Tellurium as a successor of silicon for extremely scaled nanowires: a first-principles study

Aaron Kramer1, Maarten L. Van de Put2, Christopher L. Hinkle3 and William G. Vandenberghe2

Trigonal-Tellurium (t-Te) has recently garnered interest in the nanoelectronics community because of its measured high hole mobility and low-temperature growth. However, a drawback of tellurium is its small bulk bandgap (0.33 eV), giving rise to large leakage currents in transistor prototypes. We analyze the increase of the electronic bandgap due to quantum confinement and compare the relative stability of various t-Te nanostructures (t-Te nanowires and layers of t-Te) using first-principles simulations. We found that small t-Te nanowires (≤4 nm²) and few-layer t-Te (≤3 layers) have bandgaps exceeding 1 eV, making Tellurium a very suitable channel material for extremely scaled transistors, a regime where comparably sized silicon has a bandgap that exceeds 4 eV. Through investigations of structural stability, we found that t-Te nanowires preferentially form instead of layers of t-Te since layers of t-Te have a greater number of van der Waals (vdW) interactions between the t-Te-helices. We develop a simplified picture of structural stability relying only on the number of vDW interactions, enabling the prediction of the formation energy of any t-Te nanostructure. Our analysis shows that t-Te has distinct advantages over silicon in extremely scaled nanowire transistors in terms of bandgap and the t-Te vdW bonds form a natural nanowire termination, avoiding issues with passivation.

INTRODUCTION

With the continued scaling of transistor size, the silicon (Si) mobility reduces drastically1 and at extremely small dimensions, the silicon bandgap increases dramatically (see Fig. 1). Reduced mobility gives rise to a reduced on-current, while a bandgap that is too large reduces the relative height of the gate dielectric potential barrier, increasing gate leakage current2. An increased bandgap may also lead to severe challenges in terms of doping and contacting. Graphene and topological insulators present a solution to the low mobility problem, but unfortunately have a vanishing bandgap, making the realization of a low off-state current challenging3-5. Several other alternative materials with a bandgap have been proposed, but no single material has emerged that can clearly outperform Si at the nanoscale6. Transition-metal dichalcogenides demonstrate a mobility that is lower and a bandgap that is higher than desired7-9. Phosphorene showed initial promise, but theoretical studies reveal a severely degraded mobility at small dimensions8.

Trigonal-Tellurium (t-Te) is an alternative material of interest because a high hole mobility (707 cm²Vs), low-temperature growth (≤120 °C)10, and a high current density (1 A/mm²) have all been demonstrated11. t-Te has a nearly direct and small bulk bandgap (0.33 eV)12, which has historically enabled applications in thermoelectric13, piezoelectric14, and photoconductive devices15, as well as infrared detectors16. For transistor applications, the small bandgap is detrimental, but, at scaled dimensions, quantum confinement effects are expected to increase the bandgap significantly (see Fig. 1). A significant increase in bandgap eliminates the major drawback of Te as a channel material for extremely scaled future transistors. Moreover, there has recently been an experimental demonstration of Te nanowires with a diameter down to 2 nm through the encapsulation in carbon nanotubes17.

Structurally, t-Te comprises one-dimensional (1D) helical chains of covalently bonded Te atoms (primary interaction). These Te-helices form a trigonal lattice through a mixture of covalent bonding and van der Waals (vdW) interactions (secondary interaction). The existence of the primary and secondary interactions and the overall helical t-Te structure are a consequence of Te comprising of six valence electrons18. Analogous to layered vdW materials, such as graphene19-21 and transition-metal dichalcogenides7,8,22, the vdW interactions between neighboring t-Te-helices readily yield two-dimensional (2D) and 1D nanostructures by exfoliation or a well-controlled growth.

Several low-dimensional phases of Te, such as monolayer Te, named Tellurene, have been investigated using first-principles density functional theory (DFT). A rich landscape of predicted phases has been uncovered by Zhu et al.23 (α, β, and γ), Liu et al.24 (δ and η), and Xian et al.25 (square Tellurene), where only the β-phase monolayer resembles bulk t-Te. The α, δ, and η phases were predicted to be more stable than the β-phase, with the η-phase being the most stable23,24. However, these alternative phases remain elusive since only layers of the bulk-like β phase have been successfully grown experimentally and used in field-effect transistors (FETs) so far24,10,11,12. Unfortunately, little is known about the relative stability of the bulk-like β-phase layers of Te compared to t-Te nanowires or what bandgaps are anticipated for tellurium nanostructures.

In this paper, we employ first-principles calculations within the DFT framework to compare and analyze the stability of various ideal pristine cases of t-Te nanostructures (nanowires and layers). We determine the bandgaps of t-Te nanowires and find that thin nanowires (<4 nm²) and few layers (<3 layers) of Te have bandgaps exceeding 1 eV, making t-Te a suitable channel material for extremely scaled FETs. We calculate formation energies, study the surface-to-volume ratios, and develop a simplified model to determine the
Fig. 1 Comparison of a 4 × 4 Si nanowire (0.83 nm side length) with a Te nanowire (1.2 nm side length). Both nanowires have comparable cross-sectional areas. We compute the bandgap of both structures as outlined in the “Methods” section. The silicon bandgap, exceeding 4 eV, will result in major challenges for transistor applications such as reduced mobility and contacting difficulty. A similar size tellurium nanowire has a well-suited 1.42 eV bandgap.

Electronic bandstructure

In Fig. 4, we show the conduction and valence band offsets, computed using a hybrid DFT scheme, including spin–orbit coupling (see Methods section), for all but our largest nanowires and many sheets of Te, where the computational burden becomes excessive. As explained in the “Methods” section, we use a hybrid DFT scheme that is known to vastly improve over standard DFT techniques for bandgap predictions. For example, the bulk Si bandgap is severely underestimated using standard DFT to be 0.6 eV, while the hybrid DFT technique we use predicts a much more accurate 1.2 eV bandgap (1.12 eV experiment)30. For bulk t-Te we find a hybrid DFT 0.26 eV bandgap, which is close to the experimentally measured 0.33 eV10 validating our use of hybrid DFT for Te. We found that the calculation for a single Te-helix in ref.17 does not employ hybrid functionals and underestimates the bandgap to be 1.51 eV compared to the 2.2 eV we obtained a 2 rotation about axis a, while triangular nanowires (Fig. 3a) only maintain the two screw axes. All structures maintain the vdW-linked helix structure, except for the monolayer sheet (Fig. 3g, l = 1). In the monolayer, helices are covalently bonded instead instead23,31–33.

We calculate the bulk t-Te lattice constants as $a_{\text{bulk}} = 4.40 \text{ Å}$ and $c_{\text{bulk}} = 5.93 \text{ Å}$, and the bulk intra-helix bond length as $d_{\text{bulk}} = 2.90 \text{ Å}$, which agrees with previous calculations23,34. The experimental bulk t-Te lattice constants are $a_{\text{exp}} = 4.45 \text{ Å}$ and $c_{\text{exp}} = 5.93 \text{ Å}$.

Table 1 shows the calculated lattice constants for the multi-layer sheets of Te, $a_{2D}$ and $c$, and the bond lengths $d$. The lattice constants and bond lengths quickly reach the bulk values with increasing sheet thickness with a deviation within 1% for three layers or more. In a monolayer sheet, that is, Te, neighboring helices are bound more tightly than in all other configurations. Tellurene has a secondary bond length of only 3.03 Å between nearest atoms in neighboring helices.

Table 2 shows the lattice constant along the helix axis (c), the quasi-lattice constants $\tilde{a}$ (defined in the Methods section), and the intra-helix covalent bond lengths $d$ for the various t-Te nanowires. For this case, the quasi-lattice constants are also within 1% of the bulk lattice constant, although they do not exactly approach the bulk values for the sizes we have simulated.

The lattice constants $a_{2D}$ (Table 1), the quasi-lattice constants $\tilde{a}$ (Table 2), and the bulk t-Te lattice constant (4.40 Å) all show: $\tilde{a} > a_{\text{bulk}} > a_{2D}$. t-Te nanowires and sheets of Te have a smaller lattice constant $c$ and intra-helix bond length $d$ than their respective bulk t-Te values.

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In Fig. 4a, a significant increase in bandgap is observed as quantum confinement effects become more pronounced for smaller nanowires. For the t-Te nanowires, the bandgaps range from 0.8 to 2.19 eV. For the Si nanowires, the bandgaps range from 1.7 to 4.0 eV. For sheets of Te, the bandgaps range from 0.64 to 1.43 eV. Comparing t-Te nanowires with the same number of Te-helices, the order of largest to smallest bandgaps proceeds from triangular, to rhomboid, to hexagonal nanowires.

Figure 5 shows the calculated bandstructures for monolayer and bilayer Te sheets and three t-Te nanowires ($N = 2$ hexagonal, $N = 3$ rhomboid, and $N = 4$ triangular) using the hybrid DFT scheme. Figure 5a shows that monolayer Te has a direct gap of 1.4 eV (located at $\Gamma$) and bilayer Te has an indirect bandgap of 1.2 eV. Figure 5b, d, and e shows that all three t-Te nanowires are indirect bandgap materials with bandgap values 0.98 eV (hexagonal), 1.1 eV (rhomboid), and 1.2 eV (triangular). Since bulk t-Te has a nearly direct bandgap, we expect nanowires with areas in excess of 6 nm² to have nearly direct bandgaps. As a comparison, all Si nanowires are direct bandgap (located at $\Gamma$) materials.

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To explain the different size scaling behavior of the electronic bandgap in t-Te, compared to a bulk material such as Si, we show
the dependence of the bandgap on the average number of helical neighbors per Te-helix in Fig. 6. We find that the bandgap linearly depends on $m$. Interestingly, this linear behavior also includes the edge cases of bulk and a single t-Te strand. This behavior agrees with previous findings in Selenene (2D monolayer Selenium) in ref. 37, where the authors highlight the dependence of the bandgap on the overlap of the bonding (valence band) and anti-bonding (conduction band) orbitals between adjacent Se helices rather than pure quantum confinement effects. Similarly, for t-Te, we see that increasing the number of interactions (overlaps) between neighboring Te-helices decreases the bandgap linearly. We note that, compared to Se, the Te bandgaps are smaller due to Te's stronger spin–orbit coupling (higher atomic mass).

Formation energy
Figure 7 shows the formation energies for all nanoribbons and t-Te nanowires. The nanowires have a lower formation energy compared to the nanoribbons for the same number of Te-helices (or total cross-sectional area). Hexagonal nanowires have the lowest formation energy. Rhomboid and triangular nanowires have the second and third lowest formation energies, respectively. The monolayer ribbons have an exceedingly high formation energy, while the bilayer and trilayer ribbons have formation energies closer, but still higher, than the nanowires.

| Name | $a_{2D}$ (Å) | $c$ (Å) | $d$ (Å) |
|------|-------------|---------|---------|
| 1-Layer | 4.22 | 5.61 | 2.77 |
| 2-Layer | 4.33 | 5.79 | 2.87 |
| 3-Layer | 4.36 | 5.84 | 2.87 |
| 4-Layer | 4.38 | 5.87 | 2.88 |
| 5-Layer | 4.39 | 5.88 | 2.88 |
| 6-Layer | 4.39 | 5.89 | 2.89 |
| 7-Layer | 4.40 | 5.90 | 2.89 |
| 8-Layer | 4.40 | 5.91 | 2.89 |
| 9-Layer | 4.40 | 5.91 | 2.89 |

Lattice constants $a_{2D}$ and $c$ and intra-helix bond lengths $d$ for multi-layer sheets of Tellurene.

*a1-Layer has a second bond length.
The exceedingly high formation energy of monolayer Te indicates that the experimental realization of monolayer Te without substrate support will be very unlikely. Interestingly, the formation energy cost is cut significantly for the bilayers and trilayers. We attribute this to the different fundamental structure of monolayer Te, shown in Fig. 3g. None of the known monolayer t-Te phases have clearly separated helices. The bilayer (L = 2) and trilayer (L = 3) do have distinguishable helices as illustrated in Fig. 3g. Interestingly, experimental growth also found that wires rather than layers are preferred, which agrees with our findings.

To understand the differences in the formation energies among the remaining nanostructures, we compute the surface-to-volume ratio for all t-Te nanowires and the bilayer and trilayer nanoribbons. The computed surface-to-volume ratios are shown in Fig. 8. Hexagonal nanowires have the lowest surface-to-volume ratio for the same number of Te-helices. This agrees with previous results in Fig. 7 where hexagonal nanowires have the lowest formation energy.

Unfortunately, surface-to-volume ratio does not explain all observed differences. For instance, bilayer and trilayer nanoribbons have a lower surface-to-volume ratio compared to the triangular nanowires when the nanoribbons have more than 14 and 27 helices, respectively. To explain the observation in Fig. 7, that nanowires always exhibit a lower formation energy compared to nanoribbons, we need an analysis going beyond simple surface-to-volume ratio considerations.

To this end, we propose an alternative model, based on the observation that nanostructures where Te-helices have more neighboring Te-helices have lower formation energies. In particular, Te-helices are “happy” when they have six helical neighbors, in which case their local environment resembles bulk t-Te. Nanowires will always have a higher ratio of “happy” helices to the total number of helices than Te nanoribbons.

To determine whether the number of neighboring helices is a good metric, we extract an energy penalty $\epsilon_m$ for a helix with a given number ($m \leq 6$) of missing neighboring helices. The energy penalty $\epsilon_m$ is given per unit cell. When all helices are missing, $m = 6$ and the energy penalty is the formation energy of a single helix unit cell. For $m \in \{0, 2, 3, 4\}$, the penalties are determined using an ordinary least-squares (OLS) fit on all the t-Te nanowires and nanoribbons under study, except for the structurally different monolayers. No structures were considered that contain a helix with $m = 1$ missing helical neighbors.

Figure 9 shows the resulting energy penalties per unit cell. Significant energy penalties of 0.80 to 0.40 eV are observed for helices with four to two missing helical neighbors. The maximum energy penalty for a helix without neighbors is 1.17 eV. The small value $\epsilon_0 = 0.01$ eV indicates that the OLS almost exactly reproduces the limit of bulk t-Te. Furthermore,
the energy penalties show remarkable linearity, where, on average, the energy penalty of removing a neighboring helix is ~0.20 eV. This linear scaling behavior in the energy penalty can be applied to similar trigonal vdW materials such as Selenium.

By applying these energy penalties to the nanostructures under consideration, we reproduce the order of largest to lowest formation energies, shown in Fig. 7. This demonstrates that the energy penalty picture (with a penalty due to missing neighboring helices), in contrast to the surface-to-volume ratio picture, captures correctly that t-Te nanowires have a lower formation energy compared to nanoribbon-like nanowires. The energy penalty picture also explains why hexagonal- and triangular-shaped nanowires have the lowest and highest formation energies among the nanowires. Therefore, the number of helical neighbors is a better metric for formation energy than surface-to-volume ratio in 1D vdW structures.

Considering experimental growth, we predict that growth of hexagonal nanowires will be favored. However, it is possible to envision that a surface interaction modifies the surface energy and makes surface helices “happier.” If this is the case, growth of nanowires with more missing helices can be anticipated. In the presence of such a favorable surface interaction, we expect triangular nanowires to form preferentially. This agrees with experiments where hexagonal- and triangular-shaped nanowires form under various conditions, while rhomboid-shaped nanowires are never observed38.

**METHODS**

First-principles calculations

We perform first-principles calculations with DFT as implemented in the Vienna Ab-initio Software Package (VASP) with projector augmented waves, a generalized gradient approximation using the exchange-correlation functional from Perdew–Burke–Ernzerhof (PBE)39,40, the vdW correction (DFT-D3) from Grimme, Ehrlich, and Krieg41, and a kinetic cutoff of 200 eV for the plane-wave basis set. For charge density calculations, the t-Te nanowires, the t-Te nanoribbons, the sheets of Te, and bulk t-Te calculations were performed using a 1 × 1 × 4, 1 × 1 × 4, 6 × 1 × 4, and 6 × 6 × 4 Monkhorst-Pack k-point sampling, respectively. Several studies23,24,31,34 indicate that there is “no a priori knowledge” in choosing the correct van der Waals correction. Based on a small-scale study, we found that the lattice constants change by <2% when using a different van der Waals correction (vdb-optB8843).

![](Fig. 5 Bandstructures of Tellurene sheets. a monolayer and bilayer sheets of Tellurene and the b N=2 hexagonal nanowire bandstructures. The c first Brillouin zone for sheets of Tellurene and the calculated bandstructures for d N=3 rhomboid and e N=4 triangular nanowires. The Fermi level is at 0eV. The arrows on the bandstructures indicate the conduction band minima and valence band maxima.)

**Fig. 6** Electronic bandgaps (E_g) of all t-Te nanowires and sheets of Tellurene with the average number of helical neighbors per helix m, calculated with HSE06 functionals, including spin–orbit interaction. The dotted lines represent a linear fit on the hexagonal, rhomboid, and triangular t-Te nanowires. We extrapolate the linear fit to cover the single helix, and the bulk t-Te domains, showing excellent agreement.
Calculations on bulk Si and all Si nanowires were performed with a 300 eV kinetic cutoff with Monkhorst-Pack k-point charge density sampling of 4 × 4 × 4 and 1 × 1 × 4, respectively.

To create t-Te nanowires, nanoribbons, and sheets of Te, we first construct supercells from the bulk t-Te atomic coordinates and lattice parameters. Next, we remove excess atoms, and pad with 10 Å of surrounding vacuum. We relax all structures until all forces are no <5 meV/Å. All relaxations use the PBE + DFT-D3 scheme.

The hybrid DFT schemes used HSE06 functionals for the conduction and valence band offsets. We incorporate spin–orbit coupling for all conduction and valence band offsets, and bandstructure calculations as implemented in VASP.

The formation energy is $E_f = E_{\text{tot}}/N_{\text{tot}} - \epsilon_{\text{bulk}}$, where $E_{\text{tot}}$ is the total ground state energy of a nanostructure, $N_{\text{tot}}$ is the total number of atoms per supercell of a nanostructure, and $\epsilon_{\text{bulk}}$ is the cohesive energy of bulk t-Te, which we calculate as $-3.40$ eV/atom.

Lattice constants and surface-to-volume ratio
To calculate the surface-to-volume ratio ($r$), we use the lattice constant in the periodic direction (c) in addition to a “quasi-lattice constant” ($\tilde{a}$) in the non-periodic directions.

The calculation of the quasi-lattice constant proceeds as follows: We select the three planes, perpendicular to the z-axis (crystal axis c) containing the Te atoms. Within each plane, we calculate the sum, and then average out all the nearest-neighbor distances $l_{ij}$ for each atom in the plane, where $i$ denotes the nearest-neighbor atom and $p$ denotes a plane. As a closed-form equation, the quasi-lattice constant is given by the average over the three planes:

$$\tilde{a} = \frac{1}{3} \sum_{p=1}^{3} \frac{N_p}{N} \sum_{i} l_{ij}.$$

where $N_p$ equals the total number of nearest-neighbor distances per plane. This formula averages distances across all three planes. If the entire structure retains the screw axes of bulk t-Te, then the averaging distances across one plane is sufficient. Figure 10 illustrates the methodology for the $N = 3$ rhomboid t-Te nanowire.

The surface-to-volume ratio for t-Te nanowires and nanoribbons is $r = A_s/V$, where $A_s$ is the lateral surface area and $V$ is volume (per supercell). Nanowire and nanoribbon volumes are $V = A_b c$, where $A_b$ is the
The data that support the findings of this study are available from the corresponding author upon request.

**CODE AVAILABILITY**

All data were generated using the VASP, and no custom computer code was employed.

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Fig. 10 Illustration of the calculation methodology of $\alpha$ for the $N = 3$ rhomboid nanowire. All green, blue, and red atoms are in separate planes. There are 16 distances to average to calculate $\alpha$ for the $N = 3$ rhomboid nanowire example.
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AUTHOR CONTRIBUTIONS
W.G.V. and C.L.H. conceived the project. A.K. performed the simulations and the results obtained were analyzed by A.K., M.L.V.de.P. and W.G.V. A.K. wrote the paper with all the authors contributing to the discussion and preparation of the manuscript.

COMPETING INTERESTS
The authors declare no competing interests.

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