Small compressive strain-induced semiconductor–metal transition and tensile strain-enhanced thermoelectric properties in monolayer PtTe₂

San-Dong Guo¹ and Yan Wang²

¹ School of Physics, China University of Mining and Technology, Xuzhou 221116, Jiangsu, People’s Republic of China
² School of Physics and Electronic Engineering, Jiangsu Normal University, Xuzhou 221116, Jiangsu, People’s Republic of China

E-mail: guosd@cumt.edu.cn

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Abstract

Biaxial strain effects on the electronic structures and thermoelectric properties of monolayer PtTe₂ are investigated by using generalized gradient approximation (GGA) plus spin–orbit coupling for the electron part and GGA for the phonon part. Calculated results show that a small compressive strain (about −3%) can induce semiconductor-to-metal transition, which can easily be achieved in experiment. Band convergence in the conduction bands is observed for unstrained PtTe₂, which can be removed by both compressive and tensile strain. Tensile strain can give rise to band convergence in the valence bands by changing the position of the valence band maximum, which can induce an enhanced Seebeck coefficient, and bring about high power factors. It is found that tensile strain can also reduce lattice thermal conductivity. More specifically, the lattice thermal conductivity at a strain of 4% can decrease by about 19% compared to the unstrained case at room temperature. According to the tensile strain effects on ZTₑ and lattice thermal conductivity, tensile strain can indeed improve the p-type efficiency of thermoelectric conversion. Our results demonstrate the potential of strain engineering in PtTe₂ for applications in electronics and thermoelectricity.

Keywords: strain, semiconductor–metal transition, power factor, lattice thermal conductivity

1. Introduction

Due to their potential applications in electronic and energy conversion devices, two-dimensional (2D) materials have been widely investigated both in theory and experiment [1–4]. Since the discovery of graphene, great efforts have been made to explore 2D materials, such as hexagonal boron nitride [5], germanene, silicene [6], phosphorene [7], group IV–VI compounds [8] and transition-metal dichalcogenides (TMDs) [9]. The TMD monolayer MoS₂ possesses an intrinsic direct band gap of 1.9 eV in comparison with the gapless graphene, which has been applied in field-effect transistors, photovoltaics and photocatalysis [10–12]. The thermoelectric properties related to MoS₂ have also been widely investigated [13–16]. The dimensionless figure of merit, \( ZT = S^2\sigma T/(\kappa_e + \kappa_L) \), can measure the efficiency of thermoelectric conversion in which \( S \), \( \sigma \), \( T \), \( \kappa_e \) and \( \kappa_L \) are the Seebeck coefficient, electrical conductivity, working temperature, and electronic and lattice thermal conductivities, respectively. It has been demonstrated that strain engineering is a very effective approach to tuning band structure and transport properties in MoS₂ [17–19].

Recently, the TMD monolayer PtSe₂ has been epitaxially grown with high-quality single crystal, and the local Rashba
spin polarization and spin-layer locking have been proved by spin- and angle-resolved photoemission spectroscopy, which has potential applications in electrically tunable spintronics and valleytronics [20, 21]. Biaxial strain effects on electronic structures and thermoelectric properties in monolayer PtSe\textsubscript{2} have also been investigated [22, 23], and tensile strain can improve thermoelectric properties by enhancing the power factor ($S^2\sigma$) and reducing lattice thermal conductivity ($\kappa_l$). Among PtX\textsubscript{2} (X = S, Se and Te) monolayers, PtTe\textsubscript{2} monolayer has the smallest energy band gap [24], which means small strain may induce semiconductor-to-metal transition, and has the largest lattice constant $a$ [24], which implies low lattice thermal conductivity according to the reduced lattice thermal conductivity induced by tensile strain in PtSe\textsubscript{2} [23].

Here, we investigate the biaxial strain dependence of the electronic structures and thermoelectric properties of monolayer PtTe\textsubscript{2} by first-principle calculations and Boltzmann transport theory. It has been proved that spin–orbit coupling (SOC) has important effects on electronic structures and power factors in semiconducting TMD monolayers [19, 23, 24]. Therefore, the electron part is performed using both the generalized gradient approximation (GGA) and SOC, while the lattice part is calculated using GGA. It is found that the energy band gap first increases, and then decreases from compressive to tensile strain, which is in excellent agreement with the strain dependence of the energy band gap of other semiconducting TMD monolayers, such as MoS\textsubscript{2} [17, 19] and PtSe\textsubscript{2} [22, 23]. Calculated results show that the spin–orbit splitting at the Γ point, Se-Se bond length and Se-Pt-Se bond angle monotonically decrease, while the Pt-Se bond length monotonically increases. Compressive strain can easily induce semiconductor-to-metal transition as a result of enhanced orbital overlap and hybridization. Tensile strain can induce band convergence in the valence bands by valley degeneracies, which leads to an improved Seebeck coefficient, producing enhanced $ZT_c$. Tensile strain can also reduce lattice thermal conductivity, which has been found in monolayer PtSe\textsubscript{2} [23] and ZrS\textsubscript{2} [25]. Therefore, tensile strain can indeed achieve enhanced thermoelectric properties.

The rest of the paper is organized as follows. In the next section, we shall give our computational details. In the third section, we shall present the strain dependence of the electronic structures and thermoelectric properties of monolayer PtTe\textsubscript{2}. Finally, we shall give our discussions and conclusions in the fourth section.

2. Computational detail

The first-principles calculations are carried out based on density functional theory [26] as implemented in the Wien2k package [27] within the full-potential linearized augmented-plane-waves method. For monolayer MoS\textsubscript{2}, the local-density approximation (LDA) gap of 1.86 eV is very close to the experimental value of 1.9 eV [28]. The GGA gaps of monolayer MoSe\textsubscript{2} (1.44 eV) and WSe\textsubscript{2} (1.56 eV) are very close to the experimental values of MoSe\textsubscript{2} (1.55 eV) and WSe\textsubscript{2} (1.64 eV) [29]. So, LDA or GGA should be suitable for semiconducting TMD monolayers MX\textsubscript{2} (M = Zr, Hf, Mo, W and Pt; X = S, Se and Te) to calculate the energy band gap. Here, the GGA of Perdew, Burke and Ernzerhof (GGA-PBE) [30] is used as the exchange-correlation potential to investigate the electronic structures of PtTe\textsubscript{2}. The SOC was included self-consistently for the electron part [31–34]. The 6000 k-points are used in the first Brillouin zone (BZ) for the self-consistent calculation. The free atomic position parameters are optimized using GGA-PBE with a force standard of 2 mRy au\textsuperscript{-1}. The harmonic expansion up to $l_{\text{max}} = 10$ is used in each of the atomic spheres, and $R_{\text{mt}} * k_{\text{max}} = 8$ is used to determine the plane-wave cutoff. The charge convergence criterion is used, and when the integration of the absolute charge-density difference between the input and output electron density is less than 0.0001|e| per formula unit, the self-consistent calculations are considered to be converged.

Transport calculations are carried out within the BoltzTraP code [35], which has been applied successfully to several materials [36–38]. Since accurate transport coefficients need sufficient k-points, the energy band structures are calculated using 65 × 65 × 11 k-point meshes (50000 k-points) in the first BZ. For 2D materials, larger values should usually be chosen for the LPFAC parameter. Here, we choose a LPFAC value of 20 to achieve the convergence results. Phonon frequencies are obtained by the Phonopy code [39] using a $5 \times 5 \times 1$ supercell with $8 \times 8 \times 1$ Monkhorst-Pack k-meshes. The lattice thermal conductivities are calculated within the linearized phonon Boltzmann equation, which can be achieved by using Phono3py+VASP codes [40–43]. The second-order harmonic and third-order anharmonic interatomic force constants are calculated by using a $4 \times 4 \times 1$ supercell and a $3 \times 3 \times 1$ supercell, respectively. To compute lattice thermal conductivities, the reciprocal spaces of the primitive cells are sampled using the $30 \times 30 \times 3$ meshes. It should be noted that the calculated electrical conductivity, electronic and lattice thermal conductivities of 2D materials depend on the length of the unit cell used in the calculations along the z-direction [44]. To compare these quantities of various 2D materials, the same thickness of 2D materials should be adopted, or the sheet thermal conductance should be used [44].

3. Main calculated results and analysis

The monolayer PtTe\textsubscript{2} is composed of three atomic sublayers with a Pt sublayer sandwiched between two Te sublayers, and the schematic crystal structure is shown in figure 1. The unit cell of monolayer PtTe\textsubscript{2} used in the calculations, containing two Te atoms and one Pt atom, is constructed with a vacuum region larger than 15 Å to avoid spurious interaction, and the optimized lattice constant is $a = 4.02$ Å within GGA-PBE. The GGA (LDA) is suitable for crystal structure, so the lattice constants and lattice thermal conductivity are calculated using GGA. For materials containing heavy elements, the SOC can
produce important effects on electronic structures, so the SOC should be included. This treatment can be found in many references. For example, in topological insulator Sb$_2$Se$_3$ [45], the lattice constants are predicted by GGA, while the electronic structures are performed by GGA+SOC. It has been proved that the SOC has important effects on both the electronic structures and thermoelectric properties of semiconducting TMD monolayers [19, 23, 24]. Therefore, the GGA+SOC is employed to investigate the strain dependence of electronic structures and thermoelectric properties in monolayer PtTe$_2$. The unstrained PtTe$_2$ is an indirect gap semiconductor with a gap value of 0.38 eV. The valence band maximum (VBM) and conduction band minimum (CBM) of unstrained PtTe$_2$ appear at the Γ point and between the Γ and M points, respectively. The corresponding energy band structure is shown in figure 2.

Both theoretically and experimentally, strain effects on the electronic structures of semiconducting TMD monolayers have been widely studied [13, 17, 19, 22, 23, 25], some are predicted to produce semiconductor-to-metal phase transition if suitable strain is applied. The strain can be simulated by defining $\varepsilon = (a - a_0)/a_0$, where $a_0$ is the unstrained lattice constant optimized by GGA-PBE, with $\varepsilon < 0$ ($>0$) being the compressive (tensile) strain. The energy band structures of monolayer PtTe$_2$ with strain changing from $-4\%$ to $10\%$ are plotted in figure 2 using GGA+SOC. The energy band gap, spin–orbit splitting value at the Γ point between the first and second valence bands, Pt-Se (Se-Se) bond length and Se-Pr-Se bond angle versus biaxial strain $\varepsilon$ using GGA+SOC are shown in figure 3. With strain changing from compressive to tensile, the energy band gap first increases, and then decreases, which has been found in many semiconducting TMD monolayers, such as MoS$_2$ [17, 19], ZrS$_2$ [25] and PtSe$_2$ [23]. It is noteworthy that low compressive strain (about $-3\%$) can induce semiconductor-to-metal phase transition, which is less than the critical strain of the semiconductor-to-metal phase transition of other 2D materials [17, 22, 25]. As the tensile strain increases, the CBM moves toward lower energy, while the VBM changes from the Γ point to the one along the Γ–M direction. When the VBM appears at one point along the Γ–M direction, the VBM and valence band extrema (VBE) along the Γ–K direction are almost degenerate, which can give rise to important effects on the Seebeck coefficient. With increasing compressive strain, the CBM moves from the point along the Γ–M direction to the one along the Γ–K direction. When the strain reaches about $-3\%$, both the VBM and CBM cross the Fermi level, inducing semiconductor-to-metal phase transition, which is due to enhanced orbital overlap and hybridization by reduced Pt-Se bond length. For MoS$_2$, the band gap is sensitively dependent on the S-S or Mo-S bond length and the S-Mo-S bond angle [46]. The S-S bond length and S-Mo-S bond angle monotonically decrease with increasing strain ($\leq \pm 10\%$), while the Mo-S bond length monotonically increases. Similarly, the Se-Se bond length and Se-Pr-Se bond angle monotonically decrease with the increasing strain considered in the calculations, and the Pt-Se bond length monotonically increases. When the strain increases from $-4\%$ to $10\%$, the spin–orbit splitting at the Γ point monotonically decreases from 0.66 eV to 0.13 eV. This trend of spin–orbit splitting versus strain is the same as that of monolayer PtSe$_2$ [23], while it is the opposite of that of MoS$_2$ [19].

As is well known, band convergence, including orbital and valley degeneracies, is a very effective strategy to improve the Seebeck coefficient, and hence to enhance the power factor [47]. The band convergence can be achieved by strain in many 2D materials, such as MoS$_2$, PtSe$_2$ and black phosphorus [19, 23, 48]. According to energy band structures with different strain as shown in figure 2, unstrained PtSe$_2$ nearly has a valley degeneracy of 4 due to the convergence of two conduction band extrema along the Γ–M and Γ–K directions, which produces the largest n-type Seebeck coefficient (absolute value). Tensile strain can lead to the convergence of VBE along the Γ–M and Γ–K directions, which can lead to an enhanced p-type Seebeck coefficient. Next, the transport coefficients are calculated based on the constant scattering time approximation Boltzmann theory within the rigid band approach, being effective for low doping levels [49–51]. The n-type doping (negative doping level) with the negative Seebeck coefficient can be simulated by shifting the Fermi level into conduction bands, while the p-type doping (positive doping level) with positive Seebeck coefficient can be achieved by making the Fermi level move into valence bands.

To address the enhanced power factor induced by tensile strain, the tensile strain dependence of Seebeck coefficient $S$, electrical conductivity with respect to scattering time $\sigma/\tau$ and power factor with respect to scattering time $S^2\sigma/\tau$ using GGA+SOC are plotted in figure 4 at room temperature. It is clearly seen that the unstrained PtTe$_2$ shows the largest n-type Seebeck coefficient, and that tensile strain can induce an enhanced Seebeck coefficient. Calculated results show that the PtTe$_2$ with strain from $4\%$ to $10\%$ has nearly the same Seebeck coefficient at high doping levels. These can be explained by band convergence as mentioned above. The complex strain dependence of electrical conductivity is observed due to the sensitive dependence of energy band structures on the applied strain. For the power factor combining the Seebeck coefficient with electrical conductivity, the unstrained PtTe$_2$ has the highest n-type power factor, while the strain-improved p-type power factor increases from $4\%$ to $10\%$. An upper limit of $ZT$ taking no account of lattice thermal conductivity, can be defined as $ZT_\text{e} = S^2\sigma/\tau_n e$, whose tensile strain dependence for PtTe$_2$ is shown in figure 4. The highest n-type $ZT_\text{e}$ is observed in unstrained PtTe$_2$, while the strain-improved p-type $ZT_\text{e}$ in PtTe$_2$ with

Figure 1. A sketch map of the crystal structure of monolayer PtTe$_2$. The large red balls represent Pt atoms, and the small blue balls are Te atoms.
strain from 4% to 10% at high doping levels is almost the same.

To further confirm the enhanced p-type thermoelectric properties induced by tensile strain, lattice thermal conductivities with strains of 0% and 4% are calculated. Phonon band structures of PtTe₂ with strains of 0% and 4% are plotted in figure 5. It is found that the longitudinal acoustic (LA) and transverse acoustic (TA) branches of PtTe₂ with strains of 0% and 4% are linear near the Γ point, while the z-direction acoustic (ZA) branch is quadratic near the Γ point. The dispersion of the ZA branch with strain of 4% becomes more linear than in the unstrained case in the long-wavelength limit. Calculated results also show that the optical branches with a strain of 4% move toward lower energy compared to the unstrained case. Thermal conductivity is an intensive property for bulk materials [44]. The calculated thermal conductivities for 2D materials should be normalized by multiplying $L_z/d$, where $L_z$ is the length of the unit cell along the z-direction, including the vacuum region, and $d$ is the thickness of 2D materials. However, the thickness of 2D materials is not well defined [44]. To demonstrate the reduced lattice thermal conductivity induced by tensile strain, the unnormlized lattice thermal conductivities with strains of 0% and 4% are shown in figure 6. Calculated results show that the lattice thermal conductivity (6.37 W m⁻¹K⁻¹) at a strain of 4% can decrease by about 19% compared to the unstrained case (7.89 W m⁻¹K⁻¹) at 300 K. The group velocities in the irreducible BZ with nine different bands are plotted in figure 7. It is found that the group velocities of the first band (ZA branch) with strain of 4% become lower than the unstrained case, which leads to lower lattice thermal conductivities. Similar reduced $\kappa_L$,
induced by tensile strain has also been proved in monolayer PtSe$_2$ [23] and ZrS$_2$ [25] by the first-principles calculations. To compare the lattice thermal conductivities of different 2D materials, the same thickness $d$ should be used [44]. The room-temperature lattice conductivity of PtTe$_2$ (7.89 W m$^{-1}$K$^{-1}$ with $L_z$ being 20.12 Å) is lower than that of PtSe$_2$ (16.97 W m$^{-1}$K$^{-1}$ with $L_z$ also being 20.12 Å) because of larger lattice constants $a$ [23]. According to enhanced $ZT_e$ and reduced $\kappa_L$ induced by tensile strain, tensile strain can indeed improve the efficiency of thermoelectric conversion.

**Figure 4.** At room temperature, the tensile strain dependence of Seebeck coefficient $S$, electrical conductivity with respect to scattering time $\sigma/\tau$, power factor with respect to scattering time $S^2\sigma/\tau$, and $ZT_e$ as an upper limit of $ZT$ versus doping level ($N$) using GGA+SOC are shown.

**Figure 5.** Phonon band structure of PtTe$_2$ with strains of 0% (left) and 4% (right) using GGA-PBE.

**Figure 6.** The lattice thermal conductivities of PtTe$_2$ as a function of temperature with strains of 0% and 4% using GGA-PBE.

4. Discussions and conclusion

PtTe$_2$ possesses the smallest gap among the PtX$_2$ ($X = S$, Se and Te) monolayers [24], and a semiconductor-to-metal transition can easily be produced for PtTe$_2$ by strain tuning. Calculated results show that about $-3\%$ compressive strain can induce semiconductor-to-metal transition, which is lower than the critical strain of MoS$_2$ (about 10% tensile strain and 15% compressive strain) [17] and ZrS$_2$ (about 8% compressive strain) [25]. Experimentally, such a small strain can
easily be achieved by piezoelectric stretching and exploiting the thermal expansion mismatch [52, 53]. These have potential applications in nanoelectronics by strain engineering.

The band convergence in the conduction bands for unstrained PtTe\textsubscript{2} naturally exists, which allows for better n-type thermoelectric performance (see figure 4). This is different from PtS\textsubscript{2} and PtSe\textsubscript{2}, and detailed comparisons of their electronic structures and transport properties can be found in [23, 24]. Both compressive and tensile strain can remove band convergence in the conduction bands, but tensile strain can induce band convergence in the valence bands, which supports better p-type thermoelectric properties. For PtSe\textsubscript{2}, compressive strain can produce band convergence in the conduction bands, and tensile strain can also lead to band convergence in the valence bands. The lattice thermal conductivity can be reduced by tensile strain both in PtTe\textsubscript{2} and PtSe\textsubscript{2}. Calculated results show that tensile strain can not only enhance $ZT_{\text{e}}$, but can also reduce $\kappa_{\text{L}}$, which implies that tensile strain can indeed improve the efficiency of the thermoelectric conversion of PtTe\textsubscript{2}. Similar strain-enhanced thermoelectric properties can also be found in monolayer MoS\textsubscript{2} [19], PtSe\textsubscript{2} [23] and ZrS\textsubscript{2} [25].

In summary, we investigate the strain dependence of the electronic structures and thermoelectric properties of monolayer PtTe\textsubscript{2} based mainly on reliable first-principle calculations and Boltzmann transport theory. The calculated results show that low compressive strain can give rise to semiconductor-to-metal transition. It is found that tensile strain can enhance $ZT_{\text{e}}$ and reduce lattice thermal conductivity, and then improve the efficiency of the thermoelectric conversion of PtTe\textsubscript{2}. Therefore, strain is a very effective method to achieve tuned electronic and thermoelectric properties of monolayer PtTe\textsubscript{2}, which provides great opportunities for applications in electronic and thermoelectric devices.

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