Materials Research Express

PAPER

Insights into the mechanical properties and fracture mechanism of Cadmium Telluride nanowire

Md Adnathir Munshi¹, Sourajit Majumder¹, Mohammad Motalab¹, and Sourav Saha¹,²
¹ Department of Mechanical Engineering, Bangladesh University of Engineering and Technology, Dhaka-1000, Bangladesh
² Theoretical and Applied Mechanics, Northwestern University, Evanston, Illinois, United States of America
E-mail: abdulmotalab@me.buet.ac.bd

Keywords: CdTe nanowire, zinc blende structure, fracture behavior, molecular dynamics simulations

Abstract
Semiconducting nanowires (NWs), key building blocks in nanotechnology with many potential applications, are stirring the attention of the scientific world because of their many unique properties. Cadmium telluride (CdTe) single crystal nanowires, with Zinc Blende (ZB) crystal configuration, have become the focus of interest nowadays due to its promising application in Opto-electro-mechanical nanodevices. However, due to the lack of complete insight into their mechanical deformation, it is necessary to thoroughly study the CdTe nanowires. In this study, molecular dynamics simulations have been used to investigate the mechanical behavior of CdTe nanowires (NWs) by varying size, temperature, crystal orientation, and strain rate under tension and compression. Results show that the fracture strength of the [1 1 1]-oriented CdTe NWs is always higher than that of the [1 1 0]-oriented CdTe NWs under tension whereas, in compression, the fracture strength of the [1 1 1]-oriented CdTe NWs is significantly lower than that of the [1 1 0]-oriented CdTe NWs. Moreover, upon applying the tensile load along NWs growth direction, the [1 1 1]-oriented CdTe NWs fail by creating void in [1 0 −1] direction due to bond breaking in [1 1 −2] direction regardless of temperature and NW size. Under compression, the [1 1 1]-oriented nanowires show buckling and plasticity. It has also been observed that size has a negligible effect on the tensile behavior but in compression, the behavior is size-dependent. Both tensile and compressive strengths show an inverse relation with temperature. Finally, the impact of strain rate on [1 1 1]-oriented CdTe NWs are also studied where higher fracture strengths and strains at higher strain rates have been found under both tension and compression. With increasing the strain rate, the number of voids is also increased in the NWs. This study will help to design CdTe NWs based devices efficiently by presenting an in-depth understanding of the failure behavior of the [1 1 1]-oriented CdTe NWs.

1. Introduction

Semiconductor nanowires (NWs) are one of the most basic elements of future electro-mechanical nano-devices and they work as building blocks for developing micro- (MEMS) and nano-electromechanical systems (NEMS). While nanowires (NWs) are suitable for studying the fundamental deformation mechanisms of semiconductor materials. Again, the directed growth of semiconductor nanowires has an important effect on its different properties and has attracted scientific interest in recent years as an important promoter of nanotechnology [1–4]. Moreover, the nanostructure materials are more suitable to carry the tensile and compressive load due to its enhanced mechanical properties than the traditional bulk counterpart [5–7].

To design and fabricate NW-based photo-mechanical devices it is important to describe and predict the mechanical behavior of different NWs. Mechanical properties of semiconducting NWs were studied by tensile tests [5, 8, 9], compression tests [10, 11] and bending test [12–14] in many in situ studies. Recently, molecular dynamics (MD) simulations are widely used to investigate not only the mechanical behavior but also fracture mechanisms of various NWs along with experimental and in situ studies [15–17]. Temperature, diameter, and
strain rate-dependent mechanical behavior under tension for Si NWs were investigated successfully by Kang and Cai using molecular dynamics [18]. Remarkable phenomena like shear failure and cleavage failure of Si NWs were explained in that investigation. Tsuzuki et al [19] showed the failure mechanism of SiC NWs under both tensile and compressive loading. Here, it was found that ZB SiC NWs display complex plasticity before failure while wurtzite SiC NWs are brittle in nature. Furthermore, Cheng et al [20] had reported the fracture strength due to the size dependency of SiC NWs. It was found by Pial et al that the direction of cleavage planes of ZB InP NWs change with temperature under tension while investigating the mechanical behavior of InP NWs [21]. The mechanical behavior of many other semiconductor NWs, such as Ge [22], GaN [23] and ZnO [24] was also investigated successfully with MD simulations. Recently, CdTe nanowires attracted the attention of the scientific world due to its use in high-performance photodetectors, field-effect transistors and solar cells [25, 26].

CdTe is a promising semiconductor material for electronic and optical devices [27–30]. As a group II–VI semiconductor material, CdTe has a direct bandgap of 1.5 eV and a high absorption coefficient at room temperature [31], which makes it a perfect and ideal material candidate for high-efficiency solar cells [32]. Moreover, the recent rapid growing scientific and technological interest on CdTe not only arises from its special physical properties, i.e. its mechanical, chemical and thermal stability but also for its potential in solar energy conversion devices, sensors and photonics [33], high-efficiency photovoltaic devices, [34, 35] and light-emitting diodes [36]. Previous studies of CdTe had revealed that the stable and natural phase for CdTe is the zinc-blende structure [37] and [111] is its growth direction [25]. Direct use of single-crystalline CdTe NWs makes it important to investigate its mechanical properties and fracture mechanism [25].

Previously, the melting temperature, the lowest energy, the crystalline growth, and reasonable elastic properties for zinc-blende CdTe were reported [38, 39]. However, there is hardly any research on the mechanical properties of CdTe NWs by simulations. Although the applicability of CdTe NWs requires in-depth knowledge of their mechanical properties and failure behavior, the number of experimental investigations is inadequate. Moreover, the failure behavior of CdTe NWs has yet to be discussed. Keeping this scope in mind, for the first time, this paper presents atomistic simulation results of single-crystalline CdTe NWs under uniaxial tensile and compressive load. The effects of crystal orientation, temperature, size, and strain rate on the mechanical properties of CdTe NWs are also investigated. Moreover, failure mechanisms under different conditions are elucidated to explain the failure behavior of the CdTe NWs.

2. Methodology

The uniaxial tension and compression simulations are performed for CdTe nanowire and only compression simulations are performed on nanopillar to check how ZB CdTe behaves under compression. Here, MD simulations for characterizing the mechanical behavior of CdTe nanowire is carried out using LAMMPS [40] software package and OVITO [41] is used for visualization of atomistic deformation processes. The choice of interatomic potential has a significant impact on molecular simulations. In this work, SW (Stillinger-Weber) [42] potential is used to describe the interaction between Cd and Te. This potential is incorporated because of its successful use in reproducing the melting temperature, the lowest energy, the crystalline growth, and reasonable elastic properties for zinc-blende CdTe previously [38, 39]. The SW potential consists of a two-body term and a three-body term describing the bond stretching and bond breaking interactions respectively. The mathematical expressions of these interactions are described below.

$$\Phi = \sum_{i<j} V_2 + \sum_{i<j<k} V_3$$ (1)

$$V_2 = \varepsilon A (B \sigma_{ij}^p - \sigma_{ij}^q) \exp\left(\frac{-\varepsilon A}{B - \sigma_{ij}^q}\right)$$ (2)

$$V_3 = \varepsilon \lambda \exp\left(\frac{\varepsilon A}{B - \sigma_{ij}^q + \cfrac{\varepsilon A}{B - \sigma_{jk}^q}}\right) (\cos \theta_{jk} - \cos \theta_j)^2.$$ (3)

Here, two-body and three-body terms are denoted by $V_2$ and $V_3$ respectively; $r_{ij}$ denotes the distance between atoms $i$ and $j$; $\theta_{ik}$ denotes the angle between bond $ij$ and $jk$; equilibrium angle between two bonds is denoted by $\theta_j$; $A$, $B$, and other parameters are the coefficients required to fit while developing the potential. The values of these parameters can be found in reference [42].

The aspect ratio of the nanowire height to width is kept constant as 10:1 for nanowire and 2:1 for nanopillar. Tension and compression are applied in crystal orientation of [001], [110], and [111]. CdTe has a zinc blende (ZB) structure having a lattice constant of 6.48 Å [43]. The NWs models are prepared by first creating a rectangular box of ZB CdTe with the lattice constant $a = 6.48$ Å and later nanowires of specified diameter is cut from it with the help of Atomsk tool [44]. The [111]-oriented ZB CdTe NWs are modeled with the x, y, and z axes oriented along the [1-11], [10-1], and [111] directions, respectively. A few [001] and [110]-oriented CdTe NWs and nanopillar models are also developed to test the crystal orientation effect. The periodic boundary condition is maintained along the axis of the nanowire while the other two directions are kept free. However, to simulate
the nanopillar free boundary conditions are used in all three directions. The prepared [111]-oriented ZB CdTe nanowire model is shown in figure 1. Here, D and L stand for the diameter and length of the nanowire, respectively.

To evaluate the effects of temperature, the temperature range used is from 100 K to 600 K. Meanwhile, tensile and compressive strains are applied to the 5 nm NW at 300 K to investigate the effects of strain rates. Seven strain rates are used, which are $10^8$, $5 \times 10^8$, $10^9$, $5 \times 10^9$, $10^{10}$, $5 \times 10^{10}$, and $10^{11}$ s$^{-1}$. Again, the type of structure, diameter, length of the nanowires, and the total number of atoms calculated in each model are summarized in table 1.

Before applying the tensile and compressive load, the system energy is minimized using a conjugate-gradient algorithm. A constant integration time step of 1 fs is considered which is quite good for all the simulations. Before applying the tensile and compressive load, constant NVE is performed for 10 ps. Then isothermal-isobaric (NPT) ensemble is applied for pressure equilibration at atmospheric pressure and prescribed temperature for 50 ps. Finally, the system is thermally equilibrated by the canonical (NVT) ensemble for 50 ps. To control the temperature, a Nose-Hoover thermostat is employed in these steps. To equilibrate various state variables, the timesteps mentioned are chosen by trial and error for NVE, NPT and NVT simulation. Finally, the nanowire and nanopillar are deformed along their axis at a fixed strain rate of $10^9$ s$^{-1}$. This strain rate was successfully applied to predict the result in many tension and compression based MD simulations [45–47]. Both tensile and compressive tests are conducted under the NVT ensemble using a Nose-Hoover thermostat and carried out until the failure. The simulation box is deformed uniaxially to calculate the atomic stress for obtaining stress-strain behavior. In our simulations, the atomic stresses are calculated using Virial stress theorem [38]. The equation of stress stands as

$$\sigma_{\text{virial}} = \frac{1}{\Omega} \sum_i \left( -m_i \ddot{u}_i \otimes \ddot{u}_i + \frac{1}{2} \sum_{j \neq i} f_{ij} \otimes f_{ij} \right)$$

where the summation is done over all the atoms occupying the total volume, the mass of the atom is represented by $m_i$ and displacement by $\ddot{u}_i$. The relative position vector of the atom is $r_{ij}$, the cross product is $\otimes$ and the interatomic force applied on atom $i$ by atom $j$ is $f_{ij}$.

### 3. Method validation

To validate the SW (Stillinger-Weber) potential employed in this study, Young’s modulus of [111]-oriented nanowires, lattice constants, and the cohesive energy of bulk CdTe are calculated. For Young’s modulus, nanowire having a diameter of 6 nm at 100 K is considered while for lattice constant and cohesive energy a cube

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**Table 1. CdTe nanowires and Nanopillar geometric specifications.**

| Structure type | Diameter, D(nm) | Length, L(nm) | Number of atoms |
|---------------|---------------|-------------|----------------|
| Nanowire      | 2             | 20.2        | 1872           |
|               | 3             | 29.5        | 6760           |
|               | 4             | 39.8        | 14770          |
|               | 5             | 49.4        | 28512          |
|               | 6             | 60.6        | 50976          |
| Nanopillar    | 10            | 20          | 46260          |
of 2.592 nm × 2.592 nm × 2.592 nm of bulk CdTe is used. In this study, Young’s modulus is calculated from the stress-strain graphs using linear regression.

Data obtained from the present study and data from the available literature are presented in Table 2 for comparison. It is found that the calculated lattice constants, cohesive energy, and Young’s modulus agree well with other numerical and experimental studies.

Moreover, to ensure that the results of CdTe NW under SW potential which was fitted for the simulations of liquid CdTe previously discussed here are not potential specific, additional simulation on CdTe is also performed using analytical bond order potential (BOP) [54] under the same conditions. A [111]-oriented 4 nm NW at 300K is considered for fracture strain and failure mechanism. Whereas, for lattice constant and cohesive energy a cube of 2.592 nm × 2.592 nm × 2.592 nm of bulk CdTe is considered. Data obtained from the SW and BOP are presented in Table 3 for comparison.

The proximity of the values obtained by both the potential verifies the present method and adopted potential to describe the interactions in CdTe nanowire. While previously it was reported that similar structures and formation mechanisms predicted by the SW potential having defects in the structure are also observed in the BOP simulations [55]. So, it can be said that the results and the fundamental physics discussed in this study are not potential specific.

### 4. Results and discussion

#### 4.1. Effects of Temperature and Size

The stress-strain curve of [111]-oriented 4 nm CdTe NWs under uniaxial tension and compression at strain rate $10^9$ s$^{-1}$ is shown in Figure 2(a) for different temperatures. It is observed from Figure 2(a) that at 100 K, the ultimate strength is about 7.7 GPa with a failure strain of about 20.1% in case of tension while for compression the ultimate strength is about 3.01 GPa with a failure strain of about 7.1%. Sharp fall of stress in Figure 2(a) indicates brittle type failure of the material. It is also observed that as the temperature is increased from 100 K to 600 K, the fracture strength decreases from 7.7 GPa to 4.3 GPa in case of tension while for compression it decreases from 3.01 GPa to 1.6 GPa. This type of softening behavior at higher temperatures is also observed for nanowires of other sizes in this study.

Figure 2(b) shows the stress-strain curve for [1111]-oriented CdTe NWs with different diameters at 100 K temperature, exhibiting the size effect. The diameter of the nanowires, in this case, is varied from 2 nm to 6 nm. The length of the nanowires is varied from 20.2 nm to 60.6 nm respectively to maintain the constant length to width ratio of 10:1. Here, the applied strain is $10^9$ s$^{-1}$ and the temperature is 100 K. It is observed from the graph that all of the stress-strain curves for tension follow almost the same path until fracture under tension. However, for the length of nanowires used, the results show that in compression, the stress–strain curve largely depends on the diameter of the NWs. The larger the diameter, the larger the strength and elastic modulus have been observed. A similar kind of size-dependent behavior for SiC was also found in the literature [19]. In Figure 2, the ultimate strength in all cases shows a large asymmetry between tensile and compressive loadings. This high asymmetry is because, under tension, material failure occurs due to the void formation which eventually created due to bond breaking. Breaking of bonds results in higher ultimate strength in all cases. On the contrary, nanowire failure occurs due to buckling when subjected to compressive loading. When buckling type failure occurs in material, failure occurs under comparatively a lower load.

The variation of ultimate strength with temperature and size, in case of tension in Figure 3(a) and the case of compression in Figure 3(b) are elucidated. The figure shows that the ultimate strength decreases monotonically.

### Table 2. Comparison between values obtained by the present method and existing literature.

|                | Lattice constant (Å$^*$) | Cohesive energy | Young’s modulus (GPa) |
|----------------|--------------------------|------------------|-----------------------|
| Present calculation | 6.50                     | 2.061            | 49 (NW), 42 (Bulk)    |
| Computational studies | 6.486–6.573 [48–50] | 2.068 [41]        | 49.55 [51]            |
| Experimental studies | 6.486 [52]               | 2.060 [53]       | —                     |

### Table 3. Comparison between values obtained by SW and BOP.

| Potential | Lattice constant (Å$^*$) | Cohesive Energy | Fracture strain (%) | Failure mechanism            |
|-----------|--------------------------|------------------|---------------------|-----------------------------|
| SW        | 6.50                     | 2.061            | 17.2                | Void in [10-1] direction    |
| BOP       | 6.83                     | 2.17             | 18.91               | Void in [10-1] direction    |
with temperature. Moreover, the impact of size is more prominent in the case of compression than in case of tension. The possibility for bonds to reach the critical bond length condition increases with temperatures which lead to bond breaking. The fracture is initiated imminently when a bond breaks because CdTe is a brittle type material. On the contrary, the crystal structure of ZB CdTe remains perfect at a lower temperature subjected to little or no excitation due to temperature, therefore, resulting in high tensile stress.

Figure 3(c) shows Young’s modulus of [111]-oriented CdTe NWs as a function of NW diameter at different temperatures ranging from 100 K to 600 K. It is observed that Young’s modulus decreases with temperature but increases with size. Moreover, the dependency of Young’s Modulus on diameter is greater at a higher temperature than at a lower temperature. Lower fracture strength and Young’s Modulus of CdTe NWs at the higher temperature may be attributed to a reason that the length of the chemical bonds in the NWs fluctuates with the increase of temperature. Young’s Modulus increases with the decrease of temperature because of the decrement of space between atoms which results in higher interaction force among atoms. This makes the crystal stiffer. In other words, the structure behaves like a perfect crystal that leads to this behavior at low temperatures. Similar results reported previously for InP and Si nanowires [18, 21].

4.2. Effects of crystal orientation

Figure 4(a) shows the stress-strain curves of CdTe with 4 nm diameter and 300 K temperature with [111], [110] and [001] crystal orientations. Under tension, the fracture strength for the [111], [110], and [001]-oriented NWs are 5.85 GPa, 4.82 GPa, and 3.83 GPa, respectively. So, for 4 nm diameter and at 300 K temperature, it can be said that the fracture strength of the [111] orientation is the highest and for [001] orientation, it is the lowest. Under tension, a similar kind of orientation behavior was found for Si NWs [18]. However, in the case of compression, the fracture strength is highest for the [111] direction (2.47 GPa) and it is the lowest for the [001] direction (1.81 GPa). To better observe how this ZB CdTe material behaves under compression, a compressive load is given to 6 nm nanopillar (NP) having different crystal orientations. A similar kind of behavior is found in the case of NP also. It is clear from figure 4(b) that [111] NP has less compressive strength than [110] NP. While in the case of [001], its compressive strength is lower than the other two.

Figure 4(c) represents Young’s modulus of CdTe NWs as a function of NWs crystal orientations at different temperatures. The Young’s modulus of [001], [110] and [111] oriented CdTe NWs are obtained by fitting the stress-strain curve to a straight line. It is observed that the [111]-oriented CdTe NW has the highest value of elastic modulus. Moreover, the results are close for [111] and [110]-oriented NWs while for [001]-oriented NWs, the values are significantly lower than that of those two directions. Furthermore, the stress-strain curve has two distinct regions in figure 4(b) which is similar to the study performed by Healy, et al for Fe nanopillar [36]. The stress first increases linearly up to a certain point (yielding point) and then starts to fluctuate as flow stress. It is observed that the average flow stress varies with crystal orientation. The maximum average flow stress is 3.76 GPa for the [111]-oriented NP and the minimum average flow stress for the [001]-oriented NP is 2.83 GPa. The [110]-orientation yields average flow stress of 3.24 GPa. It is also observed that the average flow stress
for the [111] direction is the highest and for [001] CdTe, it is the lowest. However, significant fluctuation in average flow stresses (figure 4(b)) is observed due to activation of several cross-slip systems in the material under compression.

Figure 5(a) shows the atomic arrangement of [001] oriented ZB CdTe, the bonds are arranged in a way that all the bonds make 45° with the loading direction (indicated by the arrow). As a result, these bonds fail at a lower compressive load. That is why [001] oriented structures have lower strength than the other two structures in both tension and compression. On the other hand, figures 5(b) and (c) show that [110] and [111] oriented structure’s atoms are singly bonded to the opposite surface or atomic layer. In both cases, the bonds are arranged in a way that all the bonds make 90° with the loading direction. Therefore, they are capable of taking higher tensile and compressive loads than the [001] oriented ZB CdTe structures. For similar reason, Young’s Modulus in [111]-orientation is the highest and [001]-orientation is lowest which is presented in figure 4(c). Furthermore, the spacing between atoms in [110] oriented structure is shorter than the spacing of [111] oriented structures and each atom is surrounded by opposite type atom resulting in higher compressive strength. On the contrary, in [111] oriented ZB CdTe, there are two types of polarities in the atomic layers. From figure 5(c), it is evident that all atoms in a layer are positively charged (Cd) and all atoms in the adjacent layer are negatively charged (Te). As a result, there is an electrostatic attraction between two adjacent planes which makes it difficult to separate when tension is applied along the [111] orientation. However, under compression, when the layers come closer to each other, atoms with the same polarity start to repel each other. Upon applying a sufficient amount of load, the repelling force becomes significantly high in magnitude. The [111]-oriented CdTe structure has a lower compressive strength than [110]-oriented structure. This is because the effective compressive load (resultant of

**Figure 3.** Variation of ultimate stresses of [111]-oriented CdTe in (a) tension and (b) compression with temperature, and for different diameters. (c) Variation of Young’s modulus of ZB CdTe nanowires with temperatures, and for different diameters.
Figure 4. Stress–strain curves of [111], [110], and [001]-oriented (a) NWs of $D = 4 \text{ nm}$ at $T = 300 \text{ K}$ under both tension and compression. (b) Nanopillars of $D = 6 \text{ nm}$ at 100k under compression. (c) Variation of Young’s modulus of ZB CdTe nanowires with temperature, and for different crystals orientation of 4 nm nanowires.

Figure 5. Representation of the atomic arrangements of (a) [001], (b) [110], (c) [111] oriented ZB CdTe, respectively.
applied compression and repelling force) increases more with a gradual increment of strain along [111]-orientation which has larger atomic layer spacing.

4.3. Failure mechanism
The [111]-oriented ZB CdTe NWs in the present study fails by creating void in [10-1] direction regardless of temperature and NW size. In figure 6, the failure phenomenon of the nanowire with a diameter of 6 nm is shown at 300 K temperature with the aid of construct surface mesh (CSM). At 15.74% strain, a void is initiated at the NW surface which is marked with a red square in figure 6(a). It is found that loading in z-direction causes very little plasticity in the nanowire and the fracture happens in a short strain region, from 15.74% to 16.71%. It is observed that the bonds are broken in [1-21] direction and void which is created due to bond breaking propagates in [10-1] direction not reported for Zinc-Blende structure in previous literature, as illustrated in figure 6.

To understand the failure mechanism profoundly, atomic arrangement analysis of [111]-oriented ZB CdTe NWs is used which is shown in figure 7. Breaking bonds along [10-1] direction require a high amount of energy because of its shorter bond gaps. Therefore, bond breaking is not seen in this [10-1] direction. On the other hand, along [1-21] direction gap between bonds is greater. Therefore, it would take less energy to break bonds along [1-21] direction. Bond breaking is a gradual process and it passes from one layer to another layer. When breaking of bonds in one layer is completed, bond breaking in another layer is initiated. So, in this way void
propagates in [10−1] direction (see figures 6(d) and (e)). Thus, a fast rate of void propagation in [10−1] direction causes a fracture in a short strain region.

For compression, [111]-oriented ZB CdTe NW with a diameter of 6 nm and temperature of 100 K exhibits mechanical behavior that is different from that of tension. For a strain rate of $-10^9$ s$^{-1}$ the structure deforms and buckles and eventually fractures the nanowire which is shown in figure 8. Similar results have been obtained for NWs of other diameters also.

4.4. Effects of Strain Rates

Finally, the influence of strain rate on the mechanical properties of CdTe NWs is depicted in figure 9. Stress-strain curves of a [111]-oriented CdTe NW with 5 nm diameter size at 300 K are shown for a strain rate range from $10^8$ s$^{-1}$ to $10^{11}$ s$^{-1}$. It is observed from the figure that for both uniaxial tension and compression, the fracture strength and the strain reduce with the decrement of strain rate. This type of phenomenon occurs because defects can nucleate easily at lower stresses if more time is given. The curves of both tension and compression for the NWs above $5 \times 10^9$ are distorted due to the disorderliness and fluctuation of atoms stemming from the impact of such unusual high strain. A similar kind of strain-dependent behavior was observed in the case of SiC [19].

The failure mechanisms of [111]-oriented ZB CdTe NW for the three tensile strain rates $10^9$ s$^{-1}$, $10^{10}$ s$^{-1}$ and $10^{11}$ s$^{-1}$ are illustrated in figure 10. The change in failure behavior for different strain rates is presented in these Figures. In figure 10(a), for the slowest strain rate, only one void is created leading to a brittle fracture. For intermediate strain rate of $10^{10}$ s$^{-1}$, more voids are observed to cause the failure (see figure 10(b)). For the highest strain rate of $10^{11}$ s$^{-1}$, a cascade of voids is nucleated throughout the [111] oriented ZB CdTe NW structure (figure 10(c)).
The mechanical behavior of [111]-oriented ZB CdTe NWS under different compressive strain rates are also distinctive. For a gradual increase of compressive strain rates, there is a clear transition in the [111]-oriented CdTe NWs behavior from single buckling to multiple buckling to homogeneous amorphization. This behavior is illustrated in figure 11. At the low strain rate of $10^9 \text{ s}^{-1}$, the nanowires develop a single buckling that leads to fracture of the nanowire. However, at the intermediate rate of $10^{10} \text{ s}^{-1}$, multiple buckling is generated along the NWs accompanied by irreversible plastic deformations, as illustrated in figure 11 (b). At the highest compressive strain rate of $10^{11} \text{ s}^{-1}$ NW is homogeneously amorphized. This behavior is consistent with some previous studies for different nanowires [19].

5. Conclusions

In this investigation, Zinc blende Cadmium Telluride nanowires are studied by molecular dynamics simulations. Here, atomistic simulations have been carried out to investigate both the tensile and compressive mechanical behavior of these nanowires considering different sizes, temperatures, crystal orientation, and strain rates. Both ultimate strength and Young’s modulus show an inverse relation with temperature under both tension and compression. It is also demonstrated that size has a negligible effect on the tensile behavior but during compression, the ultimate strength and elastic modulus are diameter dependent. However, the NWs of CdTe under tension shows considerably higher strength than NWs under compression. One of the main findings of this study is that fracture strength of the [111]-oriented CdTe NWs is always higher than that of the [110]-oriented NWs under tension, while in compression, the fracture strength of the [111] NWs is always lower.
than that of the [110] NWs. Moreover, the [111]-oriented ZB CdTe NWs fails by creating void in [10-1] direction regardless of temperature and NW size. Investigation suggests that these phenomena of ZB CdTe nanowires are controlled by bond length, atomic spacing, and electrostatic forces. Finally, it is observed that with increasing the strain rate, both the ultimate strength and strain increase. The failure mechanism for low to high strain rates is also elucidated. This investigation provides a comprehensive understanding of temperature, size, crystal orientation, and strain rate dependent mechanical properties and fracture phenomenon of ZB CdTe NWs which has enumerable application in NEMS/MEMS.

Acknowledgments

The authors of this paper would like to thank the Department of Mechanical Engineering, BUET for providing the computing resources and Multiscale Mechanical Modelling and Research Network (MMMRN) group of the same department for the technical support to conduct the research.

ORCID iDs

Mohammad Motalab @ https://orcid.org/0000-0003-2128-464X

References

[1] Huang Y, Duan X, Cui Y, Lauhon I, J, Kim K-H and Lieber C M 2001 Logic gates and computation from assembled nanowire building blocks Science 294 1313–7
[2] Duan X, Huang Y, Agarwal R and Lieber C M 2003 Single-nanowire electrically driven lasers Nature 421 241–5
[3] Tian B, Zheng X, Kemps T J, Fang Y, Yu N, Yu G, Huang J and Lieber C M 2007 Coaxial silicon nanowires as solar cells and nanoelectronic power sources Nature 449 885–9
[4] Lieber C M and Wang Z J 2007 Functional nanowires MRS Bull. 32 99–108
[5] Han X D, Zheng K, Zhang Y F, Zhang X N, Zhang Z and Wang Z J 2007 Low-temperature in situ large-strain plasticity of silicon nanowires Adv. Mater. 19 2112–8
[6] Ostlund F, Rzepiejsewa-Malyksa K, Leifer K, Hale I M, Tang Y, Ballarini R, Gerberich W W and Michler J 2009 Brittle-to-ductile transition in uniaxial compression of silicon pillars at room temperature Adv. Funct. Mater. 19 2439–44
[7] Ostlund F, Howie P R, Ghielen R, Korte S, Leifer K, Clegg W J and Michler J 2011 Ductile–brittle transition in micropillar compression of GaAs at room temperature Philos. Mag. 91 1190–9
[8] Kikuta T, Takatani Y, Asaka K and Yoshizaki R 2005 Measurements of the atomistic mechanics of single crystalline silicon wires of nanometer width Phys. Rev. B 72 035333
[9] Minamisawa R A, Süss M J, Spolenak R, Faist J, David C, Bourdelle K K and Sigg H 2012 Top-down fabricated silicon nanowires under tensile elastic strain up to 4.5% Nat. Commun. 3 1096
[10] Michler J, Wasmter K, Meier S, Ostlund F and Leifer K 2007 Plastic deformation of gallium arsenide micropillars under uniaxial compression at room temperature Appl. Phys. Lett. 90 043123
[11] Stan G, Krylyuk S, Davydov A V and Cook R F 2010 Compressive stress effect on the radial elastic modulus of oxidized Si nanowires Nano Lett. 10 2031–7
[12] San Paulo A, Bokor J, Howe R T, He R, Yang P, Gao D, Carraro C and Maboudian R 2005 Mechanical elasticity of single and double clamped silicon nanobeams fabricated by the vapor-liquid-solid method Appl. Phys. Lett. 87 053111
[13] Calahorra Y, Shtemplick O, Kotchetkov V and Yaish Y E 2015 Young’s modulus, residual stress, and crystal orientation of doubly clamped silicon nanowire beams Nano Lett. 15 2945–50
[14] Hoffmann S, Ute I, Moser B, Michler J, Christiansen S H, Schmidt V, Senz S, Werner P, Gosele U and Ballif C 2006 Measurement of the bending strength of vapor–liquid–solid grown silicon nanowires Nano Lett. 6 662–5
[15] Root S E, Savagatrup S, Pais C J, Arya G and Lipomi D J 2016 Predicting the mechanical properties of organic semiconductors using coarse-grained molecular dynamics simulations Macromolecules 49 2886–94
[16] Guineoile J, Goot J and Brochard S 2011 Deformation of silicon nanowires studied by molecular dynamics simulations Model. Simul. Mater. Sci. Eng. 19 074003
[17] Dayeh S A, Wang J, Li N, Huang J Y, Gin A V and Picraux S T 2011 Growth, defect formation, and morphology control of germanium–silicon semiconductor nanowire heterostructures Nano Lett. 11 4200–6
[18] Kang K and Cai W 2010 Size and temperature effects on the fracture mechanisms of silicon nanowires: molecular dynamics simulations Int. J. Plast. 26 1387–401
[19] Tsuzuki H, Rino JP and Brancioli P S 2011 Dynamic behaviour of silicon carbide nanowires under high and extreme strain rates: a molecular dynamics study J. Phys. Appl. Phys. 44 055405
[20] Cheng G, Chang T H, Qin Q, Huang H and Zhu Y 2014 Mechanical properties of silicon carbide nanowires: effect of size-dependent defect density Nano Lett. 14 754–8
[21] Piall T H, Rakib T, Mogejmer S, Matebal M and Akanda M A S 2018 Atomistic investigations on the mechanical properties and fracture mechanisms of indium phosphide nanowires Phys. Chem. Chem. Phys. 20 8647–57
[22] Kang K and Cai W 2007 Brittle and ductile fracture of semiconductor nanowires—molecular dynamics simulations Philos. Mag. 87 2169–89
[23] Wang Z, Zhu X, Yang L, Gao F and Weber W J 2007 Atomic simulations of the size, orientation, and temperature dependence of tensile behavior in GaN nanowires Phys. Rev. B 76 045310
[24] Dai L, Cheong W C D, Sow C H, Lim C T and Tan V B C 2010 Molecular dynamics simulation of ZnO nanowires: size effects, defects, and super ductility Langmuir 26 1165–71
[25] Ye Y, Dai L, Sun T, You I P, Zhu R, Gao J Y, Peng R M, Yu D P and Qin G G 2010 High-quality CdTe nanowires: synthesis, characterization, and application in photosresponse devices J. Appl. Phys. 108 044301
[26] Shaygan M, Davami K, Kheirabadi N, Baek C K, Cuniberti G, Meyyappan M and Lee J S 2014 Single-crystalline CdTe nanowire field effect transistors as nanowire-based photodetector Phys. Chem. Chem. Phys. 16 22687–93
[27] Dreifus D L, Kolbas R M, Harris K A, Bicknell R N, Harper R L and Schhetzina J F 1987 CdTe metal-semiconductor field-effect transistors Appl. Phys. Lett. 51 931–3
[28] Dreifus D L, Kolbas R M, Tassitino J R, Harper R L, Bicknell R N and Schhetzina J F 1988 Electrical properties of CdTe metal–semiconductor field effect transistors J. Vac. Sci. Technol. A 6 2722–4
[29] Lee Y J, Ryu H J, Lee S W, Park S J and Kim H J 2013 Comparison of ultra-high-resolution parallel-hole collimator materials based on the CdTe pixellated semiconductor SPECT system Nucl. Instrum. Methods Phys. Res. Sect. A 7529 –33
[30] Tsutsui H, Ohtuschi T, Ohmori K and Baba S 1993 CdTe semiconductor x-ray imaging sensor and energy subtraction method using x-ray energy information IEEE Trans. Nucl. Sci. 40 93–101
[31] Rakshania A E 2001 Heterojunction properties of electrodeposited CdTe/CdS solar cells J. Appl. Phys. 90 4265–71
[32] Britz J and Ferekides C 1993 Thin-film CdS/CdTe solar cell with 15.8% efficiency Appl. Phys. Lett. 62 2851–2
[33] Tang Z, Kotov N A and Giessen M 2002 Spontaneous organization of single CdTe nanoparticles into luminescent nanowires Science 297 237–40
[34] Sakoda K, Yao Y, Kuroda T, Dirin D N and Vasiliev R B 2011 Exciton states of CdTe tetrapod-shaped nanocrystals Opt. Mater. Express 1 379–90
[35] Williams B L, Halliday D P, Mendis B G and Durose K 2013 Microstructure and point defects in CdTe nanowires for photovoltaic applications Nanotechnology 24 135703
[36] Shen H, Zheng Y, Wang H, Xu W, Qian L, Yang Y, Titov A, Hyvonen J and Li L S 2013 Highly efficient near-infrared light-emitting diodes by using type-II CdTe/CdSe core/shell quantum dots as a phosphor Nanotechnology 24 475603
[37] Wei S H and Zhang S B 2000 Structural stability and carrier localization in CdX (X = S, Se, Te) semiconductors J. Phys. Chem. B 104 6944–7
[38] Ward D K, Zhou X W, Wong B M, Doty F P and Zimmerman J A 2011 Accuracy of existing atomic potentials for the CdTe semiconductor compound J. Chem. Phys. 134 244703
[39] Henager C and Morris J R 2009 Atomic simulation of CdTe solid-liquid coexistence equilibria Phys. Rev. B 80 245309
[40] Plimpton S 1995 Fast parallel algorithms for short-range molecular dynamics J. Comput. Phys. 117 1–19
[41] Stukowski A 2010 Visualization and analysis of atomic simulation data with OVITO—the open visualization tool Model. Simul. Mater. Sci. Eng. 18 015012
[42] Wang Z Q, Stroud D and Markworth A J 1989 Monte Carlo study of the liquid CdTe surface Phys. Rev. B 40 3219–32
[43] Kanou M B, Sekkal W, Aourag H and Merad G 2000 Molecular-dynamics study of the structural, elastic and thermodynamic properties of Cadmium Telluride Phys. Lett. A 272 113–8
[44] Hired P 2015 Atomusk: a tool for manipulating and converting atomic data files Comput. Phys. Commun. 197 212–9
[45] Saha S, Abdul Motalab M and Mahboob M 2017 Investigation on mechanical properties of polycrystalline W nanowire Comput. Mater. Sci. 136 52–9
[46] Mojumder S 2018 Molecular dynamics study of plasticity in Al-Cu alloy nanopillar due to compressive loading Phys. B Condens. Matter 530 86–9
[47] Muhammad Nahid S, Nahian S, Motalab M, Rakib T, Mojumder S and Mahbubul Islam M 2018 Tuning the mechanical properties of silicone nanosheet by auxiliary cracks: a molecular dynamics study RSC Adv. 8 50345–65
[48] Christensen N E and Christensen O B 1986 Electronic structure of ZnTe and CdTe under pressure Phys. Rev. B 33 4739–46
[49] Stöhrssner K, Vos S, Dieterich W, Gebhardt W and Cardona M 1983 High-pressure x-ray investigations of phase transitions in CdI—xMnTe Solid State Commun. 56 563–5
[50] Cohen M L 1985 Calculation of bulk moduli of diamond and zinc-blende solids Phys. Rev. B 32 7988–91
[51] Delgoffe G, Colakoglu K and Ciftci Y 2006 Elastic, electronic, and lattice dynamical properties of CdS, CdSe, and CdTe Phys. B Condens. Matter 373 124–30
[52] Rowe J M, Nicklow R M, Price D L and Zanio K 1974 Lattice dynamics of Cadmium Telluride Phys. Rev. B 10 671–5
[53] Harrison W A 2012 Electronic structure and the properties of solids: the physics of the chemical bond (Rockland: Courier Corporation)
[54] Ward D K, Zhou X W, Wong B M, Doty F P and Zimmerman J A 2012 Analytical bond-order potential for the Cadmium Telluride binary system Phys. Rev. B 85 115206
[55] Chavez J J, Zhou X W, Almeida S E, Aguirre R and Zubia D 2018 Molecular dynamics study of high-symmetry planar defect evolution during growth of CdTe/CdS films J. Phys. Chem. C 122 751–61
[56] Healy C J and Ackland G J 2014 Molecular dynamics simulations of compression–tension asymmetry in plasticity of Fe nanopillars Acta Mater. 70 105–12