\beta\text{-}\text{As}_2\text{Te}_3$: Pressure-Induced 3D Dirac Semi-Metal

E. Lora da Silva,1,2,* A. Leonardo,3,4 Tao Yang,5 M. C. Santos,2 R. Vilaplana,6 S. Gallego-Parra,2 A. Bergara,7,4,8 and F. J. Manjón2

1IFIMUP, Departamento de Física e Astronomia, Faculdade de Ciências da Universidade do Porto, Porto, Portugal
2Instituto de Diseño para la Fabricación y Producción Automatizada, MALTA Consolider Team, Universitat Politècnica de València, València, Spain
3Departamento de Física Aplicada II, Universidad del País Vasco, UPV/EHU, Spain
4Donostia International Physics Center (DIPC), Donostia, Spain
5College of New Materials and New Energies, Shenzhen Technology University, Shenzhen, 518118, China
6Centro de Tecnologías Físicas: Acústica, Materiales y Astrofísica, MALTA Consolider Team, Universitat Politècnica de València, València, Spain
7Departamento de Física de la Materia Condensada, Universidad del País Vasco, UPV/EHU, Spain
8Centro de Física de Materiales CFM, Centro Mixto CSIC-UPV/EHU, Donostia, Spain

Abstract

We report a theoretical ab-initio study of \beta\text{-}\text{As}_2\text{Te}_3 (R\bar{3}m \text{ symmetry}) at hydrostatic pressures up to 12 GPa. We have systematically characterized the vibrational and electronic changes of the system induced by the pressure variation. The electronic band dispersions calculated at different pressures using the Quasiparticle Self-Consistent GW approximation (QSGW) show an insulator-metal transition. At room pressure the system is a semiconductor with small band-gap, and the valence and conduction bands present a parabolic conventional dispersion. However around 2 GPa the parabolic shape of the valence and conduction bands become linear and touch at the Fermi level. This means that this compound undergoes a pressure-induced topological phase transition to a 3D analog of graphene, known as a 3D Dirac semi-metal, with gapless electronic excitations protected by topology and symmetry. At increasing pressures the gap reopens and variation of the character of the electronic band-gap from direct to indirect is evidenced. At 7 GPa we observe the formation of a negative band-gap character, which persists for pressures up to 12 GPa. Topological insulating features are evidenced from 2 to 12 GPa with a Z_4=3 topological index. Moreover by investigating the lattice thermal-conductivity at different pressures, we observe an ultra low value of \kappa_1 at 300 K for 0.5 GPa (0.294 and 0.486 Wm\text{-1K\text{-1}} for the x-y-axis and for the z-axis, respectively), which is the result of existing low-frequency optical modes which increase the scattering rate of the acoustic phonons. At 2 GPa \kappa_L increases to 1.170 and 0.669 Wm\text{-1K\text{-1}}, for the x-y and for the z-axis, respectively. At 4 GPa the thermal-conductivity values between the two distinct crystallographic axis tend to approximate, with 1.495 and 1.433 Wm\text{-1K\text{-1}}, along the x-y-axis and the z-axis, respectively.

I. INTRODUCTION

Sesquichalcogenides A_2X_3 (X=S, Se, Te) of group-15 cations (A=As, Sb, Bi) with tetradymite (R\bar{3}m) symmetry have stimulated enormous research activity, because of their exceptional thermoelectric properties. Moreover, these systems have attracted even more attention due to their unique fundamental properties since Bi_2Se_3, Bi_2Te_3 and Sb_2Te_3 were discovered to be 3D topological insulators with a single Dirac cone on the surface. This type of compounds represents a new class of material with metallic electronic states and topologically protected metallic surface states due to time-reversal symmetry and strong spin-orbit interaction; and these could be applied to spintronics and quantum computation. Most of the studies performed on the tetradymite-like A_2X_3 sesquichalcogenides have been applied to compounds with Sb and Bi species; much less attention has been paid to the As-based compounds. These latter systems do not tend to crystallize in the tetradymite structural phase at ambient conditions due to the strong lone electron pair (LEP) stereo-activity of the As cation. In particular, at room conditions As_2Te_3 crystallizes in the monoclinic C2/m phase (\alpha\text{-}As_2Te_3), showing some interesting properties and applications, including efficient thermoelectric properties, electrical threshold and memory switching properties for phase change memory (PCM) devices (similar to other group-14 and group-15 chalcogenides). More recently it has been observed incredible mechanical properties of As_2Te_3 with potential applications for superstretchable membranes. As_2Te_3 is also very interesting since it has the ability to display rich polymorphism, such as the metastable tetradymite structure (\beta\text{-}As_2Te_3) and the low-temperature phase with P21/m symmetry (\beta\text{'-}As_2Te_3). In particular, several theoretical studies have addressed the structural, electronic and mechanical properties of \beta\text{-}As_2Te_3 at room conditions and it has been shown that this phase also displays good thermoelectric properties. Moreover, recent calculations show that \beta\text{-}As_2Te_3 exhibits other interesting properties, i.e PCM, which are also related to topological insulator (TI) features. Such properties are the result of an unconventional bonding mechanism known as “metavalent bonding”. Finally, another major interest in \beta\text{-}As_2Te_3 is the possibility of finding a pressure-induced...
electronic topological transition (ETT)\textsuperscript{7}, which can result in a significant enhancement of respective thermoelectric properties.\textsuperscript{7} Very few high-pressure (HP) studies have been devoted to understand the properties of As\textsubscript{2}Te\textsubscript{3} \textsuperscript{2,7} \textsuperscript{α}-As\textsubscript{2}Te\textsubscript{3} has been shown to undergo a trivial semiconductor-metal transition above 4 GPa followed by a phase transitioning directly to a monoclinic structure (phase \textgamma\textsuperscript{7} S.G. \textit{C2/c}) above 13 GPa: and not to the \textbeta phase, as it had previously been observed by using uniaxial stress.\textsuperscript{7} Moreover, several isostructural phase transitions (IPTs) have also been suggested.\textsuperscript{7,7} As regards to the \textbeta-As\textsubscript{2}Te\textsubscript{3} phase, the strength of the spin-orbit coupling of As is smaller than that of A\textsubscript{2}Te\textsubscript{3} (A=Sb, Bi) due to the lighter mass of As. The transition from a trivial band insulator to a TI would thus require HP application on the \textbeta-As\textsubscript{2}Te\textsubscript{3} system, according to a theoretical study that shows that uniaxial strain could cause a quantum topological phase transition (QTPT) from a band insulator to a TI state at 1.8 GPa.\textsuperscript{7} Another theoretical study have shown that application of isotropic strain,\textsuperscript{7} enables an overlap of the electronic bands at the Fermi level (\textDelta V/V \sim -7\%), accompanied by a metallic state transition, characteristic of an electronic topological phase transition.\textsuperscript{7}

Finally, it must be stressed that from first-principles calculations performed on the rhombohedral tetradyomite structure of Sb\textsubscript{2}Se\textsubscript{3} (a polymorph of Sb\textsubscript{2}Se\textsubscript{2} that has not yet been experimentally reported), have shown that this compound should evidence a pressure-induced QTPT,\textsuperscript{7} thus transitioning from a trivial semiconductor to a 3D topological Dirac semi-metal (3D TDS).\textsuperscript{7}

In this work, we report a first-principles study of the electronic, vibrational and thermal-conductivity properties of \textbeta-As\textsubscript{2}Te\textsubscript{3} under hydrostatic compression, ranging between 0 and 12 GPa. We further show that this compound undergoes a pressure-induced QTPT around 2 GPa, in which a linear-type dispersion is observed at the \textGamma-point, evidencing a transition from a trivial insulator to a 3D Dirac semi-metal. This feature corresponds to a TI behaviour and which TI persists above this pressure. We also compute the lattice thermal-conductivity at three different pressure ranges, in order to compare the influence of hydrostatic pressure to \kappa\textsubscript{L} and compare the results of the obtained low values to the phonon lifetimes and low-frequency optical phonon modes.

II. THEORETICAL FRAMEWORK

The structural properties calculations were performed within the pseudopotential plane-wave DFT\textsuperscript{7} framework implemented in the Vienna Ab-initio Simulation Package (VASP) code.\textsuperscript{7} The semi-local generalized-gradient approximation functional with the Perdew-Burke-Ernzerhof parametrization revised for solids (PBEsol)\textsuperscript{7} was employed for the structural relaxations, lattice dynamics and thermal-conductivity calculations. Projector augmented-wave (PAW)\textsuperscript{7} pseudopotentials were used to treat semi-core electronic states, with the As[4s\textsuperscript{2}4p\textsuperscript{3}] and Te[5s\textsuperscript{2}5p\textsuperscript{4}] electrons being included in the valence shell. The starting point for our calculations was a full structural relaxation of the \textit{R\textipa{3}m} phase, performed with a plane-wave kinetic-energy cut-off of 800 eV. The electronic Brillouin-zone (BZ) was sampled with a \Gamma-centred Monkhorst-Pack mesh\textsuperscript{7} and defined with 14×14×14 subdivisions.

The theoretical background regarding the harmonic lattice-dynamics calculations is presented in Refs.\textsuperscript{7,7} and therefore it will not be detailed in the present work. Lattice-dynamics calculations were performed using the supercell finite-displacement method implemented in the Phonopy software package,\textsuperscript{7} with VASP used as the 2nd order force-constant calculator.\textsuperscript{7} Calculations of the phonon supercell size were carried out on 2×2×2 expansions of the primitive-cell. The phonon frequencies were sampled on an interpolated 50×50×50 \textit{q}-point mesh (tetrahedron method) when evaluating the phonon density of states (DoS) and vibrational internal energy and entropy.

The lattice thermal-conductivity and phonon lifetimes were calculated by employing the Phonopy package,\textsuperscript{7} and VASP is used as the calculator for the third-order (anharmonic) interatomic force-constants. A 2×2×2 supercell is used, with a \textit{q}-mesh of 50×50×50 with the tetrahedron method to perform the integration for the phonon lifetime calculation. The phonon lifetimes were computed with the single-mode relaxation-time approximation, to solve the Boltzmann transport equations.

Calculations to obtain the electronic band-structure for different pressure values were performed using the Questaal (formerly LMSuite) package. Questaal is an all-electron implementation of density-functional theory and the quasiparticle self-consistent form (\textit{QSGW}).\textsuperscript{7} The basis-sets applied to expand the wavefunctions are defined with a combination of smoothed Hankel functions and augmented plane-waves, known as the Plus Muffin-Tin (PMT) basis-sets.\textsuperscript{7} Spin-orbit coupling (SoC) was included for all electronic structure calculations.

For the \textit{QSGW} calculations the BZ was sampled using the tetrahedron method\textsuperscript{2} with a sampling mesh of 6×6×6 subdivisions. The plane-wave cut-off for the interstitial charge density (GMAX) was defined with a 6 Ry cut-off radius. For the \textit{QSGW} calculation the G-vector cut-offs for the interstitial part of the eigenfunctions and the Coulomb interaction matrix were set to 6.0 and 5.4 Ry, respectively.

III. RESULTS AND DISCUSSION

The obtained relaxed lattice parameters for the PBEsol+SoC calculation are shown in Table I together with other calculations from the literature as well as experimental values. Our results are found to be consistent with the rest of the calculations and overestimate the value of \textit{c} \textsubscript{0} by 3.58\% resulting in a larger unit-cell...
volume when compared to the experiments. For visualization purposes the unit-cell is shown in (Fig. 1).

Similar overestimation of lattice parameters where found with PBEsol+SoC calculations for isostructural Sb$_2$Te$_3$.\cite{Scheidemantel2017}

A. Electronic Band Structure as a function of Pressure

We have calculated the electronic band dispersions of β-As$_2$Te$_3$ (represented in $R3m$ reciprocal space-group) for different pressures values, ranging from 0 GPa up to 12 GPa (Figs. 3, 7, and 14), by employing the QSGW method (Tab. II and Fig. 2). The pressure-dependant structures were previously minimized using VASP with PBEsol+SoC, and serve as input for the QSGW calculations.

At 0 GPa (Fig. 3 we observe that the conduction band minimum (CBM) and the valence band maximum (VBM) are positioned along the high-symmetry segment Z-F with an indirect character, which we will hereafter denote as the Z'-point. The gap width is around 0.304 eV, making β-As$_2$Te$_3$ a small gap semiconductor at room conditions. These results differ from previous DFT@PBE calculations,\cite{Morin2015} where a direct band gap was observed to be 0.30 eV; where similar results are observed for Morin et al.\cite{Morin2015} Curiously enough, Pal and Waghmare\cite{Pal2015} show that at vanishing strain, the VBM and the CBM are located along different directions in the BZ evidencing an indirect band-gap around 0.22 eV; with direct band-gap of around 0.35 eV. These latter calculations have been performed by employing an all-electron full potential linearized augmented plane wave (FP-LAPW) technique, with the PBE functional, and by considering SoC effects. Moreover, Deng\cite{Deng2016} reports a direct band-gap with 0.24 eV of width, and positioned at the Γ-point: respective calculations were carried out with the PBE functional and ultrasoft pseudopotentials. For comparison we must note that our QSGW direct gap at the Γ point is found to be slightly higher with 0.45 eV. For comparison we must note that our QSGW direct gap at the Γ point is found to be slightly higher with 0.45 eV.

Scheidemantel\cite{Scheidemantel2017} has also found a direct gap for β-As$_2$Te$_3$ of 0.12 eV with FP-LAPW basis-sets and the PBE functional, while Sharma\cite{Sharma2016} found an indirect gap along Z-F direction of 0.22 eV by employing similar methodologies.

The differences observed in the character and width of the band-gaps are mainly dependent and sensitive to the applied methodologies, and therefore the differences of obtained results. In this context we must note that by applying one-shot GW calculations the band-gap character of Sb$_2$Te$_3$ has also shown different conclusions. While Lawal et al.\cite{Lawal2018} show a direct band-gap at Gamma (0.22 eV), Nechaev and co-workers\cite{Nechaev2015} have observed an indirect band-gap along Z'-Γ.

When pressure increases we observe variations not only of the electronic band dispersions, but also of the band-gap character and width. At around 1 GPa the gap starts to decrease (0.192 eV) and the CBM moves towards the Γ-point. Therefore, at 1 GPa the indirect character of the band-gap (Z'-Γ) is similar to that found for Sb$_2$Te$_3$ at 0 GPa.\cite{Scheidemantel2017}

An interesting feature occurs around 2 GPa, where we observe a direct gap at the Γ-point which closes forming a linear dispersion behavior. This feature is consistent with a previous study that found that the application of an uniaxial strain in the Z-direction of 1.77 GPa induces the system to pass through a Weyl metallic state with a single Dirac cone in its electronic structure at the Γ-point.\cite{Scheidemantel2017} Our calculations therefore evidence a pressure-induced quantum topological transition from a semiconductor-to-semi-metal, making β-As$_2$Te$_3$ a 3D Dirac semi-metal under hydrostatic pressure. These results can be compared to those found for Cd$_3$As$_2$\cite{Scheidemantel2017} a system which has attracted intensive research interest as an

| References | $a_0$(Å) | $c_0$(Å) | $V_0$(Å$^3$) |
|------------|---------|---------|-------------|
| present (PBEsol) | 4.096 | 30.592 | 444.46 |
| GGA\cite{Lawal2018} | 4.089 | 30.297 | 438.76 |
| optB88-vdW\cite{Nechaev2015} | 4.075 | 30.306 | 435.79 |
| PBE\cite{Deng2016} | 4.102 | 29.745 | 433.40 |
| Experiment 1\cite{Nechaev2015} | 4.047 | 29.498 | 418.395 |
| Experiment 2\cite{Sharma2016} | 4.0473 | 29.5018 | * |

Figure 1. Crystal structure of β-As$_2$Te$_3$ in the hexagonal unit-cell representation (the rhombohedral primitive-cell is represented in shaded green).
archetypical Dirac semi-metal, hosting three-dimensional linear-dispersive electronic bands close the Fermi level.\footnote{1}

We can argue that the observed ETT (Lifshitz type) is another interesting feature of high-pressure physics. It was firstly predicted by I. Lifshitz in 1960\footnote{2} as the existence of 2,5-order phase transitions possibly due to a topological change of the Fermi surface under special conditions. Across the ETT transition, there would be singularities in the third derivatives of the thermodynamic potentials at which the topological transition occurs.\footnote{3}

When the pressure over the system is increased beyond the 2 GPa value, calculations show that the gap reopens and it gradually transforms its character from direct to indirect. The VBM is positioned between the Γ-Z segment, which we will define as the Z"-point. At around 7 GPa we observe the formation of a negative band-gap character (-0.081 eV), which persists for pressures up to 12 GPa. Such results are consistent with discussion of Refs. \footnote{4} and \footnote{5}. Both report a band inversion with parity reversal of states close to the Fermi level, either by employing uniaxial compression ($\Delta V/V \sim -$7%) or isotropic stress ($\Delta V/V \sim -$5%), respectively. From the present calculations, hydrostatic pressure at $\sim$ 7 GPa would correspond to a higher compression with $\Delta V/V \sim$ -14.64%.

From Fig 3 we also show the contribution of the As-$p$ and Te-$p$ states to the dispersion curves. At 0 GPa the valence band are mostly dominated by the $p$-states of Te atoms (blue dispersion curves), whereas the conduction band are mostly As-$p$ states (red dispersion curves). By further increasing the pressure to values close to the Dirac semi-metal transition ($\sim$ 2.0 GPa) we observe that some As states start appearing at the high-symmetry Z-point, which are more evident at 7 GPa, when the band-inversion is observed. Moreover, at around the ETT transition a fraction of As states can be observed at the VBM, at the Γ-point. At 4 GPa, when the gap reopens we observe that the small fraction of the As-states persist at the Γ-point.

In order to confirm the possibility of inversion of states for the different pressure values, we have performed a topological analysis of the eigenvalues at the high-symmetry K-points by employing the Check Topological Materials Tools as detailed in Ref. \footnote{6} . We then obtain a set of irreducible representations at each maximal K-vec. Then, using the compatibility relations and the set of Elementary Band Representations (EBRs), it is possible to probe whether the set of bands can be linearly combined as EBRs (Tabs. III and in Sup. material IV, V, VI, VII, VIII, IX.).

The topology analysis performed on our system determines that in the 0-2 GPa range we have a trivial insulator; while for pressures above 2 GPa $\beta$-As$_2$Te$_3$ belongs to a strong topological class with $Z_4$=3 topological index (Tab. III). These systems are known as Split Elementary Band Representations (SEBR). The bands directly below and above the Fermi level form a EBR, with a topological band-gap.\footnote{7} SEBRs can be tuned either to be topologically nontrivial insulators or to be semi-metals. Dirac semi-metals are three-dimensional phases of matter with gapless electronic excitations and are protected by topology and symmetry, with well-defined 3D massless charge carriers. As three-dimensional analogs of graphene, these systems have generated much recent interest. Currently, intrinsic Dirac semi-metals are found among the following systems: Bi$_{1-x}$Sb$_x$,\footnote{7} Cd$_3$As$_2$\footnote{7} and Na$_3$Bi.\footnote{7}

Their characteristic electronic properties lead to protected surface states and novel responses to applied electric and magnetic fields.\footnote{7} The $\beta$-As$_2$Te$_3$ system therefore can be compared to prototypical graphene with large spin-orbit coupling where the valence band maximum (VBM) and conduction band minimum (CBM) touch at the Fermi level; this is what we observe at 2 GPa (Fig. 14), which corresponds to $\Delta V/V \sim$ -7.30%.

Since the effect of pressure can be mimicked by the

| Pressure [GPa] | Character (VBM-CBM) |
|--------------|-------------------|
| 0.0          | Indirect (Z"-Z')  |
| 1.0          | Indirect (Z"-Γ)   |
| 1.7          | Direct (Γ-Γ)      |
| 2.0          | Direct (Γ-Γ)      |
| 2.2          | Direct (Γ-Γ)      |
| 2.5          | Indirect (Z"-Γ')  |
| 3.0          | Indirect (Z"-Γ')  |
| 4.0          | Indirect (Z"-Γ')  |
| 5.0          | Indirect (Z"-Γ')  |
| 6.0          | Indirect (Z"-Γ')  |
| 7.0          | Indirect (Z"-Γ')  |
| 8.0          | Indirect (Z"-Γ')  |
| 9.0          | Indirect (Z"-Γ')  |
| 10.0         | Indirect (Z"-Γ')  |
| 12.0         | Indirect (Z"-Γ')  |

Figure 2. The QSGW+SoC band-gap as a function of pressure of $\beta$-As$_2$Te$_3$. 

Table II. QSGW+SoC electronic band-gap character for different pressure values.
effects of chemical doping, this opens the possibility of obtaining a Dirac semi-metal close to room conditions when introducing impurities to $\beta$-As$_2$Te$_3$.

It is noteworthy of mentioning that the Dirac cones for the present system only occurs at the $\Gamma$-point, unlike what is observed for other 3D Dirac semi-metals, e.g. Cd$_3$As$_2$, Na$_3$Bi, ZrTi$_5$ and bP. Therefore, Kohn anomalies can only occur at the BZ center. This feature would inhibit any Fermi-surface nesting and thus no Peierls distortion can appear for this $R3m$ compound.

### Table III.

| Pressure [GPa] | Topological Indices | Topological Class |
|---------------|---------------------|-------------------|
| 0.0           | Trivial Insulator   | -                 |
| 0.5           | Trivial Insulator   | -                 |
| 1.0           | Trivial Insulator   | -                 |
| 2.0           | $x_{2u,1}=0$ $x_{2u,2}=0$ $x_{2u,3}=0$ $x_{4i}=1$ | 1                 |
| 3.0           | $x_{2u,1}=0$ $x_{2u,2}=0$ $x_{2u,3}=0$ $x_{4i}=1$ | 1                 |
| 4.0           | $x_{2u,1}=0$ $x_{2u,2}=0$ $x_{2u,3}=0$ $x_{4i}=3$ | 1                 |
| 8.0           | $x_{2w,1}=0$ $x_{2w,2}=0$ $x_{2w,3}=0$ $x_{4i}=3$ | 1                 |
| 10.0          | $x_{2w,1}=0$ $x_{2w,2}=0$ $x_{2w,3}=0$ $x_{4i}=3$ | 1                 |

### B. Lattice Dynamics

#### 1. Phonon Dispersion Curves

The primitive-cell of As$_2$Te$_3$ contains five atoms: Te(1) occupying the 3a Wyckoff position, and Te(2) and As(1) both at 6c. The eigenvectors corresponding to the 3D atomic displacements of each atom will therefore total 15 modes, with the three acoustic IR-active modes formed by the irreducible representations of $\Gamma_{\text{acoustic}} = A_{2u} + E_u$ and the remaining 12 optical modes being $\Gamma_{\text{optical}} = 2E_g$ (Raman) + 2$A_{1g}$ (Raman) + 2$E_u$ (IR) + 2$A_{2u}$ (IR).

Figs. 4, 5 and 15 (and in Suppl Mat. in Sec. V B) show the phonon dispersion curves (PDC) of $\beta$-As$_2$Te$_3$ for different pressure values. We observe that the system presents dynamically stability up to 12 GPa. We must note however that at 0 GPa a small localized instability is observed at the high symmetry $Z$-point, which corresponds to the out-of-phase displacements between the As inter-layer atoms (Fig. 6; breathing mode). Such an instability persists for increasing convergence parameters (supercell size, $k$-point mesh), therefore conclud-
ing that the observed negative mode is not a numerical feature of the employed methodology. A similar imaginary mode at the same high-symmetry point has been reported by Vaney et al. at 0 K and 0 GPa for β-As$_2$Te$_3$. By increasing the pressure up to 0.5 GPa the negative frequency observed at the Z-point hardens, allowing the system to evidence dynamically stable at this pressure range. Moreover, the low-frequency phonon branches along the Γ-Z-F segment are relatively soft for low pressure values. By increasing the pressure the phonon branches located along these mentioned segments show a considerable increase in frequency and the abrupt gradient variations (kinks with abrupt drop of frequencies) tend to fade away at high pressure, namely along Γ-Z and the F-point.

Since the tetradymite structure is stable at room conditions, as demonstrated by several studies performed for this compound, we infer that the instability observed at 0 GPa at the Z-point is related to not considering the anharmonic effects for the lattice-dynamics calculations. Such effects would probably tend to stabilize the rhombohedral structure of As$_2$Te$_3$ at 0 GPa, thus suggesting that the anharmonic contributions are very important for this compound, namely at low pressures. Further calculations by including this effect should be considered to fully characterize the vibrational properties of β-As$_2$Te$_3$, however.

Figure 4. Phonon dispersion curves of β-As$_2$Te$_3$ for pressure values between 0 and 1 GPa.

Figure 5. Phonon dispersion curves of β-As$_2$Te$_3$ for pressure values between 1.5 and 2 GPa.

Figure 6. Eigenvectors associated to the negative mode at Z-point represented in the unit-cell of β-As$_2$Te$_3$. The red arrows correspond to motions of the As atom, the blue and purple arrows correspond to motions of the Te(1) and Te(2) atoms, respectively.

Figure 7. Phonon dispersion curves of β-As$_2$Te$_3$ for pressure values between 2.2 and 3.5 GPa.
this study is out of the scope of the present study.

It has been observed in other related works, that the soft phonon modes can be potentially induced by a Kohn anomaly (frequency kink/dip in the phonon dispersion at certain high symmetry points) which are associated with the topological singularities of Dirac nodes, in analogy to similar effects found for graphene\(^7\) and other Weyl semi-metals.\(^7\) A discontinuity of the derivative of the dispersion relation is observed, when an abrupt change in the electronic screening of lattice vibrations by conduction electrons occurs (anomalies of the dielectric tensors).

The Kohn anomaly is one of the most important anomalies also observed for \(d\)-block transition metals.\(^7\) The lattice vibrations are partly screened by virtual electronic excitations on the Fermi surface. This screening can change rapidly at certain wave-vector points of the Brillouin-zone so the phonon energy can vary abruptly with the wave-vector. Consequently, it usually shows a singularity or sharp dip in the phonon dispersions and a maximum in the phonon linewidth (inverse of the phonon lifetimes and detailed in Subsec. III B 3). It is believed that the Kohn anomaly can efficiently affect the superconductivity of some conventional superconductors, the lattice-dynamical instability, and the formation of spin density-waves in elemental metals.\(^7\)

It must be stressed that the observed Kohn anomalies occur at \(q=2k_F\), where \(k_F\) is the wave-vector where the Dirac cones appear. For the case of \(\beta\)-As\(_2\)Te\(_3\), the Dirac cones appear at the \(\Gamma\) point \((k_F=0)\), therefore the Kohn anomalies are only expected to occur at the zone-center. In fact, the lowest optical mode at the \(\Gamma\)-point, \(E_u\) (IR-active; Fig 8) shows a minimum frequency around 1.33 THz between 1.0 and 1.7 GPa (Fig. 10), while it increases at other pressure values. Moreover at 1.6 GPa a dip (discontinuity) is observed for which the mode increases up to 1.5 GPa, however decreasing afterwards. The second observed soft-mode, \(E_g\) (Fig ??), which is Raman-active, presents lowest frequency at 0 GPa, at 1.54 THz, increasing with ongoing pressure up to 1.79 THz at 3.0 GPa.

The presence of these soft modes, namely the \(E_u\) mode, can be seen as an evidence for the appearance of a 3D TDS for \(\beta\)-As\(_2\)Te\(_3\) at relatively low pressures, similarly as to what occurs for black phosphorus.\(^7\) It is also noteworthy of mentioning that, in agreement with our calculations, the Dirac cones are also formed at the \(\Gamma\)-point for the rhombohedral Sb\(_2\)Se\(_3\) system, for pressures close to 3 GPa.\(^7\)

We emphasize here that the present calculations can only capture the Kohn anomaly due to static electronic screening of lattice vibrations, while a full treatment including dynamic screening effect will require the calculation of dynamic electron-phonon coupling, which is out of the scope of the present work.

2. Phonon Partial Density of States

We have computed the phonon density of states (PDoS) where the atomic contributions of the three inequivalent sites are evidenced (Fig 11), namely Te(1) (3a site) and Te(2) and As(1) (both at 6c site). We show the PDoS as a function of pressure up to 4 GPa. We note that the phonon dispersion curves of the \(\beta\) phase (at 0 GPa) exhibits very low frequency modes, which do not exceed 6.0 THz, as to what occurs for the monoclinic phase of As\(_2\)Te\(_3\) (\(\beta'\)).\(^7\)
We observe that the Te(2) phonon states are quite localized around 3 THz, with large densities. These densities would correspond to interactions with the six neighboring As atoms. At 0.5 GPa, a small peak shoulder is observed around 2 THz which tends to delocalize towards lower frequencies for increasing pressures. At around 4 GPa respective states start to localize between 1 and 2 GPa.

For lower frequencies (below 2 GPa) we observe low frequency densities, namely dominated by the As and Te(1) elements. These would correspond to interactions with the six neighboring As atoms. At 0.5 GPa, a small peak shoulder is observed around 2 THz which tends to delocalize towards lower frequencies for increasing pressures. At around 4 GPa respective states start to localize between 1 and 2 GPa.

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It has been claimed that Kohn anomalies are indicative of structural instabilities. Indeed our calculations for $\beta$-As$_2$Te$_3$ show that the system is dynamically unstable at room pressure (Fig. 4). The low-energy phonons mainly at the Z-point clearly show that $\beta$-As$_2$Te$_3$ is indeed metastable above 0.5 GPa. Such a metastable state can lead to lower values of the lattice thermal-conductivity than that obtained when $\beta$-As$_2$Te$_3$ is a 3D TDS (around 2 GPa). Therefore, this work may pave the way to search for structural instabilities which occur in 3D TDS by tuning different parameters such as temperature, pressure, chemical composition, in order to search for the best conditions to obtain the lowest thermal conductivity compatible with the highest ZT value.

Moreover, we have to state that heavy atoms have low vibrational frequencies which consequently result in a low lattice thermal-conductivity. These tend to also exhibit large spin–orbit coupling necessary for certain nontrivial topological materials. In addition, TIs often have a small electronic band-gap as they lie in the vicinity of a strain dependent ETT which aids in tuning the intrinsic carrier concentration to optimize the thermal-conductivity.

Materials with resonant bonding (lead chalcogenides, SnTe, Bi$_2$Te$_3$, Bi and Sb) commonly evidence long-ranged interactions. Long-ranged interactions may be another cause for optical phonon softening, strong anharmonic scattering and large phase space for three-phonon scattering processes, for which such features can explain the reason why rocksalt IV–VI compounds have much lower thermal-conductivity than the zincblende III–V
It has been observed through first-principles calculations, that long-ranged interactions are significant in IV–VI materials owing to the strong resonant bonding resonance or hybridization between different electronic configurations.

In order to further understand the intrinsic lattice thermal-conductivity as a function of applied pressure, we have also calculated the frequency-dependent phonon lifetimes at 0.5 GPa, 2 GPa and 4 GPa (Fig. 13), all at 300 K. In principle the anharmonicity of a material will be inversely related to the phonon lifetime, and larger anharmonicity will result in lower lattice thermal-conductivity.

We find that the frequency-dependent phonon lifetimes of $\beta$-As$_2$Te$_3$ at 300K and 0.5 GPa is very short, roughly located below 0.5 ps; much lower than those found for SnSe (from 0 to 30 ps). In the mid-frequency region a larger density of phonons are located between 1.5 THz and $\sim$ 4.2 THz with maximal value at 0.2 ps. The small lifetimes of the phonons indicate a strong scattering rate, which is the main reason for the low lattice thermal-conductivity at this pressure range. At 2 GPa (Fig. 12.b), the lifetimes increase to higher values reaching 5.0 ps. The larger density of phonons are more localized and concentrated around 2.5 and 4.0 THz, with maximal value located below 2.0 ps. The densities scattered between 1 and 2 THz are related to the soft-modes which are the main source of low lattice thermal-conductivity due to the Kohn anomalies, and these evidence larger lifetimes. At 4 GPa the larger density is located between 3.5 and 4 GPa, similarly as to what occurs for 2 GPa, however with larger lifetimes (roughly below 4 ps). The larger lifetimes are observed at 8 ps and are mainly the contribution of phonons ranging between 2 and 3 THz.

IV. CONCLUSIONS

We have theoretically investigated the electronic properties, phonon dispersion curves and the lattice thermal-conductivity of $\beta$-As$_2$Te$_3$ as a function of pressure. We show the pressure-variation QSGW electronic band dispersions (gap character and width). More interestingly we observe a semiconductor to semi-metal electronic topological transition at 2 GPa, where a Dirac cone is formed at the $\Gamma$-point. At this pressure range, and by conducting a topological analysis, we observe that $\beta$-As$_2$Te$_3$ belongs to a strong topological class characterized with a topological band-gap, protected by topology and symmetry, with well-defined 3D massless charge carriers. This feature persists up to 10 GPa; however at 7 GPa (up until 12 GPa) an inversion of the band-gap is observed, where inversion of states occur close to the Fermi level.

Moreover, we have investigated the lattice dynamics and lattice thermal-conductivity of $\beta$-As$_2$Te$_3$ for different pressure points. We have identified the existence of two soft optical phonons ($E_u$ and $E_g$) at the zone-center associated to the Kohn anomaly associated with the Dirac nodes close to 2 GPa. Unlike other 3D TDS systems, however similarly to what is observed for other compounds with $R3m$ structure, $\beta$-As$_2$Te$_3$ does not show Kohn anomalies at the zone-boundaries; these are only observed at the Brillouin-zone center. This feature will inhibit the appearance of any type of Peierls distortion, as recently been questioned for related pure tetradymite-like materials.

Based on the observation of the soft modes, we explained that the low lattice thermal-conductivity is caused by the optical soft-modes which enhance the phonon-phonon scatterings, in a similar manner as to what occurs for the prototypical Dirac semi-metal Cd$_3$As$_2$, ZrTe$_5$ and Na$_3$Bi. By comparing the lattice thermal-conductivity at three different pressure points related to the ETT: before, at the transition point and after the ETT, we find that mainly at 0.5 GPa the lattice
Figure 13. Calculated phonon lifetimes of $\beta$-As$_2$Te$_3$ at 300K for 0.5 GPa (left), 2.0 GPa (middle) and 4.0 GPa (right). The color shades represent the phonon density, where darker shades refer to higher phonon densities.

thermal-conductivity is very low.
V. APPENDIX

A. Electronic Band Structure as a functions of Pressure

B. Phonon Dispersion Curves for Pressures above 4 GPa

C. Topological Data

Table IV. Band representations ordered by energy with respect to the Fermi level, and respective degeneracies below the Fermi level for the trivial insulator system at 0.0 and 0.5 GPa.

| Level | Γ | Z | F | L |
|-------|---|---|---|---|
| 1     | 5+6(2) | 5+6(2) | 2(2) | 3(2) |
| 2     | 8+9(2) | 8+9(2) | 3(2) | 2(2) |
| 3     | 5+6(2) | 5+6(2) | 3(2) | 3(2) |
| 4     | 8+9(2) | 8+9(2) | 2(2) | 2(2) |
| 5     | 5+6(2) | 5+6(2) | 3(2) | 3(2) |
| 6     | 8+9(2) | 8+9(2) | 2(2) | 2(2) |
| 7     | 8+9(2) | 8+9(2) | 3(2) | 3(2) |
| 8     | 8+9(2) | 5+6(2) | 2(2) | 2(2) |
| 9     | 5+6(2) | 7(2)  | 2(2) | 2(2) |
| 10    | 7(2)  | 8+9(2) | 3(2) | 3(2) |
| 11    | 4(2)  | 4(2)  | 3(2) | 3(2) |
| 12    | 8+9(2) | 8+9(2) | 2(2) | 2(2) |
| 13    | 7(2)  | 7(2)  | 2(2) | 2(2) |
| 14    | 8+9(2) | 5+6(2) | 2(2) | 2(2) |

Table V. Band representations ordered by energy with respect to the Fermi level, and respective degeneracies below the Fermi level for the system at 2.0 GPa.

| Level | Γ | Z | F | L |
|-------|---|---|---|---|
| 1     | 5+6(2) | 5+6(2) | 2(2) | 3(2) |
| 2     | 8+9(2) | 8+9(2) | 3(2) | 2(2) |
| 3     | 5+6(2) | 5+6(2) | 3(2) | 3(2) |
| 4     | 8+9(2) | 8+9(2) | 2(2) | 2(2) |
| 5     | 5+6(2) | 5+6(2) | 3(2) | 3(2) |
| 6     | 8+9(2) | 8+9(2) | 2(2) | 2(2) |
| 7     | 8+9(2) | 8+9(2) | 3(2) | 3(2) |
| 8     | 8+9(2) | 5+6(2) | 2(2) | 2(2) |
| 9     | 7(2)  | 8+9(2) | 3(2) | 3(2) |
| 10    | 4(2)  | 4(2)  | 3(2) | 3(2) |
| 11    | 8+9(2) | 8+9(2) | 3(2) | 3(2) |
| 12    | 7(2)  | 8+9(2) | 2(2) | 2(2) |
| 13    | 7(2)  | 7(2)  | 2(2) | 2(2) |
| 14    | 5+6(2) | 5+6(2) | 2(2) | 2(2) |

Table VI. Band representations ordered by energy with respect to the Fermi level, and respective degeneracies below the Fermi level for the topological insulator system at 4.0 GPa.

| Level | Γ | Z | F | L |
|-------|---|---|---|---|
| 1     | 5+6(2) | 5+6(2) | 2(2) | 3(2) |
| 2     | 8+9(2) | 8+9(2) | 3(2) | 2(2) |
| 3     | 5+6(2) | 5+6(2) | 3(2) | 3(2) |
| 4     | 8+9(2) | 8+9(2) | 2(2) | 2(2) |
| 5     | 5+6(2) | 5+6(2) | 3(2) | 3(2) |
| 6     | 8+9(2) | 8+9(2) | 2(2) | 2(2) |
| 7     | 8+9(2) | 8+9(2) | 3(2) | 3(2) |
| 8     | 5+6(2) | 5+6(2) | 2(2) | 2(2) |
| 9     | 7(2)  | 8+9(2) | 3(2) | 3(2) |
| 10    | 4(2)  | 4(2)  | 3(2) | 3(2) |
| 11    | 8+9(2) | 8+9(2) | 3(2) | 3(2) |
| 12    | 7(2)  | 7(2)  | 2(2) | 2(2) |
| 13    | 5+6(2) | 5+6(2) | 2(2) | 2(2) |
| 14    | 5+6(2) | 5+6(2) | 2(2) | 2(2) |

Table VII. Band representations ordered by energy with respect to the Fermi level, and respective degeneracies below the Fermi level for the topological insulator system at 8.0 GPa.

| Level | Γ | Z | F | L |
|-------|---|---|---|---|
| 1     | 5+6(2) | 5+6(2) | 2(2) | 3(2) |
| 2     | 8+9(2) | 8+9(2) | 3(2) | 2(2) |
| 3     | 5+6(2) | 5+6(2) | 3(2) | 3(2) |
| 4     | 8+9(2) | 8+9(2) | 2(2) | 2(2) |
| 5     | 5+6(2) | 5+6(2) | 3(2) | 3(2) |
| 6     | 8+9(2) | 8+9(2) | 2(2) | 2(2) |
| 7     | 8+9(2) | 8+9(2) | 3(2) | 3(2) |
| 8     | 5+6(2) | 5+6(2) | 2(2) | 2(2) |
| 9     | 7(2)  | 8+9(2) | 3(2) | 3(2) |
| 10    | 4(2)  | 4(2)  | 3(2) | 3(2) |
| 11    | 8+9(2) | 8+9(2) | 3(2) | 3(2) |
| 12    | 7(2)  | 7(2)  | 2(2) | 2(2) |
| 13    | 5+6(2) | 5+6(2) | 2(2) | 2(2) |
| 14    | 5+6(2) | 5+6(2) | 2(2) | 2(2) |

Table VIII. Band representations ordered by energy with respect to the Fermi level, and respective degeneracies below the Fermi level for the topological insulator system at 10.0 GPa.

| Level | Γ | Z | F | L |
|-------|---|---|---|---|
| 1     | 5+6(2) | 5+6(2) | 2(2) | 3(2) |
| 2     | 8+9(2) | 8+9(2) | 3(2) | 2(2) |
| 3     | 5+6(2) | 5+6(2) | 3(2) | 3(2) |
| 4     | 8+9(2) | 8+9(2) | 2(2) | 2(2) |
| 5     | 5+6(2) | 5+6(2) | 3(2) | 3(2) |
| 6     | 8+9(2) | 8+9(2) | 2(2) | 2(2) |
| 7     | 8+9(2) | 8+9(2) | 3(2) | 3(2) |
| 8     | 5+6(2) | 5+6(2) | 2(2) | 2(2) |
| 9     | 7(2)  | 8+9(2) | 3(2) | 3(2) |
| 10    | 4(2)  | 4(2)  | 3(2) | 3(2) |
| 11    | 8+9(2) | 8+9(2) | 3(2) | 3(2) |
| 12    | 7(2)  | 7(2)  | 2(2) | 2(2) |
| 13    | 5+6(2) | 5+6(2) | 2(2) | 2(2) |
| 14    | 5+6(2) | 5+6(2) | 2(2) | 2(2) |
Figure 14. QSGW+SoC electronic band structure of $\beta$-As$_2$Te$_3$ for different pressure values.

Table IX. Topological character of translation equivalent subgroups for the system at 2.0, 4.0 and 8.0 GPa, where we present the number and symbol of the space group, the transformation matrix, the possibility of forming linear combinations of the elementary band representations (EBR) below the Fermi level (the system is a topological insulator if one cannot form EBRs). Minimal subgroups are highlighted in the table.

| Symmetry Group | Transformation matrix | EBR | Topological Indices |
|----------------|-----------------------|-----|---------------------|
| $P1$           | $2/3,1/3,1/3,1/3,-1/3,-1/3,1/3,1/3,1/3,0,0,0$ | yes | $z_{2w,1}=0$ $z_{2w,2}=0$ $z_{2w,3}=0$ $z_4=3$ |
| $P-1$          | $2/3,1/3,1/3,1/3,-1/3,-1/3,1/3,1/3,1/3,0,0,0$ | no  | $z_{2w,1}=0$ $z_{2w,2}=0$ $z_{2w,3}=0$ $z_4=3$ |
| $R3$           | $1.0,0,0,1,0,0,0,1,0,0,0$ | yes | $z_{2w,1}=0$ $z_{2w,2}=0$ $z_{2w,3}=0$ $z_4=3$ |
| $R-3$          | $1.0,0,0,1,0,0,0,1,0,0,0$ | no  | $z_{2w,1}=0$ $z_{2w,2}=0$ $z_{2w,3}=0$ $z_4=3$ |
Figure 15. Phonon dispersion curves of $\beta$-As$_2$Te$_3$ for pressure values between 4 and 9 GPa.

Figure 16. Phonon dispersion curves of $\beta$-As$_2$Te$_3$ between 10 and 12 GPa.
VI. ACKNOWLEDGEMENTS

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