L^3}\left(\frac{3L^2}{4} - x^2\right) \tag{2}$$

where δ is the maximum deflection at the free end of the beam. The second derivative, which is known as the curvature, of equation:2, is,

$$\frac{d^2v}{dx^2} = \frac{24\delta}{L^3}(1 - 4\frac{x}{L}) \tag{3}$$

Young's modulus E for each nanowire is calculated at each bending increment by first inserting the calculated curvature into the strain energy expression (1), then integrating with respect to x, and finally solving for young's modulus E. This method allows for the calculation of young's modulus by utilizing only strain energy, deflection, and geometric parameters; forces or stresses are not expressly used in calculating young's modulus. The moment of inertia (I) is calculated using continuum equations. It is important to note that at the atomistic level, the moment of inertia is sensitive to the specification of the cross-sectional area. We calculate the area as a continuous entity with bounding dimensions defined as the distance between the appropriate atomic positions. While this calculation certainly influences the magnitude of the calculated modulus, the observed trends are not affected. For rectangular cross sections,

$$I = \frac{bh^3}{12} \tag{4}$$

where h and b are the height and width of the relaxed cross-section, respectively. An energy-based continuum-mechanical method for calculating young's modulus for nanowires in tension was presented in a study by Diao et al [15]. At each tensile loading increment, the axial stress in the interior of the nanowire is balanced by the externally applied quasi-static force at the end of the nanowire. Thus, the change in potential energy in the nanowire during loading is equal to the work done by the externally applied load,

$$\delta U = \int_0^{\Delta L} Fd(\Delta L) = \int_0^{\epsilon} V\sigma d\epsilon \tag{5}$$

Euler–Bernoulli beam theory (also known as engineer's beam theory or classical beam theory) [1] is a simplification of the linear theory of elasticity which provides a means of calculating the load-carrying and deflection characteristics of beams. It covers the case for small deflections of a beam that are subjected to lateral loads only. It is thus a special case of Timoshenko [16] beam theory. For the classical Euler-Bernoulli beam theory, the governing equation of the doubly clamped thin beam under pure bending is given as [17],

$$(EI)w^4 = 0 \tag{6}$$

where E is bulk young's modulus, w is the beam deflection, I is the moment of inertia. Solve Eq. 6 using the usual clamped boundary conditions at both ends, with a constant load F applied at the midpoint x=L/2 of the NW, i.e., the transverse displacement and slope are zeros at x=0, and the slope at x=L/2 is also zero because of symmetry. The force equilibria at x=0 is

$$-(EI)w^3 = \frac{F}{2}$$

The relationship between the applied load F and the resulting displacement d can be deduced as,

$$F = \frac{192(EI)}{L^3}d \tag{7}$$

The yield strength σ_y is then estimated from the yield force Fy in the F-d curve before the onset of plastic deformation according to [18]

$$\sigma_y = \frac{3F_yL}{4h^3} \tag{8}$$

According to the experimental (Heidelberg, et al., 2006) and MD results, the axial extension exerts considerable influence on the beam behaviors. So, by taking into account the axial extension effect we obtain the following solution,

$$F = \frac{192(EI)}{L^3}f(k)d \tag{9}$$

$$f(k) = \frac{k}{48 - 192tanh(\sqrt{k}/4)/\sqrt{k}} \tag{10}$$

where k is directly connected to the axial tension. Similarly, we refer to k as an axial extension effect factor. The axial extension effect factor is related to the maximum displacement d by the following transcendental equation,

$$\frac{kcosh^2(\sqrt{k}/4)}{2+cosh(\sqrt{k}/2)-6sinh(\sqrt{k}/2)/\sqrt{k}}(1-4\frac{tanh(\sqrt{k}/4)}{\sqrt{k}})=d^2\frac{EA}{EI} \tag{11}$$

Obviously, Eq. 11 is complex in nature and a numerical solution is required. Thus, the following asymptotic solution is constructed,

$$k=\frac{6s(140+s)}{350+3s} \tag{12}$$

$$s=d^2\frac{A}{I} \tag{13}$$

Parametric Study

Mechanical behavior or properties of Cu NWs using the above model as well as the parametric studies are presented in this section. Different factors such as indenter size, loading rate, and depth variation, were studied. Here, in this section, the inclusion of comparison between obtained results using both Euler-Bernoulli beam theory and modified Euler-Bernoulli beam theory has been discussed.

It is to be noted that for all the simulations the initial distance between the virtual indenter, which actually works as a tip, was set to be 0.1 nm. The indenter was of a cylindrical type with a radius of 0.8 nm circling around the z-axis. The indenter repels all atoms in the group that touch it, so it was used to push into a material. The indenter exerts a force of magnitude

$$F(r)=-K(r-R)^2 \tag{14}$$

Here, r is the distance from the atom to the center axis of the cylinder, R is the radius of the indenter and K is the specified force constant. For this simulation process, we take K = 10 Nm^2. For validation, MD results are first compared with some experimental measurements previously done by other researchers and also with the result of the tensile tests. This Fig:3 represents the F-d curve of a Cu NW during the loading process. A similar kind of curve has been obtained from previous experimental work on Au NW by Wu et al [9]. Such consistency suggests that the MD model could provide valid information about the bending deformation properties of NWs. Further investigations of our work are discussed below

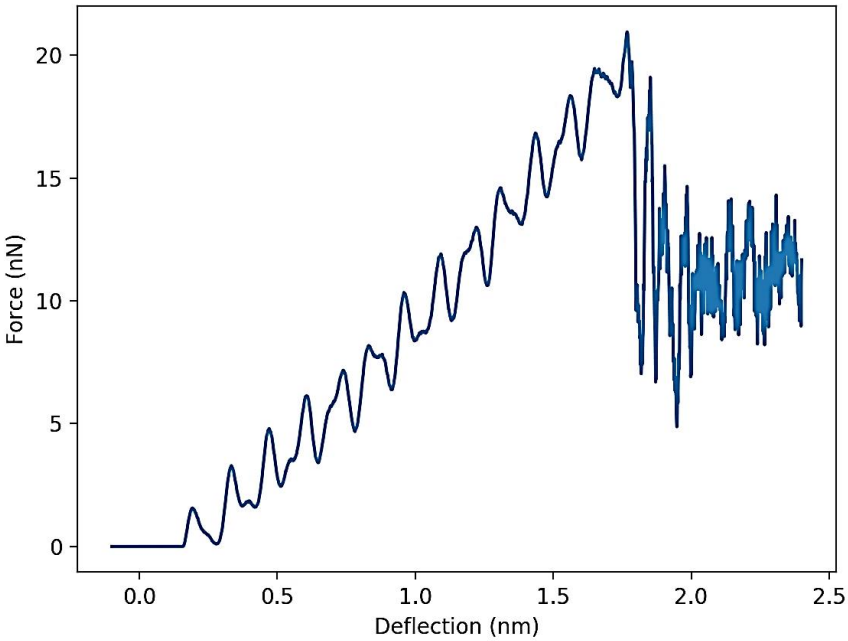
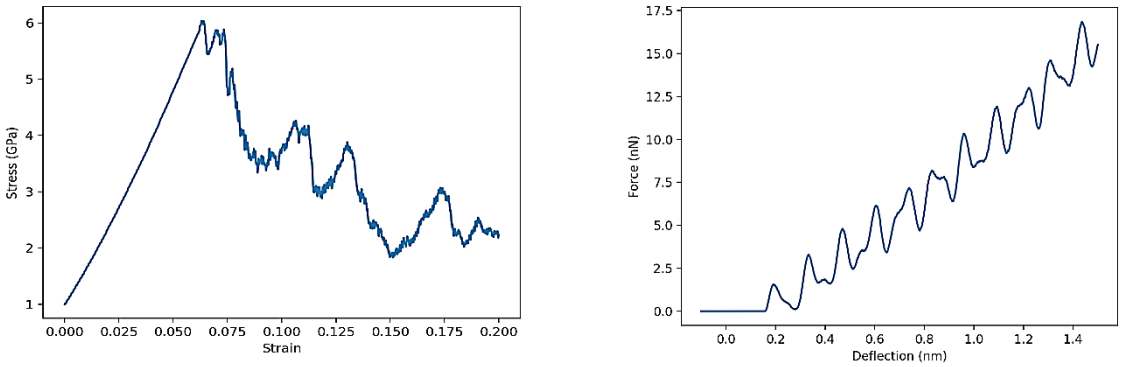


Fig. 3: Bending result of a Cu NW (20 nm X 2.5 nm X 2.5 nm) under 1m/s loading rate at 0.01k temperature

Validation with the Tensile Test Result

As it has been previously studied, the young's modulus due to the bending test is far greater than for the tensile test (diao et al). But with the evolving improvement of analysis methods and for an obvious reason, they should be similar or nearly similar to each other. An extensive study on this purpose has been done recently by zhan et al [20]. According to his study, for both cases, bending and tensile testing, young's modulus should be near to each other. For this purpose, we have chosen Cu NW with a size of 20X2.5X2.5 nm3. At first, we run the tensile test simulation on the model at a constant temperature of 0.01k and strain rate of 109. The stress-strain curve can be seen in Fig:4 (a). After that, we run a bending simulation on the same model at a force rate of 1m/s, whose force-deflection curve is depicted on Fig:4(b).



(a) **(b)**

Fig. 4: (a) Tensile result of a Cu NW (20 nm X 2.5 nm X 2.5 nm) at 0.01k temperature (b) Bending result of a Cu NW (20 nm X 2.5 nm X 2.5 nm) at 0.01k temperature

By analyzing the generated Force-Deflection curve, we obtain young's modulus for both cases as:

Young's Modulus		
Tensile Test	Euler bending Equation	Modified Euler bending equation
80.76 GPa	78.033 GPa	60.2318 GPa

Table 1: Different values of young's modulus from different analyses and comparisons among them

Such findings for NW under bending deformation are well matched with the findings of Zhan et. al [19]. We will, therefore, proceed with the process further.

Indenter Size Effect

In this process of simulation, an indenter, virtual, is employed to do the work of loading at the center of the model beam. This indenter is taken in the shape of a cylinder so that a uniform plane load over a portion of the beam can be induced. For all the simulations in this procedure, we have selected the tip radius to be 0.8 nm. This selection has done by simulating with three different tip sizes, accordingly 0.8 nm, 1 nm, and 1.2 nm, and then by analyzing their results.

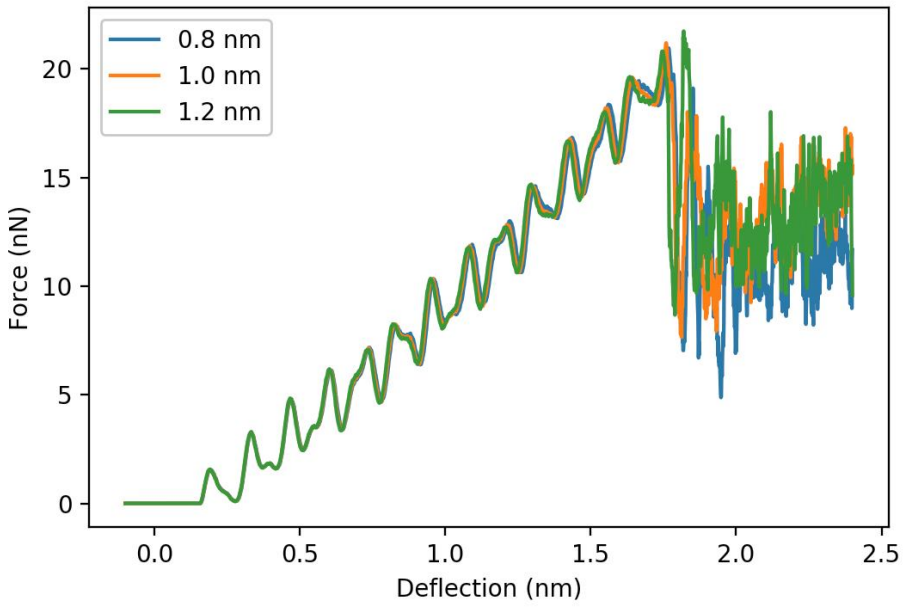


Fig. 5: F-d curve for different indenter size

Basically, it is found that from Fig:5, the F-d curves of different tip sizes almost overlap with each other, indicating the tip size exerts a minor difference in the mechanical response of the NW.

Loading Rate Effect

Due to the size of the NWs, the loading rate could exert a great influence on their performance of them. Therefore, it is crucial to examine possible loading rate effects as well as reasonable loading rate for bending. And the selection of a loading rate may save our computation time and resources yet give us fairly good results. For this task, several different loading rates including 5 m/s, 8 m/s, 10 m/s, and 100 m/s are employed.

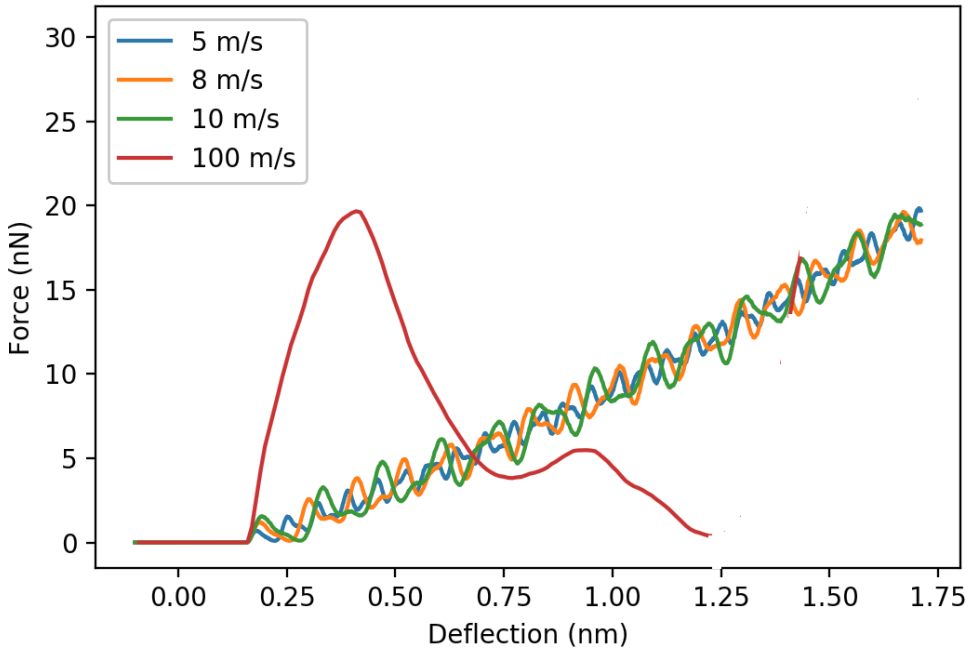


Fig. 6: F-d curve for different loading rate

Referring to the Fig:6, F-d curves under different loading rates can be seen. It can be viewed that up to a loading rate of 10 m/s the curves were obtained almost similar. The increase in loading rate may increase fluctuations in the curve more. But they are almost similar until 10 m/s. It is evident from Fig. 7 that a higher loading rate is always associated with a larger force. Such observation is consistent with the findings for NWs under tensile deformation, i.e., a higher loading rate induces larger yielding strength.

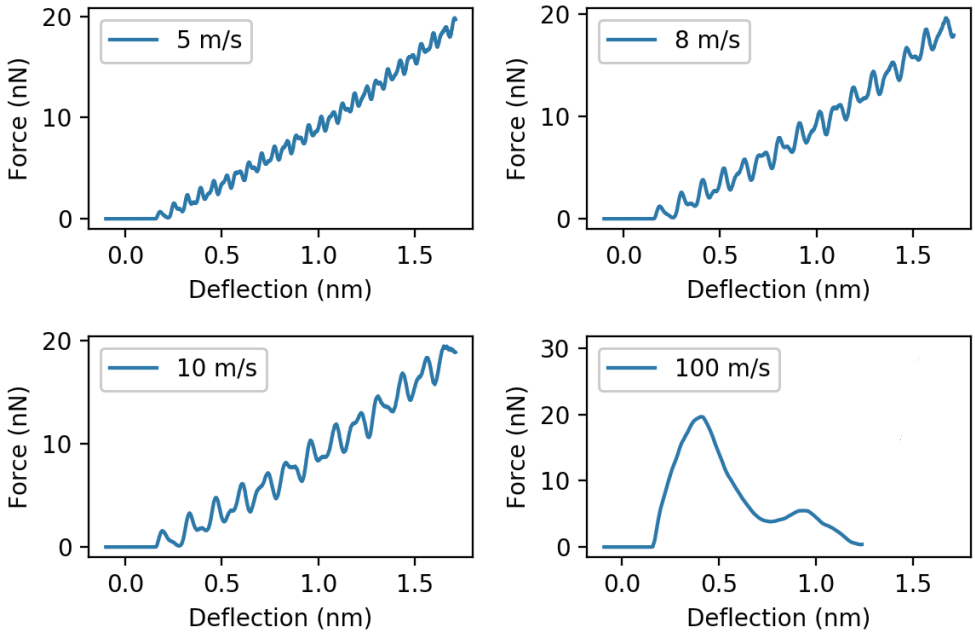


Fig. 7: F-d curve for different loading rate subplots

According to the experimental results by Wu et al [9], the asymmetry F-d curve during the whole loading circle is actually indicating the emergence of plastic deformation during loading. The high loading rate, 100m/s, behaves like an impact load, leading to severe plastic deformation. So, it can be concluded that when the loading rate is fairly slow, the loading rate effect would be negligible, and to perform a homogenous bending deformation, a reasonable loading rate should be below 10 m/s.

Therefore, for saving the computation time and resources, we choose 10m/s as our loading rate for the existing simulations.

Depth Variation Effect

The high surface-to-volume ratio of NWs makes it possible to see a variety of events. Every mechanical characteristic of a NW is heavily influenced by the free surface effect. Therefore, it is anticipated that the varying depth variations in the direction of loading will have some influence on the mechanical property of the bending test. We take a model with a length of 20 nm and a width of 2.5 nm fixed. And then run the simulation for various depths including 1 nm, 1.5 nm, 2 nm, and 2.5 nm. From Fig: 8 it can be seen that the slope for the Cu NW F-d curve is increasing with the increment of depth.

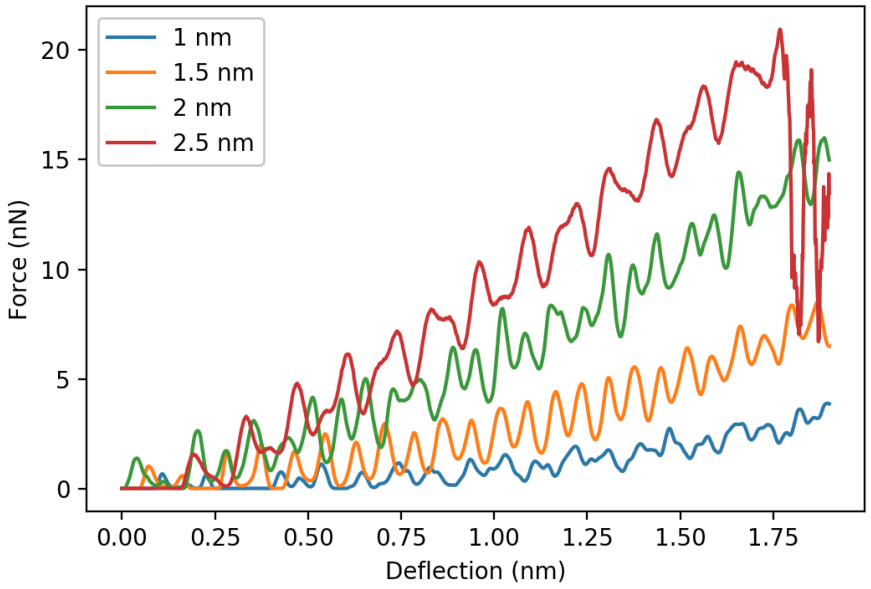


Fig. 10: F-d curve for different depth variation

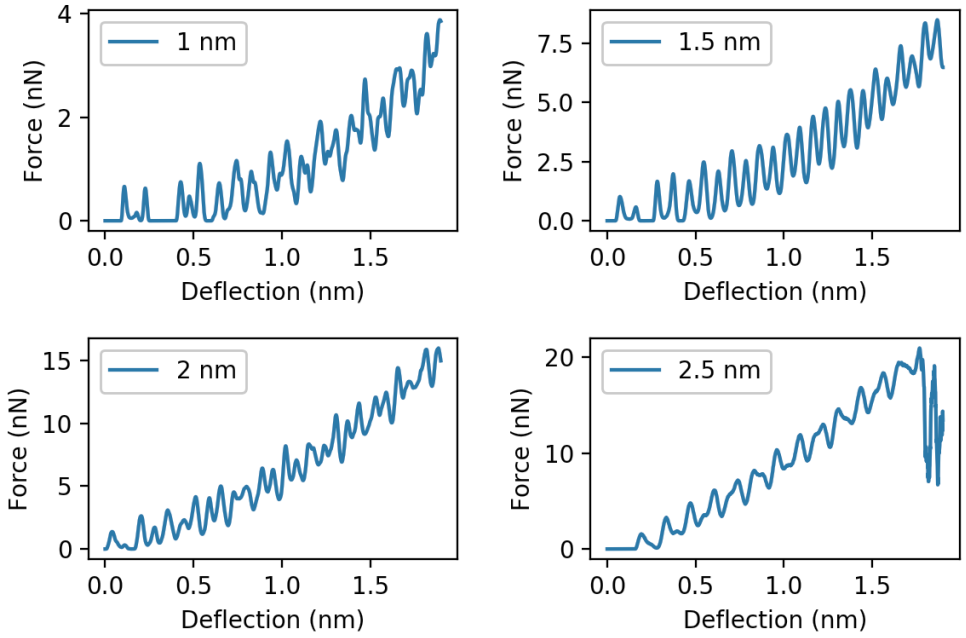


Fig. 10: Subplots of F-d curve for different depth variation

Taking these curves together and doing two different analyses, results can be seen in Fig. 11 and Fig. 12 respectively.

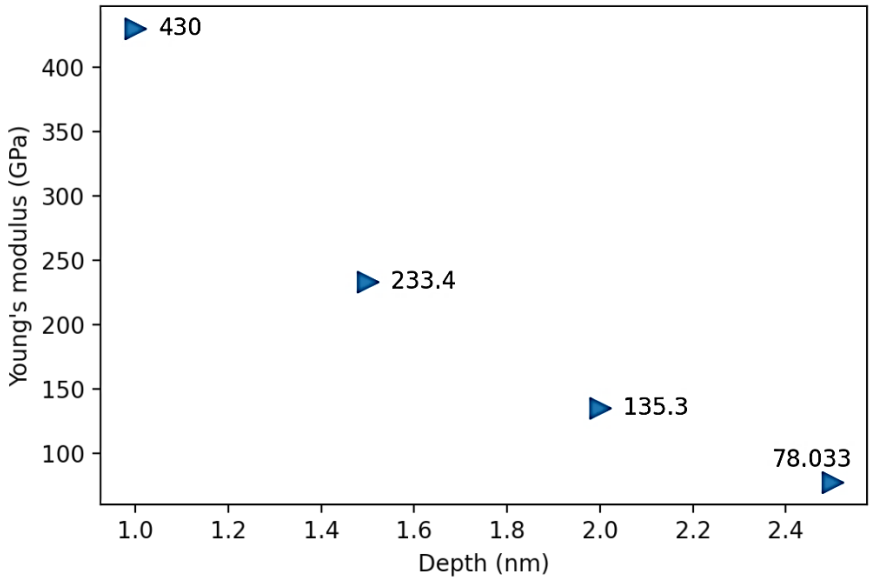


Fig. 11: Variation of young's modulus for different depth using Euler's equation

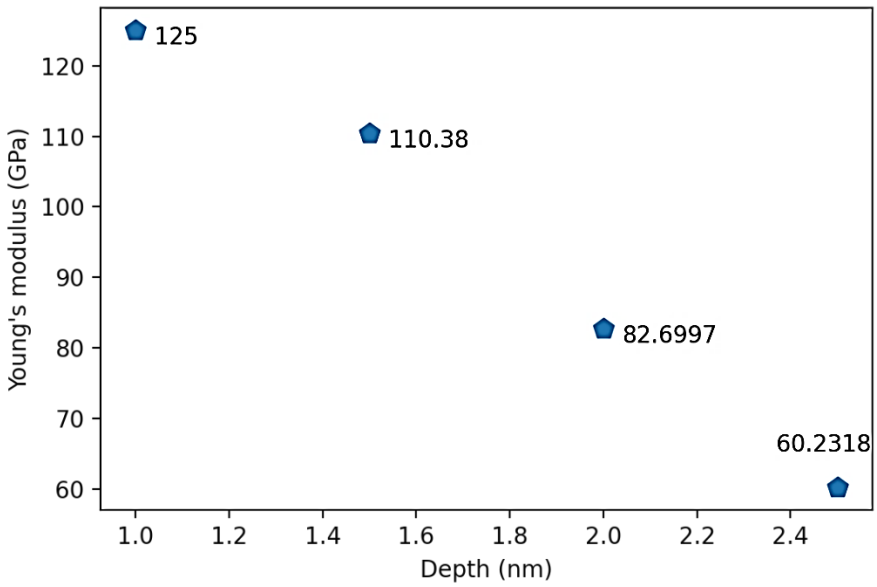


Fig. 12: Variation of young's modulus for different depth using Modified Euler's equation

These calculations for the young's modulus indicate that the young's modulus of elasticity falls as depth increases. The free surface effect is to blame for this. The material becomes more elastic as the depth drops due to the increasing effectiveness of the free surface.

Mechanical Properties

Mechanical property such as young's modulus due to different analysis is shown in this subsection. We have taken two different analysis processes, one is by using the Euler-Bernoulli equation,

$$F = \frac{192(EI)}{L^3} d$$

and another one is Heidelberg modification on Euler equation due to axial effect,

$$F = \frac{192(EI)}{L^3} f(k) d$$

$$f(k) = \frac{k}{48 - 192 tanh(\sqrt{k}/4)/\sqrt{k}}$$

$$k = \frac{6s(140 + s)}{350 + 3s}$$

$$s = d^2 \frac{A}{I}$$

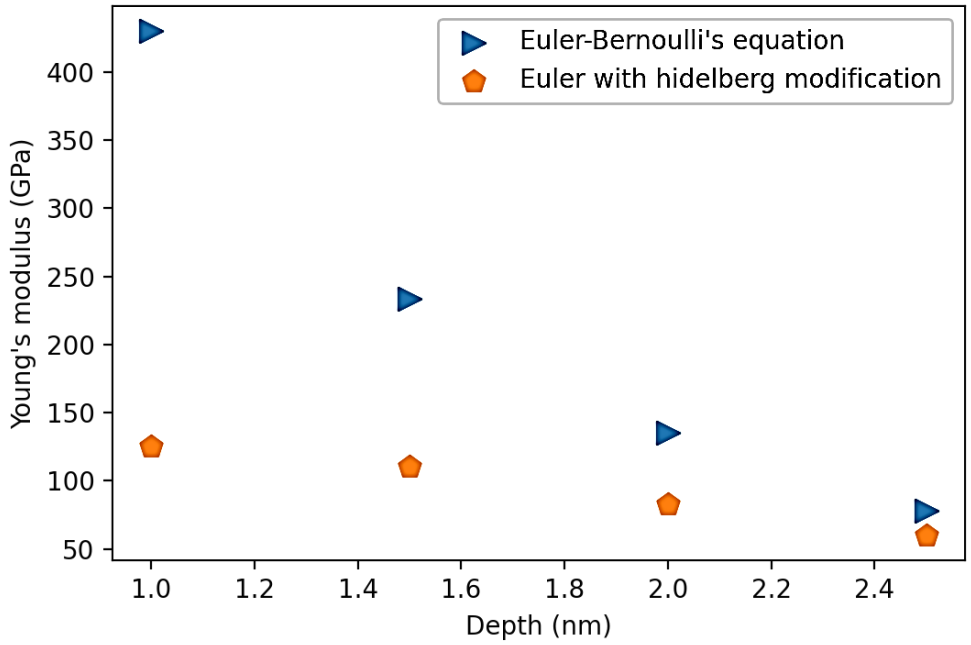


Fig. 13: Comparisional analysis of young's modulus variation due to different depth using Euler and Modified Euler equation

According to Fig. 13, the modified Euler-Bernoulli equation provides the finest analytical solution to date. Given that it accounts for the axial impact, it is evident. As it would be assumed, the axial effect cannot entirely be overcome by the model because of its nanoscale. If this is not taken into account, it could sometimes produce some unexpected effects. The values of the young's modulus, which can only be calculated via the Euler equation, can be used to detect this occurrence. It provides solid foundational assumptions for a surface effect-lighter model. So, it is safe to say that the analysis works better using a modified Euler equation.

Conclusion

Based on the AFM-bending experiments, a three-point bending model is developed that can precisely account for the complete range of mechanical characteristics of Cu NWs in a doubly clamped beam configuration, from elasticity to plasticity and failure. Major conclusions are summarized as below:

- The mechanical properties of Cu NWs are significantly influenced by the loading rate. As an impact load, a high loading rate might be effective. It is determined that a suitable loading rate for a homogenous bending deformation is less than 10 m/s.
- The F-d curve from MD simulation is highly consistent in shape with those obtained from experiments done previously by other researchers.
- When an axial effect is taken into account, MD results are exceptionally in line with the classical Euler-Bernoulli beam theory.
- The mechanical property of a beam under bending changes significantly due to the depth variation. It is the most prominent cause of surface effect i.e, greater surface-to-volume ratio.
- The mechanical characteristics obtained under bending and tensile deformations are equivalent. In particular, the modulus for these two loading techniques is approximately the same.

Author Contributions: Mohammad Din Al Amin: Conceptualization, Problem Design, Data curation, Formal analysis, Investigation, Methodology, Software, Visualization, Writing – original draft. Mohammad Minhaz Uddin: Writing – review & editing. Md Alamgir Hossain**:** Supervision, Administrative support, Writing – review & editing.

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