The strain effect on superconductivity in phosphorene: a first-principles prediction

Yanfeng Ge, Wenhui Wan, Fan Yang and Yugui Yao
School of Physics, Beijing Institute of Technology, Beijing 100081, People’s Republic of China
E-mail: ygyao@bit.edu.cn

Keywords: phosphorene, electron-phonon coupling, superconductivity, strain

Abstract
The effects of biaxial and uniaxial strains on electron–phonon coupling and superconductivity in monolayer phosphorene are systematically investigated by first-principles calculations. It is found that the electron–phonon coupling primarily comes from the low frequency optical phonon modes around $B_{1g}$, and the biaxial strain gives rise to more obvious increase in density of states around the Fermi level and phonon softening in the low frequency regime compared to the other two types of uniaxial strain. Therefore, the electron–phonon coupling is more significantly enhanced by the biaxial strain than the uniaxial strains and the superconducting transition temperature $T_c$ increases sharply from 3 K to 16 K at the typical doping concentration $n_{2D} = 3.0 \times 10^{14} \text{cm}^{-2}$ when the biaxial strain reaches 4.0%.

1. Introduction

Two-dimensional (2D) materials [1], such as graphene based materials and transition metal dichalcogenides (TMDCs), have generated intensive research interest owing to their special physical properties, some of which are not seen in their bulk counterparts. For instance, the massless Dirac fermion of graphene [2] leads to an extremely high room temperature mobility of $10^6 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ and other multitudinous electronic properties, but the absence of an energy gap results in a low on/off ratio and limits its application in the mainstream semiconductor industry. In the case of semiconducting MoS$_2$ [3, 4], though it has a moderate gap, a much lower carrier mobility than that of graphene indicates that it may not be a promising candidate for high-performance devices. Very recently, layered black phosphorus, termed phosphorene, has been experimentally isolated (mechanical exfoliation [5–7] and plasma-assisted fabrication [8]) and has good prospects in research owing to its tunable energy gap and remarkable electronic properties [9–12]. The layer-number-dependent direct energy gap [13–17], ranging from 1.51 eV in a monolayer to 0.59 eV in 5-layers [14], leads to its potential application in field-effect transistors (FETs) and photoelectric materials with a wide spectrum. In addition, previous works [6, 14, 18] have reported that its room temperature mobility is as high as $1000 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ [6] with explicit anisotropy, which even reaches $10^4 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ [14] in the theoretical prediction obtained from deformation potential approximation.

In materials science, one important application of 2D materials is in nanoscale superconducting devices, including superconducting quantum interference devices and superconducting transistors [19–21]. Previous studies of bulk black phosphorus [22, 23] have observed a superconducting phase in the metallic state under high pressures, when $T_c$ is above 10 K. Regarding phosphorene, there has been a first-principles calculation predicting superconductivity [24] when $T_c$ is about 4 K at a typical doping concentration of $3.0 \times 10^{14} \text{cm}^{-2}$. However, a feasible experimental method to further improve $T_c$ still needs to be explored. As a common approach, strain has long been successfully used to tune electronic properties of 2D materials [25–35]. In phosphorene, it is found that its layered structure can sustain a wide range of strains [36], which gives rise to the semiconductor–metal transition and rotates the preferred conducting direction by 90 degrees [18, 36–38].
Motivated by the effects of strain on the electronic properties of phosphorene, we employ first-principles calculations in the present work to obtain further insight into the evolution of superconductivity with respect to the magnitude and type of strain. The strain-dependent electron–phonon coupling constant $\lambda$ and superconducting transition temperature $T_c$ are systematically investigated in electron-doped phosphorene. It is found that the low frequency optical phonon modes around $B_{1g}$ play a key role in the electron–phonon coupling. Through modulating the band structure and phonon spectrum, the strains prominently enhance the electron–phonon coupling and the superconductivity, especially in the case of biaxial strain ($\epsilon = 4.0\%$), improving the $T_c$ from 3 K to 16 K at the typical doping concentration $n_{2D} = 3.0 \times 10^{14}$ cm$^{-2}$.

2. Methodology

2.1. Electron–phonon coupling formalism

The calculation of electron–phonon coupling is carried out in a many-body formalism. The matrix element $M_{k\epsilon(k+q)}^{\nu}$ illustrates the interaction between the electrons and phonons, expressed as [39]

$$M_{k\epsilon(k+q)}^{\nu} = \frac{\hbar}{2m_0a_{q,\nu}} \langle k\epsilon \mid \delta^{q,\nu}V \mid (k+q)\rangle,$$

where $|k\epsilon\rangle$ is the Kohn–Sham electronic eigenstate with wavevector $k$ and band index $\epsilon$, and $m$ is the atomic mass. $\delta^{q,\nu}$ is the derivative of the Kohn–Sham potential with respect to atomic displacement along the $\nu$ phonon mode with wavevector $q$ and the corresponding phonon frequency is $\omega_{q,\nu}$.

The electron–phonon coupling strength $\lambda_{q,\nu}$ for mode index $\nu$ and wavevector $q$ is given by [39],

$$\lambda_{q,\nu} = \frac{2}{N_F N_k a_{q,\nu}} \sum_{k,\epsilon} |M_{k\epsilon(k+q)}^{\nu}|^2 \delta(\epsilon_{k\epsilon} - \epsilon_F) \delta(\epsilon_{(k+q)\epsilon} - \epsilon_F),$$

where $N_F$ is the density of states at the Fermi level, $N_k$ is the total number of $k$ points and $\epsilon_{k\epsilon}$ is the band energy of the Bloch electron.

The dimensionless parameter electron–phonon coupling constant $\lambda$ is given by the average coupling [39],

$$\lambda = 2 \int_0^\infty a^2 F(\omega) \frac{d\omega}{\omega} = \frac{1}{N_q} \sum_{q,\nu} \lambda_{q,\nu}.$$

$a^2 F(\omega)$ is the Eliashberg spectral function, written as [39],

$$a^2 F(\omega) = \frac{1}{2N_q} \sum_{q,\nu} \omega_{q,\nu} \delta(\omega - \omega_{q,\nu}),$$

where $N_q$ is the total number of $q$ points.

Based on the isotropic approximation in the Eliashberg theory, which describes the conventional electron–phonon coupling superconductors very well, we estimate $T_c$ using the Allen–Dynes-modified McMillan equation [39],

$$T_c = \frac{\langle \omega \rangle_{\log} \log 1.2}{1.2} \exp \left( -\frac{1.04(1 + \lambda)}{\lambda - \mu^*(1 + 0.62\lambda)} \right),$$

where $\mu^*$ is the effective Coulomb repulsion with a reasonable value of 0.1 [24, 40] and $\langle \omega \rangle_{\log}$ is the logarithmically averaged phonon frequency,

$$\langle \omega \rangle_{\log} = \exp \left( \frac{2}{\lambda} \int_0^\infty a^2 F(\omega) \log \frac{d\omega}{\omega} \right).$$

2.2. Technical details

All of the first-principles calculations in the present work were carried out with the QUANTUM ESPRESSO package [41], using the norm-conserving pseudopotentials [42]. The Perdew, Burke and Ernzerhof parameterized generalized-gradient approximation (PBE-GGA) [43] was used to describe the exchange-correlation effect. The kinetic energy cutoff of 40 Ry was used in all the calculations. The energy and force convergence criteria for fully relaxing atomic positions were $10^{-5}$ Ry and $10^{-4}$ Ry a.u.$^{-1}$, respectively. A Monkhorst–Pack $k$-mesh of $42 \times 30 \times 1$ was used for electronic calculations. In our slab model, a vacuum layer of 15 Å was set to avoid interactions between the adjacent atomic layers. In order to be a metallic state, the electron-doped phosphorene was achieved by increasing the valence charge while simultaneously introducing...
the same amount of uniform background charge. The strains were introduced by adjusting the lattice constants with uniaxial strain capacity $\varepsilon_x = a_0 - a_0 \times 100\%$ and biaxial strain capacity $\varepsilon = \varepsilon_x = \varepsilon_y$, where $a_0 (b_0)$ is the lattice constant along the $x (y)$ direction for the strained-free structure. The phonon spectrum and $\lambda$ were calculated on a $14 \times 10 \times 1$ $q$-grid by using the density functional perturbation theory (DFPT) [44].

3. Results and discussion

3.1. Band structure and phonon spectrum

Unlike graphene, the lattice structure of monolayer phosphorene has a puckered structure (figure 1), because of the five valence electrons of phosphorus the atom and the $sp^3$ hybridization [38]. In our calculations, the in-plane lattice constants $a_0$ and $b_0$ are optimized to be 3.30 Å and 4.62 Å, respectively, similar to previous works [5, 36]. In our calculations for different doping concentrations, we have used fixed lattice constants of a unit cell and allowed the atomic positions to be determined by full relaxation for every calculation. As summarized in table 1, $R_2$ increases by 0.033 Å from $n_{2D} = 0.26 \times 10^{14}$ cm$^{-2}$ to $n_{2D} = 2.6 \times 10^{14}$ cm$^{-2}$, whereas $R_1$ grows only by 0.002 Å. The bond angles, $\alpha$ and $\beta$, decrease by 0.15° and 0.26°, respectively.

In the band structure, there is an energy gap of 0.91 eV at the $\Gamma$ point, which is in agreement with previous theoretical calculations [36]. We define the first and second conduction band minima at the $\Gamma$ point to be $\Gamma_1$ and $\Gamma_2$, in the high doping level (figures 2(b) and (c)). Similar behavior—the shift of the conduction band with doping—has also been found in other layered materials [45–47]. Monolayer phosphorene has twelve branches of phonons and belongs to the non-symmorphic space group D$_{2h}$. The eight irreducible representations at the $\Gamma$ point help to denote the vibration modes and figure 2(e) shows the three main optical vibration modes in the following discussions. Comparing the phonon spectra at different doping concentrations (figure 2(d)), one finds that the optical phonons around the $\Gamma$ point are greatly changed with doping. In the low frequency branches of the phonon spectrum, the $y$ direction stretching optical mode [24, 48] $B_{2g}^3$ softens evidently and other low frequency modes are nearly invariable. Another remarkable softening appears in the high frequency branches, which are the outplane optical modes [24, 48] stretching $A_{1g}$ and interlacing $B_{2g}^3$. The significant phonon softening in the doping condition may be attributed to the changes of bond lengths (table 1), the Kohn effect, and the nesting effect around the Fermi surface [24], which are also found in graphene and MoS$_2$ [35, 49].

When strains are turned on, they show significantly different effects on the different electronic eigenstates owing to their different bonding natures [36]. The application of biaxial strain $\varepsilon$ brings $\Gamma_1$ and $\Gamma_2$ close to each other and also leads to the apparent decline of the conduction band whose bottom is along the $\Gamma$–$Y$ line. As a

\begin{table}
\centering
\caption{Structure information for different doping concentrations.}
\begin{tabular}{lcccc}
\hline
$n_{2D}$ (10$^{14}$ cm$^{-2}$) & 0.26 & 1.30 & 1.80 & 2.60 \\
\hline
$R_1$ (Å) & 2.224 & 2.225 & 2.226 & 2.227 \\
$R_2$ (Å) & 2.275 & 2.300 & 2.303 & 2.308 \\
$\alpha$ (°) & 95.96 & 95.91 & 95.87 & 95.81 \\
$\beta$ (°) & 104.04 & 103.87 & 103.83 & 103.78 \\
\hline
\end{tabular}
\end{table}

Figure 1. (a) Lattice structure of phosphorene. (b) Side and (c) top views of the structure.
result, the five conduction band bottoms are simultaneously located in a small energy window around the Fermi level (figures 3(a)–(c)). Similar behaviors are also observed in the case of strain along the zigzag (x) direction (\(\varepsilon_z = 4.0\%\)) (figure 3(d)), but with a greater energy difference between \(\Gamma_1\) and \(\Gamma_3\) than under of biaxial strain (\(\varepsilon = 4.0\%\)) (figure 3(c)). The effect of strain along the armchair (y) direction on the conduction band (figure 3(e)) is far less obvious than the other two types of strain.

In the effect of strains on the phonon spectrum, the biaxial strain weakens the bond energy which, overall, lowers the atomic vibration frequencies, as shown in figures 4(a) and (b). In particular, the \(B_{2g}\) mode exhibits conspicuous softening, which plays a crucial role in enhancing the superconducting \(T_c\) via equation 2. In the case of uniaxial strains (figures 4(c) and (d)), both uniaxial strains affect the phonon spectrum in the low frequency branches less than the biaxial strain. In addition, due to the direction of vibration of the \(B_{2g}\) mode, i.e. the y direction (figure 2(e)), the strain along the armchair (y) direction has more influence on the \(B_{2g}\) mode than that of the zigzag direction. By comparison, in the high frequency branches of the phonon spectrum there is more obvious phonon softening under strain along the zigzag direction.

3.2. Electron–phonon coupling

The above obvious changes of electronic band structure and phonon spectra indicate a strong dependence of electron–phonon coupling on the strains. To further substantiate this statement, we have calculated the Eliashberg spectral function \(\lambda^2 F(\omega)\) and the electron–phonon coupling constant \(\lambda\) under different strains (figure 5).

As shown in figure 5(a), the \(\lambda^2 F(\omega)\) spectrum spreads through all phonon frequencies with three major parts lying on different frequency ranges. The stronger peaks of the spectrum lie in the low frequency regime around 150 cm\(^{-1}\) and primarily come from the coupling between the electrons and phonons, with frequencies around that of the \(B_{2g}\) mode. Those of \(A_{1g}\) and \(B_{2g}\) modes lead to the two relatively small peaks around 300 cm\(^{-1}\) and (c) \(1.3 \times 10^{14}\) cm\(^{-1}\) under the strain-free condition. After applying the biaxial strains, the peaks around 150 cm\(^{-1}\) are strengthened and shift to lower frequencies because of the visible phonon softening around the \(B_{2g}\) mode, while other peaks have no significant change. Figure 5(b) shows the comparison between \(\lambda^2 F(\omega)\) under the same magnitude of biaxial and uniaxial strains. The enhancing effects of the two types of uniaxial strain in the low frequency regime are much smaller than that of the biaxial strain due to the lesser phonon softening there. In addition, as a result of the different phonon softening effects under the two types of uniaxial strain (figures 4(c) and (d)), the peaks of the \(\lambda^2 F(\omega)\) spectrum in the low frequency regime in the case along the armchair direction are slightly higher than in the case along the zigzag direction. However, the opposite effect of the uniaxial strains on the \(\lambda^2 F(\omega)\) spectrum occurs in the high frequency regime.

Figure 2. (a) Band structure at \(n_{F1} = 0.26 \times 10^{14}\) cm\(^{-2}\) under the strain-free condition. The inset shows the Brillouin zone. \(\Gamma_1\) and \(\Gamma_2\) represent the first and second conduction band minima at the \(F\) point, respectively. \(X_1\) and \(X_2\) mark the two valleys around the \(X\) point. Band structures at doping concentrations (b) \(n_{F1} = 1.3 \times 10^{14}\) cm\(^{-2}\) and (c) \(1.8 \times 10^{14}\) cm\(^{-2}\) under the strain-free condition. One band falls from above to somewhere between \(\Gamma_1\) and \(\Gamma_2\) with the increase of doping concentration. (d) Phonon spectra at different doping concentrations under the strain-free condition, \(n_{F1} = 0.26 \times 10^{14}\) cm\(^{-2}\) red dashed line and \(1.3 \times 10^{14}\) cm\(^{-2}\) (back solid line). (e) Schematic diagram of main optical vibration modes (the y direction stretching optical mode \(B_{2g}\), the outplane stretching optical mode \(A_{1g}\) and the outplane interlacing optical mode \(B_{3g}\)).
The doping-dependent total electron–phonon coupling constant $\lambda$ under the strains is shown in figure 5(c) and (d). It is usually expected that the increase of doping concentration strengthens the electron–phonon coupling as verified by the overall increasing trend in figure 5(c), but a local decline of $\lambda$ appears in a small range around $n_{2D} = 1.3 \times 10^{14}$ cm$^{-2}$. The $I_1$ and $I_2$ are close to each other, especially obvious under the biaxial strain and the uniaxial strain along the zigzag direction.

Figure 3. (a)–(c) Effect of the biaxial strains ($\epsilon = 0.0\%$, $2.0\%$ and $4.0\%$) on the band structure at $n_{2D} = 1.3 \times 10^{14}$ cm$^{-2}$. (d)–(f) Effect of the uniaxial strains ($\epsilon_x = 4.0\%$, $\epsilon_y = 4.0\%$ and $\epsilon_z = 5.0\%$) at $n_{2D} = 1.3 \times 10^{14}$ cm$^{-2}$. The $I_1$ and $I_2$ are close to each other, especially obvious under the biaxial strain and the uniaxial strain along the zigzag direction.

Figure 4. Phonon spectra at $n_{2D} = 1.3 \times 10^{14}$ cm$^{-2}$ under different strains, (a) $\epsilon = 2.0\%$, (b) $4.0\%$, (c) $\epsilon_x = 4.0\%$ and (d) $\epsilon_y = 4.0\%$. By contrast, the red dashed lines show the phonon spectrum under strain-free condition.

The doping-dependent total electron–phonon coupling constant $\lambda$ under the strains is shown in figure 5(c) and (d). It is usually expected that the increase of doping concentration strengthens the electron–phonon coupling as verified by the overall increasing trend in figure 5(c), but a local decline of $\lambda$ appears in a small range around $n_{2D} = 1.5 \times 10^{14}$ cm$^{-2}$ under the low strains $\epsilon < 2.0\%$ (we shall explain this in the next paragraph). It is important that the biaxial strain ($\epsilon = 4.0\%$) markedly enhances the electron–phonon coupling, improving $\lambda$ from 0.4 to 1.6 at $n_{2D} = 3.0 \times 10^{14}$ cm$^{-2}$. In the case of uniaxial strains (figure 5(d)), due to the obvious changes of electronic band structure and the high frequency branches of the phonon spectrum under the strain along the zigzag direction, it has more influence on the electron–phonon coupling than the uniaxial strain along the armchair direction. But both effects of the uniaxial strains are far less obvious than those of the biaxial strain. It is
also found that the increase of strain does not always enhance the electron–phonon coupling. As shown in figure 5(d), the electron–phonon coupling of $\varepsilon_x = 5.0\%$ is slightly below that of $\varepsilon_x = 4.0\%$.

In order to more clearly decipher the relative contributions of phonons with different wave vectors to the electron–phonon coupling, we introduce the distribution map of the wave-vector-resolved electron–phonon coupling parameter $\lambda = \sum_\mathbf{q} \lambda_{\mathbf{q}k}$, as plotted in figure 6. We define the region around $\Gamma$ point as I and its adjacent highlight region as II (figure 6(b)). In the strain-free condition, the strong electron–phonon coupling in area I is mainly attributed to the appearance of $X_1$ and $X_2$ near the Fermi level (figures 2(b)), while the electron–phonon coupling in area II (figure 6(a)) mainly originates from the electrons on the lowest conduction band around the $\Gamma$ point. With the increase of doping concentration, the lower of the conduction band minima, $\Gamma_1$, and the band which falls from above to somewhere between $\Gamma_1$ and $\Gamma_2$ (figure 2) lessen the electron population on the $X_1$ and $X_2$ valleys. This significantly weakens the electron–phonon coupling in area I but hardly affects it in area II (figure 6(c)), so that the decline of $\lambda$ appears around $n_{2D} = 1.5 \times 10^{14} \text{ cm}^{-2}$.

The application of biaxial strains obviously strengthens the electron–phonon coupling in area I, while in area II it is enhanced slightly (figures 6(d) and (e)). The reason is that the biaxial strain, on the one hand, impacts the conduction band to increase the density of states near the Fermi level (figures 3(b) and (c)) and, on the other hand, clearly softens the phonons in the low frequency regime (figures 4(a) and (b)). The two effects are advantageous for strengthening the electron–phonon coupling. Based on the study for the changes of electron–phonon coupling caused by different phonon modes, one can mainly attribute the enhancement of the electron–phonon coupling in area I to the increase of the contribution from the low frequency optical phonon modes around $B_{3g}$, which sharply soften with increasing biaxial strain.

In the case of uniaxial strains (figures 6(f)–(g)), the increase of electron–phonon coupling in area I is far less significant than in the case of biaxial strains because of the weaker phonon softening in the low frequency regime under uniaxial strain. In addition, the effect of strain along the armchair direction on the electron–phonon coupling in area I is slightly stronger than that along the zigzag direction, consistent with the softening of the $B_{3g}$ phonon mode above (figures 4(c) and (d)). When increasing the strain along the zigzag direction to 5% (figures 6(h)), the electron–phonon coupling is weaker than in the case of $\varepsilon_y = 4.0\%$, because $X_1$ and $X_2$ are far away from the Fermi level and lower the density of states (figure 3(f)).
3.3. Superconductivity

The superconducting transition temperature $T_c$ under different strains was estimated by using equation 5 with a reasonable $\mu^*$ of 0.1 [24, 40], as shown in figure 7. Table 2 also summarizes the results of $T_c$ in a reasonable range of $\mu^*$ (e.g., 0.1 $\sim$ 0.15). In the strain-free condition, we got $T_c = 3$ K with $\lambda = 0.4$ at the typical doping concentration $3.0 \times 10^{14}$ cm$^{-2}$. More importantly, $T_c$ can be enhanced to 16 K at the same doping concentration with a biaxial strain of 4.0%. However, the uniaxial strain can only enhance the $T_c$ to 10 K (8 K) for $\epsilon_x$ ($\epsilon_y$) = 4.0%

**Figure 6.** Distribution map of wave-vector-resolved electron–phonon coupling parameter $\lambda_q$ at $n_{2D} = (a) 0.26 \times 10^{14}$ cm$^{-2}$, (b) $1.3 \times 10^{14}$ cm$^{-2}$ and (c) $1.8 \times 10^{14}$ cm$^{-2}$ under the strain-free condition. The regime around the $\Gamma$-point is defined as I and its adjacent highlight region is II. The largest values of $\lambda_q$ in area I are 0.23 and 0.12 for $n_{2D} = 1.3 \times 10^{14}$ cm$^{-2}$, $1.8 \times 10^{14}$ cm$^{-2}$, respectively. Distribution map of $\lambda_q$ under the strain of (d) $\epsilon = 2.0\%$, (e) $4.0\%$, (f) $\epsilon_x = 4.0\%$, (g) $\epsilon_y = 4.0\%$ and (h) $\epsilon_x = 5.0\%$ at the doping concentration of $n_{2D} = 1.3 \times 10^{14}$ cm$^{-2}$.

**Figure 7.** Superconducting transition temperature $T_c$ versus doping concentrations under different strains. The solid (dashed) lines show the curves of biaxial (uniaxial) strains.

**Table 2.** $T_c$ with a small range of $\mu^*$ (0.1 $\sim$ 0.15) at $n_{2D} = 3.0 \times 10^{14}$ cm$^{-2}$ under strain.

| strain          | $T_c$ (K)       |
|-----------------|-----------------|
| $\epsilon = 0.0\%$ | $3.0 \sim 1.5$  |
| $\epsilon = 2.0\%$ | $7.9 \sim 5.3$  |
| $\epsilon = 4.0\%$ | $16.0 \sim 12.9$ |
| $\epsilon_x = 4.0\%$ | $12.5 \sim 8.6$ |
| $\epsilon_y = 4.0\%$ | $7.5 \sim 5.0$  |
| $\epsilon_x = 5.0\%$ | $12.0 \sim 8.4$ |
at $n_{\text{D}} = 3.0 \times 10^{14} \text{ cm}^{-2}$, which is below the value in the case of biaxial strain. For this reason, the uniaxial strains cannot bring about the enhancement of density of states around the Fermi level and obvious phonon softening simultaneously, which are the major factors in enhancing the $T_c$ of phonon-mediated superconductivity. Compared to graphene [50], there are both similar and different aspects of the enhancing effect of biaxial tensile strain on superconductivity. In both systems, strain gives rise to the softening of the phonon mode, while in graphene the mode is the shear horizontal optical in-plane C–C stretching mode, in phosphorene it is the $y$ direction stretching optical mode. However, the strain in graphene has little effect on the conduction band, which is in contrast to phosphorene. According to the enhancement of $T_c$ under strain, our results effectively serve as guidance for experimentalists to improve the superconductivity of phosphorene.

4. Summary

In the present work, we investigate the effects of strain on electron–phonon coupling and superconductivity in monolayer phosphorene using first-principles calculations. We found that the low frequency optical phonon modes around $B_{1g}$ mainly contribute to electron–phonon coupling. Our important discovery is that the biaxial strain enhances the electron–phonon coupling significantly and hence raises the superconducting transition temperature from 3 K to 16 K at the typical doping concentration $3.0 \times 10^{14} \text{ cm}^{-2}$ used here. The boosting of $T_c$ is attributed to the simultaneous increases of the density of states around the Fermi level and the softening of the phonons. Furthermore, the anisotropy in phosphorene leads to different effects on the electron–phonon coupling under uniaxial strain along different directions. Unlike the high $T_c$ in the case of biaxial strain, the uniaxial strains of $e_x = 4.0\%$ and $e_y = 4.0\%$ enhance $T_c$ to 10 K and 8 K, respectively, at a doping concentration of $3.0 \times 10^{14} \text{ cm}^{-2}$.

Acknowledgments

This work was supported by the MOST Project of China (grant no. 2014CB920903 and 2011CBA00100), the NSFC (grant no. 11174337, 11225418, 11274041 and 11334012), the Specialized Research Fund for the Doctoral Program of Higher Education of China (grant no. 2012110110046) and the NCET program under the grant no. NCET-12-0038.

References

[1] Geim A K and Grigorieva I V 2013 Nature 499 419
[2] Castro Neto A H, Guinea F, Peres N M R, Novoselov K S and Geim A K 2009 Rev. Mod. Phys. 81 109
[3] Radisavljevic B, Radenovic A, Brivio J, Giacometti V and Kis A 2011 Nat. Nanotechnology 6 147
[4] Wang Q H, Kalantar-Zadeh K, Kis A, Coleman J N and Strano M S 2012 Rev. Mod. Phys. 84 17
[5] Liu H, Neal A T, Zhu Z, Luo Z, Xu X, Tomanek D and Ye P D 2014 ACS Nano 8 4053
[6] Li L, Yu Y, Ye G, Ge Q, Ou X, Wu H, Feng D, Chen X H and Zhang Y 2014 Nat. Nanotechnology 9 372
[7] Koenig S P, Doganov R A, Schmidt H, Castro Neto A H and Ozyilmaz B 2014 Appl. Phys. Lett. 104 103106
[8] Shao D F, Nan H Y, Hong H, Chen Y M, Zhu C, Liang Z, Ma X Y, Ni Z H, Jia C H and Zhang Z 2014 Nano Res. 7 853
[9] Engel M, Steiner M and Avouris P 2014 Nano Lett. 14 6414
[10] Buscema M, Groenendijk D J, Steele G A, van der Zant H S J and Castellanos-Gomez A 2014 Nat. Commun. 5 4651
[11] Xia F, Wang H and Jia Y 2014 Nat. Commun. 5 4458
[12] Low T, Engel M, Steiner M and Avouris P 2014 Phys. Rev. B 90 081408
[13] Rudenko A N and Katsnelson M I 2014 Phys. Rev. B 89 201408
[14] Qiao J, Kong X, Hu Z, Yang F and Ji W 2014 Nat. Commun. 5 4475
[15] Tran V, Soklaski R, Liang Y and Yang L 2014 Phys. Rev. B 89 235319
[16] Guan J, Zhu Z and Tomanek D 2014 Phys. Rev. Lett. 113 046804
[17] Guo H Y, Lu N, Dai J, Wu X J and Zeng X C 2014 J. Phys. Chem. C 118 14051
[18] Fei R and Yang L 2014 Nano Lett. 14 2884
[19] Delahaye J, Hassel J, Lindell R, Sillanpää M, Paalanen M, Seppä H and Hakonen P 2003 Science 299 1045
[20] Franceschetti S D, Kouwenhoven L, Schönenberger C and Wernsdorfer W 2010 Nat. Nanotechnology 5 703
[21] Saira O, Meschke M, Gazotto F, Savin A M, Möttönen M and Pekola J P 2007 Phys. Rev. Lett. 99 027203
[22] Kawamura H, Shirioti I and Tachikawa K 1984 Solid State Commun. 49 879
[23] Wittig J and Matthias B T 1968 Science 160 994
[24] Shao D F, Lu W J, Lv H Y and Sun Y P 2014 arXiv: 1405.0092
[25] Metzger C, Rémi S, Liu M, Kusminskiy S V, Castro Neto A H, Swan A K and Goldberg B 2010 Nano Lett. 10 4651
[26] Ding F, Ji H X, Chen Y H, Herklotz A, Dör R K, Mei Y F, Rastelli A and Schmidt O G 2010 Nano Lett. 10 3453
[27] Conley H J, Wang B, Ziegler J I, Haglund R F Jr, Pantelides S T and Bolotin K I 2013 Nano Lett. 13 3626
[28] Ni Z H, Yu T, Lu Y H, Wang Y Y, Feng Y P and Shen Z X 2008 ACS Nano 2 2301
[29] Guinea F, Katsnelson M I and Geim A K 2010 Nat. Phys. 6 30
[30] Johari P and Shenoy V B 2012 ACS Nano 6 5449
[31] Feng J, Qian X, Huang C W and Li J 2012 Nat. Photonics 6 866
[32] He K, Poole C, Mak K F and Shan J 2013 Nano Lett. 13 2831
[33] Chang C H, Fan X F, Lin S H and Kuo J L 2013 Phys. Rev. B 88 195420
[34] Wan W H, Ge Y F, Yang F and Yao Y G 2013 Europhys. Lett. 104 36001
[35] Ge Y F, Wan W H, Feng W X, Xiao D and Yao Y G 2014 Phys. Rev. B 90 035414
[36] Peng X, Wei Q and Copple A 2014 Phys. Rev. B 90 085402
[37] Lv H Y, Lu W J, Shao D F and Sun Y P 2014 Phys. Rev. B 90 085433
[38] Rodin A S, Carvalho A and Castro Neto A H 2014 Phys. Rev. Lett. 112 176801
[39] McMillan WL 1968 Phys. Rev. 167 331
[40] Grimvall G 1981 The Electron-Phonon Interaction in Metals (Amsterdam: North-Holland)
[41] Giannozzi P et al 2009 J. Phys.: Condens. Matter 21 395502
[42] Vanderbilt D 1990 Phys. Rev. B 41 7892
[43] Perdew J P, Burke K and Ernzerhof M 1996 Phys. Rev. Lett. 77 3865
[44] Baroni S, Gironcoli S D, Corso A D and Giannozzi P 2001 Rev. Mod. Phys. 73 515
[45] Ge Y and Liu A Y 2013 Phys. Rev. B 87 241408
[46] Topsakal M and Ciraci S 2012 Phys. Rev. B 85 045121
[47] Brumme T, Calandra M and Mauri F 2015 arXiv: 1501.07223
[48] Fei R and Yang L 2014 Appl. Phys. Lett. 105 083120
[49] Savini G, Ferrari A C and Giustino F 2010 Phys. Rev. Lett. 105 037002
[50] Si C, Liu Z, Duan W H and Liu F 2013 Phys. Rev. Lett. 111 196802