Unraveling the dislocation core structure at a van der Waals gap in bismuth telluride

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Tetradymite-structured chalcogenides such as bismuth telluride (Bi\textsubscript{2}Te\textsubscript{3}) are of significant interest for thermoelectric energy conversion and as topological insulators. Dislocations play a critical role during synthesis and processing of such materials and can strongly affect their functional properties. The dislocations between quintuple layers present special interest since their core structure is controlled by the van der Waals interactions between the layers. In this work, using atomic-resolution electron microscopy, we resolve the basal dislocation core structure in Bi\textsubscript{2}Te\textsubscript{3}, quantifying the disregistry of the atomic planes across the core. We show that, despite the existence of a stable stacking fault in the basal plane gamma surface, the dislocation core spreading is mainly due to the weak bonding between the layers, which leads to a small energy penalty for layer sliding parallel to the van der Waals gap. Calculations within a semidiscrete variational Peierls-Nabarro model informed by first-principles calculations support our experimental findings.
Layered, tetradymite-structured chalcogenides are of tremendous technological interest due to the novel electronic and thermal transport properties that are imparted by their quasi-two-dimensional (2D), sheet-like structures. In such structures, thin sheets composed of several atomic layers weakly interact with each other by van der Waals forces across interlayer regions called van der Waals gaps. These materials have long been of great interest as thermoelectrics1–7 and, more recently, have been of intense focus in the context of topological insulators8–12. It is important to understand the nature of extended crystallographic defects, such as dislocations, in these materials. Dislocations are 1D topological defects in crystalline materials whose glide in certain crystallographic planes constitutes the main mechanism of plastic deformation13. A typical dislocation consists of a core region with large atomic displacements from perfect-lattice positions, and an elastic strain field extending deep into the surrounding crystal lattice. Dislocations in the layered chalcogenides are relevant to both the processing and functional properties of these materials. Polycrystalline bulk thermoelectrics have long been processed by thermomechanical means that introduce dislocations through plastic deformation in order to improve their densification and control their crystallographic texture14. Dislocations are also relevant in the context of chalcogenide nanostructures and epitaxial films, for which growth spirals and low-angle grain boundaries associated with threading dislocations are commonly reported15–17.

Dislocations in quasi-2D chalcogenides can also strongly affect functional properties of these materials by several mechanisms. For example, recent work has suggested that dislocations present at low-angle grain boundaries in Bi2Te3-based alloys effectively scatter phonons in the mid-frequency range18,19, providing a grain-boundary design strategy for engineering new materials with improved thermoelectric energy conversion efficiency. The core structure of the dislocations affects their mobility under applied mechanical stresses and thus the dislocation density in the microstructure, as well as the effectiveness of phonon scattering by individual dislocations. The large strain fields near dislocation cores can also affect the electronic band structure. For instance, scanning tunneling microscopy measurements near low-angle grain boundaries in Bi2Se3 thin films grown by the molecular beam epitaxy method have demonstrated shifts in the energy of the Dirac state, which were attributed to the large strain field extending deep across the van der Waals gap in Bi2Se3 strongly affects the atomic structure of the material has a rhombohedral crystal structure (R3m, a = 0.438 nm, c = 3.05 nm)26–28 consisting of hexagonal sheets of alternating bismuth and tellurium atoms stacked along the c-axis in 5-plane groupings, or quintuple layers, of the form Te(1)-Bi-Te(2)-Sb-Te(1). Three of such quintuple layers constitute a single unit cell. The van der Waals gap is parallel to the basal plane and corresponds to the region between abutting Te(1):Te(1) planes. The material is isomorphous with Sb2Te3 and Bi2Se3, which are typically alloyed with Bi2Te3 for thermoelectric applications4, and which are of interest in their own right as topological insulators10. All these materials fall within the broader class of tetradymite-type compounds29, which possess similar layered structures.

Previous work has identified two primary types of dislocation in Bi2Te3 and the isomorphous compounds: dislocations with Burgers vector, b, of type \( \frac{1}{2}(2110) \)30–34, which lies parallel with the basal plane (Fig. 1b, c), and those with b of type \( \frac{1}{2}(0111) \), which has a large component normal to the basal plane. The Burgers vector b characterizes the magnitude and direction of the lattice translation produced by the dislocation. Operationally, it is given by the closure failure, when mapped onto the perfect lattice, of an imaginary closed loop constructed around the region including the dislocation (the so-called Burgers circuit)13. We focus in this paper on the b = \( \frac{1}{2}(2110) \)-type dislocations as their structure is directly related to the fundamental interactions across the interlayer gap. Since this Burgers vector is parallel to the basal plane, the dislocations can glide on this plane under applied shear stresses.

The presence of \( \frac{1}{2}(2110) \) dislocations in Bi2Te3 has long been recognized. In fact, the pioneering electron microscopy study of \( \frac{1}{2}(2110) \) dislocation networks in Bi2Te3 and Sb2Te3 by Amelinkx and Delavignette30 and Delavignette and Amelinkx31 provided one of the first direct observations of dislocations in non-metallic materials. The assumption has long been that the cores of such dislocations would be localized at the van der Waals gap between the Te(1):Te(1) planes, where the bonding is weakest. Indeed, in situ observations of gliding dislocations in Bi2Te3-based alloys provide some evidence supporting this assertion18,23. Recently, Fu et al.34 have shown that the cores of \( \frac{1}{2}(2110) \) dislocations in Sb2Te3 are localized in the Te(1):Te(1) layers. However, direct proof of this localization in Bi2Te3 or detailed knowledge of the core structure of such dislocations have been missing. It was hypothesized31 that the core was dissociated into \( \frac{1}{2}(0110) \)-type Shockley partials by analogy with similar dissociation taking place.
in close-packed metals. However, the microscope resolution at the time did not permit the authors to test this hypothesis. As demonstrated in the present paper, the suggested dissociation into partials does not occur in Bi$_2$Te$_3$.

To directly determine the core structure of the $\frac{1}{3}$(2110) dislocations, we conducted an electron microscopic study of a polycrystalline sample of Bi$_2$Te$_3$ consolidated through a thermal process expected to produce dislocations. We employed the technique of high-angle annular dark-field (HAADF) scanning transmission electron microscopy (STEM), using a probe-corrected instrument operated at 300 keV (see Methods for further details). This technique allows the Te and Bi layers to be distinguished due to their large difference in atomic number. Figure 1d shows an atomically resolved HAADF-STEM image of Bi$_2$Te$_3$, revealing the atomic-plane positions on either side of the slip plane from the positions of {101} crystal planes, one of which terminates at the dislocation core. The scale bar represents 2 nm.

The image itself is projected along a (2110)-type orientation. Assuming that the line direction of the dislocation is along this projection, the Burgers vector is inclined by ±60° with respect to the dislocation line. Thus, the dislocation is of 60° mixed type, one of which terminates at the dislocation core. The scale bar represents 2 nm.

### Fig. 1 Crystallographic details of Bi$_2$Te$_3$ and the dislocation.

**a** Atomic arrangements in Bi$_2$Te$_3$. The space between the Te(1):Te(1) planes is the van der Waals gap. **b** Projection of the structure on the basal plane showing the Burgers vectors of dislocations. The unit cell is shaded in blue. The heavy black arrows show the Burgers vectors for the $\frac{1}{3}$(2110) -type perfect-lattice dislocations, whereas the smaller orange arrows show the $\frac{2}{3}$(1010) -type Burgers vectors that would result if Shockley partial dislocations were to form. **c** Orientation of the Cartesian axes relative to the dislocation line. **d** High-resolution transmission electron microscopy (HRTEM) image of Bi$_2$Te$_3$ projected along (2110) direction, showing the quintuple layers and the Burgers circuit construction for calculation of the dislocation Burgers vector (see Supplementary Note 2 for detail). The basal planes are horizontal and the yellow lines trace (1015) crystal planes, one of which terminates at the dislocation core. The scale bar represents 2 nm.
Calculation of the dislocation core structure. To understand the nature of the unusually wide and yet undissociated dislocation core, the gamma-surface on the basal plane was computed by first-principles DFT methods. The challenge of this calculation was that different exchange-correlation functionals available in the literature produce qualitatively different shapes of the gamma-surface, which in turn leads to different predictions of the detailed core structure. To arrive at definitive conclusions, several different DFT functionals were tested, including the local-density approximation (LDA)\(^{40}\), the non-local correlation functionals optPBE-vdW and optB88-vdW\(^{41-44}\) accounting for dispersion interactions, and the DFT-D2 functional\(^{45}\) introducing semi-empirical van der Waals corrections (see Methods for details). The gamma-surface was computed with each of these functionals (Fig. 3a). All functionals predict the existence of a stable stacking fault (SF) on the basal plane, which is obtained by a relative translation of the \(\text{Te}^{(1)}\) layers across the van der Waals gap. An SF is a planar (2D) defect of a crystal structure obtained by relative translation of two half-crystals to create the wrong stacking sequence of the crystal planes. While the translation vector corresponding to the local minimum of the fault energy \(\gamma_{\text{sd}}\) remains approximately the same, the depth of the minimum and the respective SF energy depend on the functional. The LDA approximation predicts a large SF energy and a shallow minimum, whereas the DFT-D2 functional predicts the lowest SF energy with a broad minimum surrounded by relatively high barriers.

Based on the computed gamma-surface \(\gamma(t)\), the disregistry function \(\delta(x)\) in the dislocation core region can be predicted theoretically using one of the Peierls–Nabarro-type models\(^{13,46}\). The classical Peierls–Nabarro model represents an edge dislocation by a continuous function \(\delta(x)\) satisfying the boundary condition \(\delta(\infty) - \delta(-\infty) = b\), where \(b\) is the magnitude of the Burgers vector. It additionally postulates a sinusoidal shape of the gamma-surface in the \(x\)-direction, which is not suitable for our purposes. Instead, we employed a semidiscrete variational Peierls–Nabarro (SDVPN) model\(^{47-49}\), which was properly generalized in this work to capture the elastic anisotropy of the \(\text{Bi}_2\text{Te}_3\) crystal structure. In this model, the disregistry \(\delta_i\) is a vector (with three components labeled by index \(i\)) and is evaluated at discrete values of \(x\) equally spaced by \(\Delta x\). The latter corresponds to a spacing of atomic columns parallel to the \(x\)-direction. The model can be applied to an arbitrary (mixed-type) dislocation. The dislocation core is represented by a discrete set of imaginary partial dislocations running parallel to the actual dislocation line. The core energy is the sum of the elastic strain energy arising from the interaction of the partial dislocations, plus the crystal misfit energy due to the core spreading. The latter contribution depends on the shape of the gamma-surface provided as input to the model. In the variational formulation of the model, the disregistry function \(\delta(x)\) is found by minimizing the total energy.
Further details of the model are described in the Supplementary Note 1.

**Discussion**

Figure 2c compares the SDVPN model predictions with the experimental disregistry function. We emphasize that the SDVPN calculations did not involve any fitting to experimental data. The immediate conclusion is that the model predicts the core shape in very reasonable agreement with experiment, confirming that the wide spread of the dislocation core is primarily due to the weak van der Waals bonding across the gap, not a result of dissociation into two discrete partials separated by a SF ribbon as in low SF energy face-centered cubic (FCC) metals. In the latter case, the disregistry function would have a well-pronounced flat region at the center of the core, which is not observed in Fig. 2c. This conclusion is additionally supported by the disregistry trajectories (Fig. 3a), showing the edge ($\delta_1$) and screw ($\delta_3$) components. The trajectories pass close to the SF position but never reach it, showing that a real SF ribbon does not form. (A similar situation with very narrow dissociation without the formation of a real SF ribbon is found in high SF energy FCC metals such as Al^{50}, but then the dislocation core is much more compact than in Bi$_2$Te$_3$).

A closer inspection of Fig. 2c reveals that the different exchange-correlation functionals utilized for the DFT gamma-surface calculations lead to slightly different shapes of the disregistry plots. The LDA approximation underestimates the core width, which is consistent with the prediction of the high SF energy (cf. Figure 3b). The optPBE-vdW and especially DFT-D2 functionals create a kink at the center of the core that is not supported by the experimental disregistry function within the statistical error bars. This kink arises from the relatively low SF energy and the wide separation of the energy barriers around the energy minimum (cf. Figure 3b). Thus, an additional outcome of the present calculations is that they provide a useful benchmark of the DFT functionals, pointing to optB88-vdW as an accurate model for van der
Waals materials such as Bi$_2$Te$_3$. The SF energy $\gamma_{sf}$ predicted by this functional is 46 mJ m$^{-2}$ (Supplementary Table 1).

These results indicate that the wide spreading of the dislocation core is primarily caused by the weak van der Waals bonding between the quintuple layers. This weak bonding results in the relatively low unstable SF energy $\gamma_{su} = 60$ mJ m$^{-2}$ (the maxima in Fig. 3b) compared to 65–200 mJ m$^{-2}$ or higher in FCC metals$^{51-54}$. In other words, the penalty for the translations of the layers parallel to the van der Waals gap in Bi$_2$Te$_3$ is relatively small. Perhaps, more importantly, the depth $(\gamma_{su} - \gamma_{sf})$ of the local energy minimum corresponding to the stable SF in Bi$_2$Te$_3$ is unusually small, about 10 mJ m$^{-2}$. For comparison, in Cu$_{4}Fe$ is about the same as in Bi$_2$Te$_3$ but $\gamma_{su}$ is about 160–180 mJ m$^{-2}$$^{51,54}$. As a result, the stable SF minimum is surrounded by much higher (about 100 mJ m$^{-2}$) energy barriers. These high barriers lead to the dissociation of the dislocation core structure into cleanly separated, discrete Shockley partials. As another comparison, the so-called MAX phases$^{56}$ also have a hexagonal layered structure, but the bonding between the layers is not van der Waals type. Unlike in Bi$_2$Te$_3$, the full dislocations in the basal plane dissociate into discrete Shockley partials separated by a SF$^{57}$. The energy minimum corresponding to the SF is relatively shallow, but the absolute values of all energies on the gamma-surface are at least an order of magnitude higher than in Bi$_2$Te$_3$, including the minimum depth $(\gamma_{su} - \gamma_{sf})$. Similarly, in Ti the prismatic SF along the $\{1120\}$ direction has a relatively shallow minimum, but the absolute values of all energies are significantly higher than in Bi$_2$Te$_3$.$^{58-60}$

The unique feature of the basal dislocations in Bi$_2$Te$_3$, and most likely in other tetradyline-structured chalcogenides, is the combination of the low unstable SF energy with the shallowness of the stable SF minimum. This combination prevents any significant localization of the dislocation content into partial dislocations. Even if such dislocations hypothetically formed, their cores would be wide and would strongly overlap, making the very concept of dissociation meaningless. Thus, despite the existence of a stable SF in the gamma-surface, the wide spreading of the dislocation core in Bi$_2$Te$_3$ is not accompanied by dissociation into two discrete partials. The core remains wide but undissociated. This important conclusion is supported by calculations within a semidirect Peierls–Nabarro model with input from DFT calculations, showing excellent agreement with experiment.

In summary, we have been able to resolve the detailed basal dislocation core structure in the layered chalcogenide Bi$_2$Te$_3$, and to quantify the atomic-plane disregistry across the dislocation core using atomic-resolution electron microscopy. The wide spreading of the dislocation core is mainly due to the weak, van der Waals type bonding between the quintuple layers of the structure, which leads to relatively low energy barriers for the SF formation and annihilation. As an additional finding, we have identified the exchange-correlation functional (optB88-vdW) that should be most appropriate for future dislocation modeling in Bi$_2$Te$_3$ and, by extension, other materials composed of van der Waals bonded atomic layers.$^{61}$ As discussed in the beginning of the paper, the dislocation core structure in Bi$_2$Te$_3$ can impact many functional properties of the material. As additional evidence, Supplementary Note 3 reports on preliminary DFT calculations of the electronic properties for an idealized SF in Bi$_2$Te$_3$. The results suggest that the SF is likely to affect the concentration of free charge carriers in the SF region. A more detailed analysis of the electronic structure on the variation of the disregistry on the basal plane would be a useful future step toward predicting the electronic properties of the actual basal plane dislocations in Bi$_2$Te$_3$ and related materials that exhibit a spread core.

### Methods

#### Experimental methodology.

The observations were conducted on polycrystalline Bi$_2$Te$_3$ material that had been initially consolidated by spark-plasma sintering and then further processed by hot extrusion. This extrusion technique is convenient for the present study since the deformation introduces dislocations and can drive a preferential crystallographic texture of (21T08)$^{62}$, which is an ideal imaging direction for atomically resolving the dislocation core and its displacements. The samples were extruded at $T = 750$ °C.$^{63}$ Following extrusion, the Bi$_2$Te$_3$ puck was subjected to extrusion to increase its density. During preparation, the puck was coated with a high temperature graphite lubricant to ensure smooth movement through the tooling. The tooling was heated to 400 °C and held at this temperature for 30 min to enhance Bi$_2$Te$_3$ plasticity during the extrusion treatment. The puck was then pressed through a tool steel die with a reduction ratio of 4:1 using a force of $\sim 10^4$ kg at a strain rate of 0.1 s$^{-1}$.

The Bi$_2$Te$_3$ specimen for electron microscopy analysis was thinned to electron transparency by mechanical grinding and dimpling, followed by Ar$^{+}$ ion milling using a Fischione Model 1010 ion milling system. The specimen was cooled during each milling using a liquid nitrogen stage. Analysis was conducted by HAADF-STEM using a probe-corrected 80–300 keV Titan instrument operated at 300 keV. Images were collected with the local grain region oriented along a (21T0)-type direction. In order to efficiently identify dislocations over a large field of view, initial imaging was conducted at low magnification with a scan sampling frequency and scan orientation selected to provide strong Moiré contrast from the dislocation. By imaging at low magnification, we also took care to ensure that the analyzed dislocations were chosen to be well separated from grain boundaries and other dislocations by a radius of at least 75 nm. After identifying and focusing on each dislocation from its Moiré image, higher magnification, atomic-resolution images were collected. Image analysis was conducted using ImageJ and custom routines written in MATLAB.

The disregistry across the dislocation slip plane was measured from the atomically resolved HRSTEM images. A total of six dislocations were analyzed from images with a sampling of 77 pixels/nm. Multiple images were analyzed for each dislocation (two images for one of the dislocations; two images each for the remaining five dislocations). We employed a template averaging and matching approach$^{64}$ to determine the atomic-plane positions on either side of the slip plane. We then computed the difference in these positions as a function of distance to determine the disregistry. An example illustrating the template matching approach is shown in Fig. 2a. In detail, the images were first digitally rotated to align the average (1015) plane orientation parallel with the horizontal image axis. Next, an initial, trial template region was defined by selecting a rectangular region of the image encompassing a single Te$(1+2)$–Bi$_2$Te$_3$(1+2)–Te$(1+2)$ unit along a (1015) plane. The trial template was then cross-correlated with the starting image. Image patches centered on the peaks in the cross-correlation function were then averaged to give a refined template pattern. Finally, the refined template pattern was cross-correlated with the starting image, and the peaks from this function were extracted to determine the atomic motif positions, and hence the local position (1015) planes on either side of the slip plane.

The disregistry at the slip plane was determined by projecting the (1015) planes from above and below the slip plane to the mid-plane between Te$(1+2)$–Bi$_2$Te$_3$(1+2) layers and calculating the distance between these intersections. Since the (1015) planes are aligned parallel with the $x$-axis of the analysis coordinate frame, the disregistry, $\delta = (u_x - u_x)\sqrt{1 + m^2}$, was calculated for each plane intersection from the equation

$$u_x - u_x = (y_x - y_x)\sqrt{1 + m^2} \tag{1}$$

where $y_x$ and $y_x$ are the $y$-coordinates of the motifs measured on the two sides of the slip plane. $m$ is the slope of the mid-plane line calculated by fitting lines to the motif positions on the sides of the slip plane and taking the average slope for these two lines.

#### Simulation methodology.

First-principles DFT calculations were performed using projector-augmented wave pseudopotentials as implemented in the electronic structure Vienna Ab initio Simulation Package$^{55,56}$. Gamma-surface calculations were performed using 6-quintuplet slabs, with changes in total energy obtained after translating the upper 3 quintuplets parallel to the hexagonal basal plane. The translation vector $\mathbf{T}$ sampled the lateral area of the conventional unit cell on a uniform 10 × 10 mesh. After each translation, the atomic positions were relaxed in the direction normal to the fault. The lateral lattice vectors (in Cartesian coordinates) $\mathbf{a}_1 = (a_1, 0, 0)$ and $\mathbf{a}_2 = (a_2/\sqrt{3}, 1, 0)$ and the initial atomic positions were obtained for the lattice parameter $a_0$ computed by relaxing forces and stresses for bulk Bi$_2$Te$_3$. Convergence with respect to the Brillouin zone sampling was achieved using a uniform 10 × 10 × 10 mesh. A smooth function $\gamma(x)$ was obtained by interpolating between the measured points using a multiquadratic radial basis function. Several exchange-correlation functionals were employed, namely, LDA$^{49}$, optPBE-vdW and optB88-vdW$^{41,42}$, and DFT-D$^{26}$. The lattice parameters and elastic constants obtained with these functionals are summarized in Supplementary Table 1 and are in good agreement with previous DFT calculations$^{67}$.

In the SDVPN model used here, the disregistry function $\delta(x)$ was discretized on a mesh $\{x_i\}_{i=1,\ldots, N}$ of $N = 300$ points with the spacing $\Delta x = a/\sqrt{3}$. The total
dislocation energy is \( E_{\text{dis}} = E_{\text{elastic}} + E_{\text{mobility}} \), where the elastic strain energy \( E_{\text{elastic}} \) depends on the energy coefficients \( C_i \) which in turn depend on the elastic constants \( C_{ijkl} \). The misfit energy \( E_{\text{mis}} = \sum_{\alpha} \gamma_0 \Delta x^\alpha \Delta x \) was obtained from the DFT gamma-surface. The equilibrium disregistry \( \delta(x) \) was found by numerical minimization of \( E_{\text{total}} \) under appropriate boundary conditions. As the initial guess, we used the arc tangent disregistry function predicted by the classical Peierls–Nabarro model. A continuous disregistry curve was obtained by smooth interpolation between the \( x^\alpha \) points. The calculations were performed separately for each of the DFT functionals. Further technical details of the SDVPN calculations can be found in the Supplementary Note 1.

**Data availability**

Calculations within the SDVPN model were implemented in Python and are openly available as part of the atomman Python package at https://github.com/unistigon/atomman. All data that support the findings of this study are available in the Supplementary Information file or from the corresponding author upon reasonable request.

Received: 8 October 2018 Accepted: 27 March 2019

**References**

1. Yin, W., Fitzer, E. & Rosi, F. Thermoelectric properties of Bi\(_2\)Te\(_3\)-Sb\(_2\)Te\(_3\)-SbSe\(_3\), pseudo-ternary alloys in the temperature range 77 to 300 K. J. Mater. Sci. 1, 52–65 (1966).
2. Bulman, G. et al. Superlattice-based thin-film thermoelectric modules with high cooling fluxes. Nat. Commun. 7, 1–7 (2016).
3. Chowdhury, I. et al. On-chip cooling by superlattice-based thin-film thermoelectric devices with high room-temperature figures of merit. Nat. Materials 4, 593–602 (2005).
4. Ye, H. et al. High efficiency thin film superlattice thermoelectric cooler modules enabled by low resistivity contacts. Adv. Electron. Mater. 4, 1700381 (2018).
5. Chen, Y. et al. Experimental realization of a three-dimensional topological insulator, Bi\(_2\)Te\(_3\). Science 325, 178–181 (2009).
6. Hasan, M. & Kane, C. Colloquium: topological insulators. J. Phys. Condens. Matter 22, 093201 (2010).
7. Heremans, J., Cava, R. & Samarth, N. Tetradymites as thermoelectrics and crystal lattice defects of Bi\(_2\)Te\(_3\) Pelletier device structures. Phys. Stat. Sol. (a) 187, 585–600 (2001).
8. Poudel, B. et al. High-thermoelectric performance of nanostructure bismuth telluride bulk materials. Science 340, 634–638 (2013).
9. Venkatasubramanian, R., Siivola, E., Colpitts, T. & O’Handley, R. L. Device modules enabled by low resistivity contacts. J. Phys. Condens. Matter 22, 1700381 (2010).
10. Dion, M., Rydberg, H., Schroder, E., Langreth, D. C. & Lundqvist, B. I. Van der Waals density functional for general geometries. Phys. Rev. B 88, 195131 (2013).
11. Medlin, D., Ramasse, Q., Spataru, C. & Yang, N. Structure of the (0001) basal plane boundary in Bi\(_2\)Te\(_3\). J. Appl. Phys. 108, 045317 (2010).
12. Vitek, V. Intrinsic stacking faults in body-centred cubic crystals. Philos. Mag. 18, 773–786 (1968).
13. Vitek, V. Theory of the core structures of dislocations in bcc metals. Cryst. Lattice Defects 5, 1 (1974).
14. Medlin, D., Ramaque, Q., Cattan, C. & Yang, N. Structure of the (0001) basal twin boundary in Bi\(_2\)Te\(_3\). J. Appl. Phys. 108, 045317 (2010).
15. Kohn, W. & Sham, L. J. Self-consistent equations including exchange and correlation effects. Phys. Rev. 140, A1133–A1138 (1965).
16. Bhogra, M., Ramamurty, U. & Waghmare, U. V. Temperature-dependent dislocation properties of aluminum. Philos. Mag. Lett. 83, 096102 (2009).
17. Klimeš, J., Bowler, D. R. & Michaelides, A. Chemical accuracy for the ab initio approaches. J. Chem. Phys. 135, 174105 (2011).
18. Klimeš, J., Bowler, D. R. & Michaelides, A. Stacking fault energy of face-centered cubic metals: a review for current opinion in solid and interface science. Curr. Opin. Colloid Interface Sci. 14, 226–235 (2009).
19. Liu, Y. et al. Tuning Dirac states by strain in the topological insulator Bi\(_2\)Se\(_3\). Nat. Phys. 10, 294–299 (2014).
20. Hao, G. et al. Spiral growth of topological insulator Sb\(_2\)Te\(_3\) nanoribbons. Appl. Phys. Lett. 101, 013105 (2012).
21. Fehrat, M., Tedena, J. & Nagojo, J. Mechanisms of spiral growth in Bi\(_2\)Te\(_3\) thin films formed by hot-wall epitaxy technique. J. Cryst. Growth 218, 250–258 (2000).
22. Kim, S. et al. Dense dislocation arrays embedded in grain boundaries for high-performance bulk thermoelectrics. Science https://doi.org/10.1126/science.aat6166, 109–114 (2015).
23. Park, J. & Lee, Y. High thermoelectric performance of Bi-Te alloy: defect engineering strategy. Curr. Appl. Phys. 16, 1202–1215 (2016).
24. Yang, W. et al. Tuning of topological Dirac states via modification of van der Waals gap in strained ultrathin Bi\(_2\)Se\(_3\) films. J. Phys. Chem. A 122, 23739–23748 (2018).
25. Hu, L. et al. Synergistic compositional-mechanical-thermal effects leading to a record high zT in n-type V\(_1\)V\(_1\) alloys through progressive hot deformation. Adv. Funct. Mater. 28, 1803617 (2018).
26. Jung, S. J. et al. Impurity-free, mechanical doping for the reproducible fabrication of the reliable n-type Bi\(_2\)Te\(_3\)-based thermoelectric alloys. Acta Mater. 150, 153–160 (2018).
56. Barsoum, M. W. The M$_{3AX_4}$Ax$_4$ phases: a new class of solids: thermodynamically stable nanolaminates. *Prog. Sol. State Chem.* **28**, 201–281 (2000).

57. Higashi, M., Momono, S., Kishida, K. & Okamoto, N. L. Anisotropic plastic deformation of single crystals of the MAX phase compound Ti$_3$SiC$_2$ investigated by micropillar compression. *Acta Mater.* **161**, 161–170 (2018).

58. Benoit, M., Tarrant, N. & Morillo, J. Density functional theory investigations of titanium surfaces and stacking faults. *Model. Simul. Mater. Sci. Eng.* **21**, 015009 (2013).

59. Closet, E., Caillard, D., Chaaari, N., Onimus, F. & Rodney, D. Dislocation locking versus easy glide in titanium and zirconium. *Nat. Mater.* **14**, 931–937 (2015).

60. Ready, A. J., Haynes, P. D., Rugg, D. & Sutton, A. P. Stacking faults and the surface on first-order pyramidal planes in α-titanium. *Philos. Mag.* **97**, 1129–1143 (2017).

61. Tawfik, S. A., Gould, T., Stampfl, C. & Ford, M. J. Evaluation of van der Waals density functionals for layered materials. *Phys. Rev. Mater.* **2**, 034005 (2018).

62. Miura, S. et al. Texture and thermoelectric properties of hot-extruded Bi$_2$Te$_3$ compound. *Mater. Sci. Eng. A* **277**, 244–249 (2000).

63. Zhang, Z., Sharma, P., Lavernia, E. & Yang, N. Thermoelectric and transport properties of nanostructure Bi$_2$Te$_3$ by spark plasma sintering. *J. Mater. Res.* **26**, 475–484 (2011).

64. Paciornik, S., Kilaas, R., Turner, J. & Dahmen, U. A pattern recognition technique for the analysis of grain boundary structure by HREM. *Ultramicroscopy* **62**, 15–27 (1996).

65. Kresse, G. & Furthmüller, J. Efficiency of ab-initio total energy calculations for metals and semiconductors using a plane-wave basis set. *Comput. Mater. Sci.* **6**, 15 (1996).

66. Kresse, G. & Joubert, D. From ultrasoft pseudopotentials to the projector augmented-wave method. *Phys. Rev. B* **59**, 1758 (1999).

67. Björkman, T., Golans, A., Krasheninnikov, A. V. & Nieminen, R. M. van der Waals bonding in layered compounds from advanced density-functional first-principles calculations. *Phys. Rev. Lett.* **108**, 235502 (2012).

**Acknowledgements**

Y.M. acknowledges support from the US Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering, the Physical Behavior of Materials Program, through Grant No. DE-FG02-01ER45871. The research at Sandia National Laboratories was developed with funding from the Defense Advanced Research Projects Agency (DARPA) (C.D.S.) and the Laboratory Directed Research and Development program (D.L.M. and N.Y.). Sandia National Laboratories is a multiprogram laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the US Department of Energy’s National Nuclear Security Administration under contract DE-NA0003525. This paper describes objective technical results and analysis. The views, opinions, and/or findings expressed are those of the authors and should not be interpreted as representing the official views or policies of the Department of Defense, Department of Energy, or the US Government. Certain commercial instruments, materials or processes identified in this paper to adequately specify the experimental procedure. Such identification does not imply recommendation or endorsement by the National Institute of Standards and Technology, nor does it imply that the instruments, materials, or processes identified are necessarily the best available for the purpose.

**Author contributions**

D.L.M. performed the TEM observations of the Bi$_2$Te$_3$ dislocations and measurements of the disregistry, and prepared a draft of the introduction and experimental part of the paper. N.Y. was responsible for processing the Bi$_2$Te$_3$ material used in this study. C.D.S. performed the DFT calculations and described the results and methodology, while L.M. conducted the calculations within the SDVPN model and prepared a draft of this part of the work. D.L.M. and Y.M. conceived this project and coordinated the collaborations among the co-authors. Y.M. produced an initial draft of the complete manuscript. All co-authors were engaged in discussions, contributed ideas at all stages of the work, participated in the manuscript editing, and approved its final version.

**Additional information**

Supplementary Information accompanies this paper at https://doi.org/10.1038/s41467-019-09815-5.

**Competing interests:** The authors declare no competing interests.

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