

Theoretical study in carrier mobility of two-dimensional materials

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Abstract. Recently, the theoretical prediction on carrier mobility of two-dimensional (2D) materials has aroused wild attention. At present, there is still a large gap between the theoretical prediction and the device performance of the semiconductor based on the 2D layer semiconductor materials such as graphene. It is particularly important to theoretically design and screen the high-performance 2D layered semiconductor materials with suitable band gap and high carrier mobility. This paper introduces some 2D materials with fine properties and deduces the formula for mobility of the isotropic materials on the basis of the deformation potential theory and Fermi golden rule under acoustic phonon scattering conditions, and then discusses the carrier mobility of anisotropic materials with Dirac cones. We point out the misconceptions in the existing literature and discuss the correct ones.

1 Introduction

With Geim's team in the University of Manchester successfully isolating the single atomic layered graphene by 2004, 2D materials with huge potential for the field of basic science and applied research has drawn widespread attention. For instance, as the electrical materials with great properties, they can be made into excellent field effect transistors(FET).

In general, the excellent FET requires a suitable band gap and high mobility. Materials with Dirac cones such as graphene own the extremely high electron mobility due to the low electron effective mass ($2 \times 10^5 \text{ cm}^2 / \text{V}^{-1} \text{ S}^{-1}$ [1]). However, to obtain a suitable band gap needs to modify the material. Unfortunately, most modification methods expanding the band gap of graphene will inevitably reduce the mobility [2]. Meanwhile, 2D semiconductor materials have gradually came into view [3], such as black phosphorus [4,5], graphyne [6], transition metal dichalcogenides (TMDs) [7,8], transition metal carbides and nitrides (MXene) [9,11], etc. They own the suitable band gap as well as the high mobility, which can be the potential candidate material for the high-performance FET.

These semiconductor materials are usually anisotropic, which can lead to the mechanical, optical and electrical response depended on the angle. It also illustrates the potential application value of anisotropic semiconductor materials as sensors. Therefore, it is especially important to understand the anisotropic carrier mobility. This paper will focus on the calculation of carrier mobility of the anisotropic material.

2 Dirac material

Dirac cone is a unique band structure, whose band looks like two inverted circular cone with their apexes connected at the separated Fermi level of filled and unfilled electrons. Since the structure satisfies the Dirac equation which describes the energy-momentum relation of relativistic particles, it is called Dirac cone. The low-energy behavior of the electrons in the two-dimensional Dirac system re-



quires a Dirac equation description, which behaves as a relativistic particle behavior with an effective mass of zero and a velocity close to the speed of light. Materials with a Dirac cone structure have many excellent physical properties, such as high carrier mobility and anomalous quantum Hall effect.

Graphene is a 2D monolayer material, which is a 2D hexagonal honeycomb lattice structure formed by the carbon atom in the sp^2 hybridization. The atomic structure is Fig. 1 (a). According to the first principle and tightly bound Hamiltonian the band structure can be shown in Fig. 1 (b) [13].

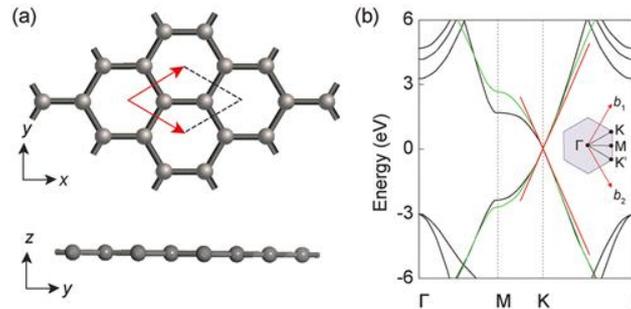


Figure 1. (a)Graphene atomic structure (b)Graphene band structure

However, in the case of isotropic materials such as graphene, the modification of the band gap will reduce its mobility, while the 2D semiconductor material, which is an anisotropic Dirac material, has an appropriate band gap and a good mobility, with a broader application prospects. Daniel Malko [6] et al. studied several graphyne such as α -graphyne and 6,6,12-graphyne with the Dirac cone structure. Fig. 2 shows their atomic structure [6].

Fig. 3 and 4 illustrate the band structure of α -graphyne and 6,6,12-graphyne respectively. It is worth noting that α -graphyne has the same hexagonal symmetry as graphene, which is generally considered to be a necessary condition for the existence of the Dirac cone. However, the band structure of the 6,6,12-graphyne has proved this view is wrong. The 6,6,12-graphyne has a rectangular symmetry but there are still two pairs of Dirac points in the Brillouin area. Fig. 5(d) and (e) show the valence and energy band of the 6,6,12-graphyne at two adjacent Dirac points.

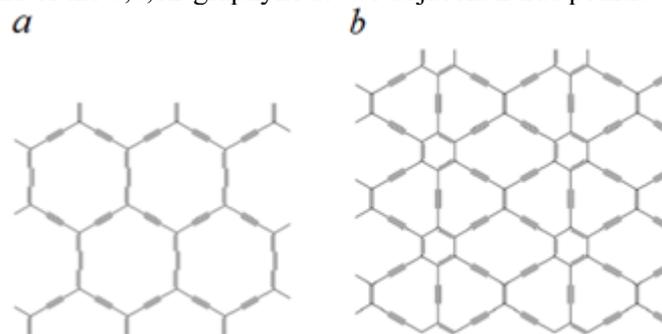


Figure 2. (a). α -graphyne atomic structure (b)6,6,12-graphyne atomic structure

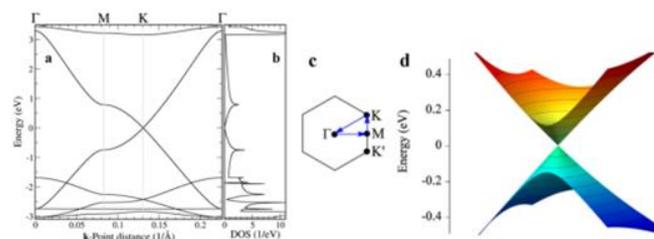


Figure 3. α -graphyne band structure

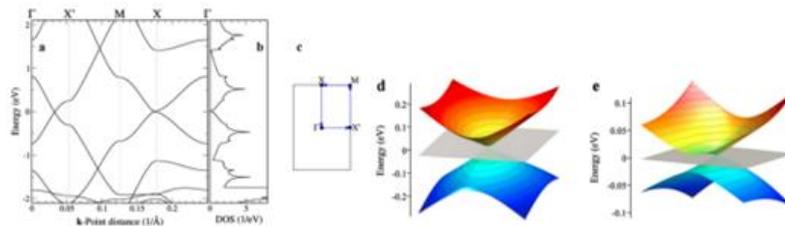


Figure 4. 6,6,12-graphyne band structure

The results of Daniel Malko et al. show that the chemically equivalent carbon atoms and hexagonal symmetries in graphene are not necessary conditions for the existence of Dirac cone, suggesting that the 2D materials which are composed of non-carbon atoms and do not even have hexagonal symmetry may also have Dirac cone as well as the excellent electrical properties. Take black phosphorus firstly prepared in 1914 for instance. In the periodic table, the elemental phosphorus in the lower right corner of the carbon element has an atomic structure similar to that of carbon. Two-dimensional crystal black phosphorus is the most stable allotrope of phosphorus. Different from the sp^2 hybrid bonds of carbon atoms in the graphite, phosphorus atoms have five valence electrons, forming the sp^3 hybrid bond with the adjacent three phosphorus atoms, which determines the differences between the 2D plane of phosphorus and elements in group IV that the plane of phosphorus has anisotropic folds, which can be seen in Fig.5[5]. Figure 6 [4] shows the black phosphorus band structure solved by density functional theory [14,15,16].

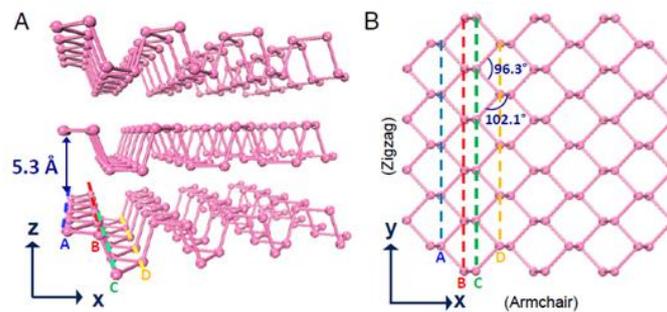


Figure 5. (a)Side view of black phosphorus crystal (b)Top view of single layer black phosphorus

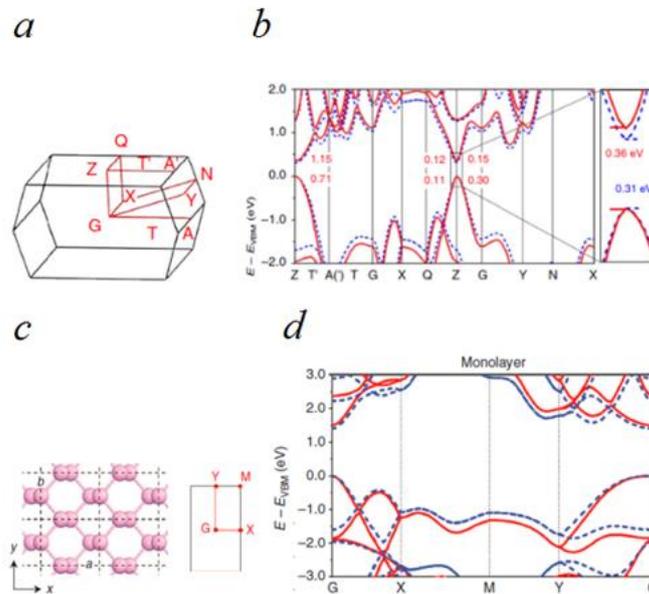


Figure 6. (a) Electron band structure of bulk black phosphorus; (b) Brillouin area of bulk black phosphorus; (c) Electron band structure of monolayer black phosphorus; (d) Brillouin area of monolayer black phosphorus

3 Deformation potential theory and the general process of calculating the carrier mobility

The deformation potential theory was first proposed by J. Bardeen et al., which converts the phonon scattering process into a change of an effective potential field that can be perceived by electrons. According to the theory, the energy change is proportional to the size of the lattice deformation. Based on the general theory of scattering, the transition probability can be given, and then the physical quantities such as relaxation time and carrier mobility can be calculated.

At room temperature, based on the deformation potential theory and Fermi golden rule, including the acoustic phonon scattering, the isotropic semiconducting state and the probability of scattering:

$$W_{\vec{k},\vec{k}'} = \frac{E_1^2 \pi k_B T}{A \hbar C_{11}} \delta(\varepsilon_{\vec{k}} - \varepsilon_{\vec{k}'}) \quad (1)$$

Where E_1 is the deformation potential constant, which describes the vertical movement of band under the strain; C_{11} is the elastic modulus mainly affecting the velocity and number of scattered phonons; A is the 2D semiconductor area; \hbar is Planck constant; T is temperature; k_B is the Boltzmann constant; $\delta(\varepsilon_{\vec{k}} - \varepsilon_{\vec{k}'})$ is the state of the electron energy.

For graphene, at room temperature, based on the deformation potential theory and Fermi golden rule, including the acoustic phonon scattering, the isotropic semiconducting state and the probability of scattering:

$$W_{\vec{k},\vec{k}'} = \frac{\pi k_B T}{A \hbar C_{11}} \delta(\varepsilon_{\vec{k}} - \varepsilon_{\vec{k}'}) \left[E_1^2 \cos^2 \frac{\theta' - \theta}{2} + E_{\beta,11}^2 \cos^2 \left(\frac{3}{2} (\theta' + \theta) \right) + \frac{C_{11}}{C_{44}} E_{\beta,44}^2 \sin^2 \left(\frac{3}{2} (\theta' + \theta) \right) \right] \quad (2)$$

Note that the difference with the two-dimensional semiconductor is that there is a parameter E_{β} , which is called the deformation transition constant mainly reflecting the Dirac cone in the horizontal

movement under the strain. Due to its linear dispersion and zero band gap characteristics, the horizontal movement effect of the energy band in Dirac cone cannot be neglected (negligible in the semiconductor). Also due to this effect, the influence of the transverse wave phonon must be considered. $E_{\beta,44}$ is the deformation constant corresponding to the tensile strain; C_{44} is the elastic modulus component corresponding to the transverse wave phonon; $E_{\beta,11}$ is the deformation constant corresponding to the tangential strain; C_{11} is the elastic modulus component corresponding to the longitudinal wave phonon; θ is the argument of \mathbf{k}' ; θ' is the argument of \mathbf{k} .

Then the relaxation time can be calculated:

$$\frac{1}{\tau(\vec{k})} = \frac{A}{4\pi^2} \int W_{\vec{k},\vec{k}'} \left(1 - \frac{\vec{v}_{\vec{k}} \cdot \vec{v}_{\vec{k}'}}{|\vec{v}_{\vec{k}}|^2} \right) d^2k' \quad (3)$$

The conductance and carrier mobility can be calculated based on the Boltzmann equation:

$$\sigma_{xx} = ge \int \tau(\vec{k}) \frac{\partial n_F}{\partial \mathcal{E}} (\vec{v}_{\vec{k}} \vec{v}_{\vec{k}})_{xx} e^{-\frac{d^2k}{(2\pi)^2}} \quad (4)$$

$$n = g \int n_F \frac{d^2k}{(2\pi)^2} \quad (5)$$

$$\mu_x = \frac{\sigma_{xx}}{ne} \quad (6)$$

Where $\tau(\mathbf{k})$ is the relaxation time depending on energy; σ_{xx} is the conductivity; g is degeneracy; n_F is the Fermi-Dirac distribution; n is the carrier density; μ_x is the carrier mobility.

For isotropic 2D semiconductors, the result is:

$$\mu_x = \frac{2e\hbar^3 C_{11}}{k_B T (m^*)^2 E_1^2} \quad (7)$$

4 The misconception on anisotropic semiconductor

There are a lot of related work on the calculation of two-dimensional semiconductor electron mobility, but they have a misunderstanding of the mobility formula, using the relevant formula [2] as follows:

$$\mu_{2D} = \frac{e\hbar^3 C_{2D}}{k_B T m_e^* m_d (E_1^i)^2} \quad (8)$$

Where m_e^* is the effective mass of the transmission direction; m_d is the average effective mass determined by $m_d = (m_x^* m_y^*)^{1/2}$; E_1 is the deformation potential constant; C_{2D} is the elastic modulus of the longitudinal wave phonon.

The formula has no problem with the handling of anisotropic effects of effective mass, but they believe that the electron mobility in the x direction is only related to the x component of the deformation potential tensor and the elastic modulus. Obviously this is an erroneous understanding, since electrons in the x-direction motion are inevitably scattered by the phonons of the y-direction so that their mobility must also be related to the y component of the deformation potential tensor and the elastic modulus.

5 The result of anisotropic Dirac cone

The mobility formula for the Dirac cone material of the anisotropic deformation potential constant has been related to the theoretical derivation. The difference from the isotropic ones is that the deformation potential constant becomes a second order tensor. Correspondingly, the change of the effective potential needs to be calculated by the transvection of the strain tensor and the deformation potential tensor. Hence E_l in Eq.(2) should be replaced by $E_l(\mathbf{q})$:

$$\begin{aligned}
E_1(\vec{q}) &= E_{1x} \cos^2 \theta_{\vec{q}} + E_{1y} \sin^2 \theta_{\vec{q}} \\
&= \frac{E_{1x} + E_{1y}}{2} + \frac{E_{1y} - E_{1x}}{2} \cos(2\theta_0 + \theta)
\end{aligned} \tag{9}$$

Where θ is the angle between \mathbf{k}' and \mathbf{k} ; θ_0 is the angle between \mathbf{k} and coordinate axis; θ_q is the argument of \mathbf{q} .

Correspondingly, $E_{\beta,11}$ should be replaced by $E_{\beta,11}(\mathbf{q})$:

$$\begin{aligned}
E_{\beta,11}(\vec{q}) &= \frac{E_{\beta,11x} + E_{\beta,11y}}{2} \\
&+ \frac{E_{\beta,11y} - E_{\beta,11x}}{2} \cos(2\theta_0 + \theta)
\end{aligned} \tag{10}$$

Based on Eq. (2)(3)(4)(5)(6)(9)(10), the carrier mobility can be calculated:

$$\begin{aligned}
\mu_x &= \frac{2e\hbar^3 C_{11} v_F^4}{0.82 (k_B T)^3} \left[\bar{E}_1^2 + \frac{1}{2} (\Delta E_1)^2 \right. \\
&\left. + 2 \left(\bar{E}_{\beta,11}^2 + \frac{1}{2} (\Delta E_{\beta,11})^2 + \frac{C_{11}}{C_{44}} E_{\beta,44}^2 \right) \right]^{-1}
\end{aligned} \tag{11}$$

Where $\bar{E}_1, \Delta E_1, \bar{E}_{\beta,11x}, \Delta E_{\beta,11x}$ can be seen as follows:

$$\left\{ \begin{aligned}
\bar{E}_1 &= \frac{E_{1y} + E_{1x}}{2} \\
\Delta E_1 &= \frac{E_{1y} - E_{1x}}{2} \\
\bar{E}_{\beta,11x} &= \frac{E_{\beta,11y} + E_{\beta,11x}}{2} \\
\Delta E_{\beta,11x} &= \frac{E_{\beta,11y} - E_{\beta,11x}}{2}
\end{aligned} \right. \tag{12}$$

6 Conclusion

Since the graphene has been successfully prepared, 2D material has been widely concerned. The semiconductor 2D crystal material, typical of graphene, graphyne and black phosphorus, has excellent characteristics such as high carrier mobility due to its novel and unique Dirac cone structure. For the isotropic material, based on the deformation potential theory and acoustic phonon scattering, the transition probability based on the general theory of scattering can be given. Then the physical quantities such as relaxation time and carrier mobility can be calculated by solving the Boltzmann equation. For anisotropic materials, the conclusions of carrier mobility calculations in most existing literature have misinterpretation of variables affecting the electron mobility in the x direction. In fact, for the anisotropic material, the deformation potential constant becomes a second order tensor. Hence E_l in the transition probability expression needs to be replaced by a second order tensor, $E_l(\mathbf{q})$. Finally, we summarize the carrier mobility calculation results of the anisotropic Dirac cones.

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