A first-principles study of structural, electronic and optical properties of $\alpha$-Te tubular nanostructures modulated by uniaxial strain

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Abstract
First-principles calculations were performed to study the effect of uniaxial strain on the electronic properties of $\alpha$-Te nanotubes (NTs) of different configurations and tube sizes. Our $ab$ initio molecular dynamics simulation and phonon dispersion calculation indicate that both armchair (5, 5) and zigzag (10, 0) $\alpha$-Te NTs are thermodynamically stable and exhibit good dynamic stability at room temperature. Under compressive and tensile strains of $\pm$10%, the atomic structure of the $\alpha$-Te NTs remains stable, demonstrating they have good flexibility. An increase in uniaxial strain leads to a progressive decrease in the band gap for both armchair and zigzag $\alpha$-Te NTs. Interestingly, it is found that armchair (5, 5) $\alpha$-Te NTs experience an intriguing semiconductor–metal transition at a critical strain, while other $\alpha$-Te NTs are semiconducting with an adjustable band gap. In addition, the valence band maximum and conduction band minimum charge density between the interlayers has an impact on the type of band gap in the (5, 5) and (10, 0) NTs. Finally, we found the optical properties can be significantly modulated under strain in the $z$ direction. Increasing our understanding of the electronic and optical properties of $\alpha$-Te NTs under strain modulation helps shed light on the properties of new nanomaterials more generally, paving the way for future optoelectronic applications. These findings highlight the tunable electronic and optical properties of $\alpha$-Te NTs, which is promising for applications in nanodevices such as opto-electronics, electrical switches, and nanoscale strain sensors.

1. Introduction
Nanomaterials have become the focus of research in materials science due to their unique structure and extraordinary physical properties. Graphene was the first two-dimensional (2D) material discovered [1], and after graphene, a large number of experimental and theoretical studies were conducted on 2D nanostructures, including elemental 2D materials such as silicone [2], germanene [3], antimonene [4], and transition-metal dichalcogenides (TMDs). Among TMDs, the novel nanomaterial MoS$_2$ has attracted both fundamental and technical interest because of its relatively large and direct band gap as well as its good...
carrier mobility [5–7]. Recently, Zhu et al predicted one emergent 2D material, tellurene [8]. This material has a higher carrier mobility than monolayer MoS$_2$ and can be stabilized in three different structures, 1T-MoS$_2$-like (α-Te), metastable tetragonal (β-Te) and 2H-MoS$_2$-like (γ-Te). The intrinsic multivalent property of tellurium (Te) contributes to the formation mechanism of these structures and exhibits superior electronic and optical properties [9]. In addition, Te is an important p-type semiconductor with a band gap of about 0.35 eV [10]. It exhibits good photoconductivity, a thermoelectric effect, catalytic activity, high piezoelectricity [11, 12] and is particularly useful for potential applications in piezoelectric devices [13], topological insulators [14], gas sensors [15], and other various optoelectronic devices [16]. Subsequently, tellurene with different configurations were successfully prepared experimentally [8, 9, 17], and it has been fabricated as a field-effect transistor with air-stable performance and high carrier mobility [7]. Over the last two decades, despite thousands of scientists researching 2D nanostructures, their development has slowed. In recent years, however, one-dimensional (1D) nanostructures, including nanowires (NWs), nanotubes (NTs), nanobelts and nanorods, have been regarded as the most promising building blocks for nanoscale electronic and optoelectronic devices [18–20]. Such 1D nanomaterials possess significant nanoscale effects and quantum confinement effects when compared to 2D nanomaterials. The intrinsic multivalent property of Te contributes to the formation mechanism of these structures and exhibits superior electronic and optical properties [9]. The inherent anisotropic crystal structure of Te has a strong tendency to grow 1D Te NWs and NTs obtained by syntheses using different methods and techniques [21, 22]. Recently, large-sized hexagonal Te NTs have been successfully synthesized experimentally [23, 24]. The morphology of 1D Te nanostructures can be controlled by light irradiation and the thermal effect [25]. The synthesis of different 1D Te nanostructures provides opportunities for various nanodevice-related applications of Te and tellurides. The size and shape of Te nanostructures can be adjusted by controlling various parameters (such as growth time and concentration), which are critical to the manufacture of functional nanodevices. Moreover, Te-NWs and Te derivatives have also been used for gas sensing probes, optoelectronics, sensors, radiative cooling devices, magnetic memory and topological insulators [26, 27].

It is theoretically predicted that α-Te NTs can be regarded as α-Te sheets rolled into a cylindrical structure. In our previous study, we investigated the effect of changes in tube size on electronic and optical properties for armchair and zigzag α-Te NTs, finding that armchair NTs transition from an indirect to a direct band gap as their tube diameter is reduced to a certain size, while zigzag NTs always remain as direct bandgap semiconductors [28]. Furthermore, in order to find wider applications in a more diverse environment, it is worth noting other methods of modulating electronic properties. In addition to doping various types of heteroatoms and adsorbing heteroatoms or molecules to adjust the electronic properties of 1D nanomaterials, another effective method to expand their potential application is to apply external strain. Depending on the strain direction and chirality of NTs, the band gap of MoS$_2$ NTs can be decreased or enhanced by uniaxial strain along the axial direction [29]. Mechanical strain usually has a surprising effect on the electronic properties of nanomaterials, and often greatly changes the inherent properties of the material.

In the present study, first-principles calculations were performed to investigate the structural and electronic properties of armchair and zigzag α-Te NTs with various tube sizes under various strains. Interestingly, both the band gap and electronic properties of α-Te NTs can be tuned by strains, showing promise for device applications in electronic and optoelectronic devices.

The rest of this paper is organized as follows: section 2 will present the computational details. In section 3, the effect of uniaxial strains on the electronic properties for α-Te NTs of various tube sizes are discussed. Further investigations of the optical properties of strained α-Te NTs are presented. Finally, the paper is summarized by a conclusion and perspectives.

2. Computational details

Our calculations were carried out using the density functional theory (DFT), implemented in the Vienna *ab initio* simulation package (VASP) with the projector augmented wave (PAW) method [30, 31]. The interactions between ion cores and valence electrons were treated by using such a PAW method. DFT structural relaxation and electronic band structure calculations were performed using the Perdew–Burke–Ernzerhof (PBE) generalized gradient approximation for the exchange–correlation functional [32]. Brillouin zone (BZ) sampling was represented by a Monkhorst–Pack [33] with k-points meshes of $1 \times 1 \times 10$ along the tube axis and was increased to a $1 \times 1 \times 80$ grid for k-point sampling for further calculations of band structure and density of states. The plane-wave cutoff energy of 218 eV was utilized in the calculations and was expanded to a cutoff of 400 eV for further computations of phonon dispersion relation. Periodic boundary conditions were adopted along the tube axis (taken as the z axis) and a sufficient vacuum thickness of 15 Å was applied in both x and y directions to eliminate the interaction.
between neighboring NTs. All structures were optimized until the interatomic forces were less than 0.02 eV Å\(^{-1}\).

The phonon dispersion relation was computed by Phonopy code [34], and the real space force constants of a 1 × 1 × 3 supercell were calculated by density function perturbation theory implemented in VASP. In order to investigate thermodynamic stability, \textit{ab initio} molecular dynamics (AIMD) simulations were carried out under 300 K, where the NVT canonical ensemble was utilized. Temperature control was achieved by using the Nosé–Hoover thermostat [35, 36]. The time step was set to be 3.0 fs.

Calculations on optical properties were carried out based on independent particle approximation as implemented in VASP. The quasiparticle self-energy corrections, excitonic contributions, and local-field effects are ignored in our computations.

3. Results and discussion

Similar to carbon NTs and 1T-MoS\(_2\) NTs, \(\alpha\)-Te NTs are constructed by rolling up a 2D \(\alpha\)-Te sheet along different orientations in order to obtain NTs with different helicities. Figure 1 shows the stress applied along the axis for typical armchair (10, 10) and zigzag (10, 0) \(\alpha\)-Te tubular geometrical structures. In this work, we explore armchair \((n, n)\) \(\alpha\)-Te NTs with \(n\) ranging from 5 to 12, and zigzag \((n, 0)\) \(\alpha\)-Te NTs with \(n\) ranging from 10 to 17. These \(\alpha\)-Te NTs were subjected to stress along the tube direction, and the strain is defined as \(\varepsilon = (L - L_0)/L_0\), where \(L\) is the strained tube length and \(L_0\) is the original tube length. Negative values of \(\varepsilon\) indicate that the NTs are compressed, while positive values indicate that they are stretched.

In order to explore the relaxed optimized geometry of armchair and zigzag \(\alpha\)-Te NTs with different diameters under external strains, we examine the variation of total energy per atom with respect to strains, sketched in figure 2. As the strain changes from \(-10\%\) to \(+10\%\), we can find that all energy–strain curves can be well-fit with quadratic functions, which demonstrates that \(\alpha\)-Te NTs have excellent flexibility under appropriate uniaxial strain. As we can conclude from the result, strain changing from \(-10\%\) to \(10\%\) will not destroy the original structures of the NTs.

The bandgap values varying under uniaxial strain of armchair and zigzag \(\alpha\)-Te NTs are plotted in figure 3, where the band gaps are generally reduced as either compressive or tensile strains increase. Specifically, it is found that the band gaps of armchair and zigzag \(\alpha\)-Te NTs quickly decrease with an increase in compressive strain, indicating that the band gap of \(\alpha\)-Te NT is more sensitive to compressive strain. Overall, the tendency of band gap changes in strained-armchair (6, 6) to (12, 12) NTs are similar. In our previous work [28], we found that without uniaxial strain, i.e., \(\varepsilon = 0\%\), armchair (6, 6) to (12, 12) NTs are indirect bandgap semiconductors, while armchair (5, 5) \(\alpha\)-Te NT is a direct bandgap semiconductor. The main reason for this indirect-to-direct transition can be ascribed to the modification of the electronic
structure resulting from tube curvature. Interestingly, figure 3(a) implies that the semiconductor-metal transition of \((5, 5)\) α-Te NT occurs at around \(ε = −8\%\).

As is known, structural stability is crucial for practical applications. The thermodynamic and lattice dynamic stability are calculated for unstrained armchair \((5, 5)\) and zigzag \((10, 0)\) α-Te NTs. The fluctuations of the total potential energies (P-energy) and the geometric structures at the end of the AIMD simulations for armchair \((5, 5)\) and zigzag \((10, 0)\) α-Te NTs are presented in figure 4. It can be seen from the left-hand side of figure 4 that the fluctuations are very small and the atomic configurations at the end of 15 ps simulation basically maintain their initial patterns. In further examination of lattice dynamics stability, we calculate the 0 K phonon dispersion curves of both types of NTs, as displayed on the right-hand side of figure 4. No imaginary frequencies are found in the phonon dispersion of either armchair \((5, 5)\) or zigzag \((10, 0)\) NTs, which indicates they are dynamically stable.
To investigate the electronic properties of $\alpha$-Te NTs, band structures for armchair $$(5, 5)$$ and zigzag $$(10, 0)$$ NTs under different uniaxial strains are simulated in figure 5. The armchair $$(5, 5)$$ NT is a direct bandgap semiconductor under uniaxial strain ($$\varepsilon = 0\%$$). However, further uniaxial tensile strain ($$\varepsilon = 4\%$$ to 10\%) and uniaxial compressive strain ($$\varepsilon = -4\%$$ to $-6\%$$) induce a direct-to-indirect bandgap transition (figure 5(a)). Such a fascinating bandgap transition for armchair $\alpha$-Te NTs is of great importance for use in optoelectronic devices. Unlike the armchair $$(5, 5)$$ NT, the zigzag $$(10, 0)$$ NT under uniaxial tensile strain ($$\varepsilon = 4\%$$ to 8\%) and uniaxial compressive strain ($$\varepsilon = -4\%$$ to $-8\%$$) is an indirect bandgap semiconductor. Under other uniaxial strain, it is a direct bandgap semiconductor. In figure 5(a), it is noteworthy that when armchair $$(5, 5)$$ NT is applied with a large uniaxial compressive strain ($$\varepsilon = -8\%$$ to $-10\%$$), the valence band crosses the Fermi level and it changes from semiconductor to metal. Note that such a standard DFT method usually tend to underestimate band gap but hybrid functionals such as HSE06 improve the band gap. For instance, with such a HSE06 approximation, the computed band gap of unstrained armchair $$(5, 5)$$ $\alpha$-Te NT is 0.952 eV, apparently larger than PBE results and in good agreement with our previous work [28] as well. The resulting band structure and band gap of the strained armchair $$(5, 5)$$ NTs obtained from HSE06 calculations can be found in supplement (https://stacks.iop.org/NJP/24/053037/mmedia). However, the overall trend of the closing of the band gap as the strain increase was accurately identified.

To obtain a more complete explanation for such an indirect-to-direct bandgap transition for armchair $$(5, 5)$$ and zigzag $$(10, 0)$$ NTs under different uniaxial strains, the change of the bonding mode between the atoms and the composition of the s- and p-orbitals of Te atoms requires further investigation. The total and partial density of states, the latter of which can be decomposed into inner, middle, and outer Te atom parts, are illustrated in figure 6 for armchair $$(5, 5)$$ and zigzag $$(10, 0)$$ $\alpha$-Te NTs at different uniaxial strains.

What it most crucial is the electron near the Fermi level, for it directly decides the electric property in all kinds of structures. We can see from figures 6(a) and (b) that the contributed p-electron of Te plays a dominant role compared to the s-electron of Te. When a stretching force is applied, the p-electron of the tri-layer (the inner, the middle and the outer) Te atoms enact different trends in the valence band and the conduction band. From further analyses on the components of s-orbitals and p-orbitals of Te atoms, shown in figures 7(a) and (c), the density of middle-p in conduction band minimum (CBM) drops by some extent in both NT structures, especially in armchair $$(5, 5)$$ $\alpha$-Te NTs. More specifically, it is the drop of Te-p$_x$ and Te-p$_y$ that matters most. The Te-p$_x$ and Te-p$_y$ drop as much as 10% in the armchair $$(5, 5)$$. However, when
we compress the NTs, the density of the bottom of the electron in the CBM increases in both NT structures. There is a rise in p-electron for all the inner, middle and outer layers of the Te atom, whereas no significant change is found in the s-electron, meaning that the p-electron plays the leading role in the determination of the electric property.

Further analysis of the components of s- and p-orbitals of Te atoms as well as corresponding charge densities are plotted in figure 7. As for the valence band, the p-electron of inner and outer Te atoms is decisive. Most notably, an increase of the stretching makes more states available for occupation in the top (−0.2 to 0 eV) of the valence band maximum (VBM). In figures 7(a) and (c), the Te-p, and the Te-p vary over a wide range when force is applied, which results in the middle Te atom tending to bond with outer Te atoms rather than inner Te atoms in the armchair (5, 5), possibly causing the bandgap transition from direct to indirect.

The analyses of the band structure and DOS suggest that the composition of the s- and p-orbitals of Te atoms around VBM and CBM play a major role and should be the focus of research. In figure 7(a), for (5, 5) α-Te NTs (ε = 0%), the components of the VBM edges mainly come from p, orbitals. When tensile strain (ε = 4% to 6%) is applied, however, the contributions of the p, p, and p, orbital components to the edge of the VBM become almost equal. Therefore, the contribution of different p orbitals near the edge of the VBM causes the change in VBM located in the BZ. In addition, for (5, 5) α-Te NTs (ε = 0%), the components of the CBM edge mainly come from p, and p, orbitals. When compressive strain is applied (ε = −4% to −6%), however, the contributions of the p, p, and p, orbital components to the edge of the CBM are also almost equal. By comparison, in figure 7(c), for (10, 0) α-Te NTs (ε = 0%), the components of the VBM (CBM) edge mainly come from p (i.e., p, p, and p,) orbitals. When tensile strain (ε = 4% to 6%) is applied, however, the components of the VBM edge are mainly the p, and p, orbitals. Moreover, when compressive strain (ε = −4% to −6%) is applied, the components of the CBM edge are mainly p, orbitals.

From the partial charge density of the VBM and CBM, as shown in figures 7(b) and (d), one can see that the hybridization effect between the middle and inner Te atoms occurs in (5, 5) and (10, 0) NTs. The charge densities of the VBM and CBM show different characteristics for different conformations depending on whether their band gaps are direct or indirect. There is a significant overlap of VBM charge density between the Te atoms in the middle layer and the Te atoms in the inner layer. Interestingly, at zero strain, (5, 5) and

![Figure 5. Calculated energy band structures for (a) armchair (5, 5) and (b) zigzag (10, 0) α-Te NTs under uniaxial strain. The Fermi level was assigned at 0 eV.](image-url)
(10, 0) NTs show strong interlayer coupling, as well as a shorter interlayer distance and a direct band gap. With increasing tensile (compressive) strain, the coupling interaction between the middle and inner layers becomes weaker. The coupling effect mainly occurs between the neighboring atoms in the same layer. Because of this, the VBM (CBM) charge density between the interlayers has an impact on the type of band gap in (5, 5) NT and (10, 0) NT. This implies that the VBM (CBM) charge density between the interlayers is key in deciding the direct or indirect band gap in (5, 5) NT and (10, 0) NT under tensile (compressive) strain. Hence, the effect of strain leads to the modification of the electronic structure in the α-Te NT and is the main factor for the indirect-to-direct bandgap transition found in armchair (5, 0) and zigzag (10, 0) NTs at different uniaxial strains. The Fermi level was assigned at 0 eV.
Figure 7. The PDOS near the VBM and CBM as well as corresponding charge densities in the \( x-y \) plane of the VBM and CBM at different strains for (a) and (b) armchair (5, 5) NT and (c) and (d) zigzag (10, 0) NT. The Fermi level was assigned at 0 eV.

\( \alpha \)-Te NTs. The effect of deformation along the tube axis on an armchair tube causes the change in energy bands and electron charge density distribution, which is the main factor for the semiconductor–metal transformation of (5, 5) \( \alpha \)-Te NT under high compressive strain.
Physically, compression pushes atoms closer while stretching pulls them farther apart. As stretched, the distances between the atoms become longer than the original bonding length at $\varepsilon = 0\%$, which will change the bonding mode in the $\alpha$-Te NTs. In figure 8, we can directly observe the bonding mode change in the middle Te atoms.

For such $\alpha$-Te tubular structures, there are two kinds of Te atoms in the system, middle layer atoms, and the inner and outer layer atoms. When different strains are applied, a corresponding response in the distance between the outer, middle and inner layers can be achieved. Thus, the bond length of the nearest and second nearest neighbor atoms from the middle layer to the outer and inner layers should be analyzed. For armchair (5, 5) NTs, the nearest neighbor curves for middle-inner and middle-outer cross at around $\varepsilon = -6\%$, which is the point where semiconductor–metal transition occurs. A top view of tube axes projected onto the horizontal plane indicates that the outer layer of the NT tends to shrink. The density of the CBM indeed falls between the outer and middle layers in figure 7. A similar situation appears in zigzag (10, 0); however, the cross occurs at the second nearest neighbor curves between the middle-inner and middle-outer layers at around $\varepsilon = +6\%$. When force constantly increases, the bond length of the second nearest neighbor also continues to increase, with the whole tube having a tendency to fracture. In figure 7, such a resulting weaker force is due to the tube axial direction influenced by the VBM of the outer and middle layers.

The optical properties are determined by energy dependence of the complex dielectric function $\varepsilon(\omega)$ [37]. The imaginary component of the dielectric function $\varepsilon_2(\omega)$ can be determined by using a weighted sum over all possible transitions from the occupied valence band states to unoccupied conduction band states.

$$\varepsilon_2(\omega) = \frac{8\pi^2e^2}{\omega^2m^2V} \sum_{\nu} \sum_k |\langle c,k|\hat{e}\cdot p|\nu,k\rangle|^2 \delta(E_c(k) - E_v(k) - \omega),$$

(1)

where $V$ is the effective unit cell volume of the NT as determined by Machón et al [38], and $\nu$ and $c$ represent the valence and conduction bands, respectively. The terms $|\nu,k\rangle$ and $|c,k\rangle$ are the eigenstates obtained from band structure calculation, $\hat{e}$ is the external field vector, $p$ is the momentum operator, and $E$ is the energy of the incident photon. The real part of the dielectric function $\varepsilon_1(\omega)$ can be evaluated from the imaginary part $\varepsilon_2(\omega)$ by a Kramer–Kronig transformation. The refractive index, the extinction coefficient and the absorption coefficient can be obtained from the dielectric function.

Figures 9(a) and (b), respectively, are the calculated real and imaginary parts of the dielectric constant of the armchair (5, 5) $\alpha$-Te NT. It can be seen from this figure that the dielectric constant along the $x$ and $y$ directions, i.e. $\varepsilon_x$ and $\varepsilon_y$, are isotropic, while the dielectric constant along the $z$ direction, i.e. $\varepsilon_z$, exhibits different properties from that along the $x$ and $y$ directions. Compared with monolayer Te, the static dielectric constant $\varepsilon_1(0)$ of the armchair (5, 5) NT along three directions is larger than that of monolayer Te [39], and the $\varepsilon_1(0)$ of armchair (5, 5) NT along the $z$ direction is greater than that along the $x$ and $y$
Figure 9. Calculated real ($\varepsilon_1$) and imaginary ($\varepsilon_2$) parts of the dielectric function as a function of energy for the armchair (5, 5) $\alpha$-Te NT without (a) and (b) and with (c)–(f) strains along the $x$, $y$ and $z$ directions. Here, the $z$ direction, which is orthogonal to $x$ and $y$, is directed along the NT axis.

The imaginary part of the dielectric constant, $\varepsilon_2$, reflects the absorption properties of the material, where the peaks of $\varepsilon_2^x$ and $\varepsilon_2^y$ are found at 1.6 eV, and the peak of $\varepsilon_2^z$ is near 0.9 eV.

Figures 9(c)–(f) show the influence of five representative stresses on the dielectric constants of the armchair (5, 5) NT, where it is clear that strain has little effect on the optical properties along the $x$ and $y$ directions. When the strain changes from $-10\%$ to $+10\%$, the static dielectric constant, $\varepsilon_1^x(0)$, gradually decreases. The first peak position of $\varepsilon_1^x$ moves to a lower energy direction and the peak height decreases slightly. The first peak position of $\varepsilon_2^x$ is almost unchanged, while the peak height decreases. Under compressive stress, the imaginary part of the dielectric constant, $\varepsilon_2^x$, appears as a second peak near 2.8 eV, but disappears under tensile stress. Since the strain is applied along the $z$ direction in the armchair (5, 5) NT, as the strain changes, the distance between atoms along the $z$ direction changes significantly, and the interaction between atoms will significantly affect the optical properties along the $z$ direction. It can be seen from figure 9(e) that the static dielectric constant continues to decrease, the position of the first peak moves to higher energy direction, and the peak height also decreases. The first peak of the imaginary part of the dielectric constant moves in the higher energy direction, and the height increases slightly.

Figure 10 shows the dielectric constant of the zigzag (10, 0) $\alpha$-Te NT. Without stress, the dielectric constants of zigzag (10, 0) NT along the $x$ and $y$ directions are similar to those of armchair (5, 5) NT; i.e., $\varepsilon_x$ and $\varepsilon_y$ are isotropic, while $\varepsilon_{1z}$ is different from $\varepsilon_{1x}$ and $\varepsilon_{1y}$. Different optical properties in the $z$ direction are exhibited by zigzag (10, 0) and armchair (5, 5) NTs; the static dielectric constant $\varepsilon_{1z}(0)$, is smaller than that of $\varepsilon_{1x}(0)$, but the difference is very small, with the first peak height of $\varepsilon_{1z}$ being lower than that of $\varepsilon_{1x}$. The position of the first peak of the imaginary part of the dielectric constant is the same, but the peak value of $\varepsilon_{2z}$ is much smaller than $\varepsilon_{2x}$, while the second peak of $\varepsilon_{2z}$ at 2.5 eV is clearly higher than that of $\varepsilon_{2x}$.

Figures 10(c)–(f) are the curves of the effect of five representative stresses on the dielectric constants of the zigzag (10, 0) NT. It can be seen that the main influence of strain on $\varepsilon_{1x}$ is the static dielectric constant, and the minimum value of $\varepsilon_{1x}(0)$ gradually decreases when the strain moves from $-10\%$ to $+10\%$, although the first peak position and peak height of $\varepsilon_{1x}$ are almost unchanged. The absolute value of the minimum value of $\varepsilon_{1x}$ increases with the change in strain, while the position of the first peak of the imaginary part $\varepsilon_{2x}$, is almost unchanged, and the peak height changes very little. The shoulder on the right of the first peak of
Figure 10. Calculated real ($\varepsilon_1$) and imaginary ($\varepsilon_2$) parts of the dielectric function as a function of energy for the zigzag (10, 0) $\alpha$-Te NT without (a) and (b) and with (c)–(f) strains along the $x$, $y$, and $z$ directions. Here, the $z$ direction, which is orthogonal to $x$ and $y$, is directed along the NT axis.

$\varepsilon_2$ gradually evolves into the second peak as the strain changes. The strain has a very obvious influence on the dielectric constant along the $z$ direction. It can be seen from figure 10(e) that the static dielectric constant continuously decreases, the positions of the first and second peaks move to higher energy direction, and the peak height also continuously decreases. The positions of the first and the second peaks of the imaginary part of the dielectric constant move towards the high-energy direction, and the peak heights of the two peaks also continuously decrease.

4. Conclusions

In summary, the structural and electronic properties of armchair and zigzag $\alpha$-Te NTs under various strains were investigated by first-principles investigations. Both armchair (5, 5) and zigzag (10, 0) NTs are dynamically stable and exhibit good thermal stability at room temperature based on our phonon dispersion computations and AIMD simulations, respectively. All these $\alpha$-Te NTs exhibit excellent toughness under strains ranging from $-10\%$ to $10\%$. Remarkably, as the compressive strain increases to $8\%$, the armchair (5, 5) $\alpha$-Te NT will undergo a semiconductor–metal transition, while other strained $\alpha$-Te NTs always remain as a semiconductor with an adjustable band gap. Moreover, we found the effect of compressive strain on the band gap of $\alpha$-Te NTs is stronger than that of tensile strain. Our findings indicate that for VBM, the charge density of the inner and outer p-electron plays a key factor in producing either the direct or indirect band gap in the (5, 5) NT and (10, 0) NT, while for CBM the charge density of the middle p-electron is the key factor driving the phenomenon. The bonding mode between middle and inner layer has a high correlation to the semiconductor–metal transition in the armchair (5, 5) NT. Extraordinary optical properties are exhibited in both armchair (5, 5) and zigzag (10, 0) NTs. The optical properties along the tube direction can be significantly modulated under strain ranging from $-10\%$ to $10\%$ in the $z$ direction. This study shows that strain engineering is an effective modification method, further progressing novel nanomaterials towards becoming attractive materials for optoelectronic devices.
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Conflict of interest

There are no conflicts to declare.

Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

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