

Research progress on the calculation of carrier mobility for two-dimensional Dirac material

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Abstract: With the development of integrated devices in the direction of increasingly miniaturization, from the end of the last century, computing, communications, automatic control and other aspects of science and technology expressed the urgent expectation of new materials. With the discovery of graphene, the study of two-dimensional material system began to reveal new vitality. The special properties of these two-dimensional materials are often related to the carrier mobility. Therefore, studying how to calculate the carrier mobility of two-dimensional materials, especially the Dirac materials, is of double significance for theoretical calculation and application of nanomaterials. In this paper, the theoretical development of the two-dimensional Dirac material mobility is studied in detail. This paper summarizes the commonly used methods and principles in theoretical calculations of materials, including Bloch's theorem and Density functional theory. The main methods for calculating carrier mobility in two-dimensional materials are introduced in detail, namely Tight-binding models and deformation potential theory.

1. Introduction

Since the graphene has been successfully synthesized, two-dimensional materials have been attracted widespread concern. The reason is that they have great potential in basic science and applied research, for example, as excellent electrical materials, it can be made into excellent performance of the field effect transistor.

In general, excellent field-effect transistors require proper bandgap and high mobility. The Dirac system, represented by graphene, has a Dirac cone at point K with a linear band dispersion relationship. The electrons near the Fermi surface are massless dirac fermi, with ultra-high current-carrying. These properties open the door to researching fundamental physics problems [1-4]. The mobility of a material is an important aspect of measuring the performance of a material device. In 2007, Das Sarma's group at the University of Maryland studied the transport properties of charge carriers in graphene with random charged impurity scattering [5].

The properties of the electrons in the solid near the Fermi surface to some extent determine the physical properties exhibited by the electrons in the solid. The theory of the solid energy band developed gradually after the quantum theory was established in the 1920s. In 1928, Bloch pointed out that the quantum nature of the motion of electrons in solids is the movement of electrons in the periodic potential field of the lattice [6]. In order to calculate the electron levels in atoms and molecules, Hartree proposed a self-consistent method of calculation, yet this method does not consider the antisymmetry of the wave function due to the exchange-related effects of electrons, which was revised by Fock later [7] and was developed into the Hartree-Fock method. This can be used to calculate the structure of the solid electron band. In the 1960s, with the development of electronic computers, a large number of theoretical calculation methods developed rapidly. One of the biggest advances was none other than the Density



Functional Theory (DFT) developed by Hohenberg, Kohn and Sham [8]. The innovation of the DFT method is that the nature of the ground state electrons is regarded as a function of the electron density. Today, the DFT method has become a reliable method for calculating the ground state properties and the band structure of electrons.

This paper first summarizes the theoretical basis and method of first principles calculation of solid materials, and finally summarizes the calculation method of two-dimensional Dirac material such as graphene. It is in hope to provide reference and guidance to researchers in the calculation of two-dimensional material mobility.

2. Bloch's theorem

On the basis of the mean field approximation, if the potential field of the electron motion environment is periodic, then according to Bloch's theorem, the solution of Schrödinger equation with periodic potential field has the following form:

$$\psi_k(\mathbf{r}) = u_k(\mathbf{r}) \exp(i\mathbf{k} \cdot \mathbf{r}), \quad (1)$$

Where $u_k(\mathbf{r})$ has the periodicity of the lattice: $u_k(\mathbf{r}) = u_k(\mathbf{r} + \mathbf{T})$. Here \mathbf{T} is the translation vector of the lattice. Equation (1) is a formulation of Bloch's theorem, which shows that for a wave equation in a periodic potential field, its eigenfunction consists of a plane wave $\exp(i\mathbf{k} \cdot \mathbf{r})$ multiplied by a function $u_k(\mathbf{r})$ with a lattice period. Under this circumstance, the wave function of a single electron given by the formula is a Bloch function, which can be expressed as the addition of traveling waves. In the meantime, the Bloch waves can be superimposed as wave packets to represent electrons that freely propagate in the real field of ions [9].

3. The first-principles calculations

First principles calculation refers to the method of solving material properties based on the basic principles of quantum mechanics without introducing empirical models and parameters. It includes Hartree-Fock method, post-Hartree-Fock method (such as multi-body perturbation theory, configuration interaction method, coupled cluster method) and multi-reference state method. Density functional theory (DFT) is also commonly considered as first-principles calculations in solid computing.

3.1 Density functional theory (DFT)

In 1964 and 1965, Kohn and Hohenberg jointly published the basic theory on the nature of electronic ground states, which became the basis of the famous theory of density functional theory. Hohenberg and Kohn pointed out that there exists a universal electron density function $F(n(\mathbf{r}))$ in the presence of an external potential field $v(\mathbf{r})$. It has no dependence on the external potential field $v(\mathbf{r})$. This conclusion applies to all ground state electronic systems. Therefore, once we know that the electron Density function, then the ground state energy in the external potential field can be easily calculated, that is, $E \equiv \int v(\mathbf{r})n(\mathbf{r})d\mathbf{r} + F(n(\mathbf{r}))$ [8].

3.2 Exchange associated functional

The Kohn-Sham equation depends largely on the choice of exchange-related functionalities, and approximation of local density, generalized gradient approximation and hybrid functional approximation are usually used to approximate the exchange-related functional. Among them, local density approximation is the assumption that when the solid is in a very small range, its electron can be seen as homogeneous. At this time in this local area, the exchange correlation function is the same for the exchange of related electron and electron density system of uniform electron gas. Therefore, the exchange-related functionalities can be written as a function of local electron density,

$$E_{xc}[n] = \int n(\mathbf{r}) \varepsilon_{xc}(n(\mathbf{r})) d\mathbf{r} = \int n(\mathbf{r}) [\varepsilon_x(n(\mathbf{r})) + \varepsilon_c(n(\mathbf{r}))] d\mathbf{r}, \quad (2)$$

Where $\varepsilon_{xc}(n(\mathbf{r})) = \varepsilon_x(n(\mathbf{r})) + \varepsilon_c(n(\mathbf{r}))$ is the density of related energy exchange.

4. Tight-binding models

Among the carbon materials, besides diamond, π -electron is the most relevant to transport of carbon material or other solid-state properties; Tight Binding calculation gives the band structure of π -electron system simply and accurately.

Tight binding approximation is not a self-consistent method of calculation, however, the occupation of an electron in the band structure must be self-consistent. Therefore, to get a given electronic occupancy, the corresponding Hamiltonian potential can be calculated first, and then the electronic occupancy status is continually updated, such as using the Mulliken gross population analysis. Within the accuracy range, when the input and output of electronic occupancy are consistent, it can be said that the calculation of the energy eigenvalue has reached a self-consistent.

In the practical application of the above calculation method, the symmetry of the solid is usually carefully considered, which not only can simplify the calculation, moreover, on the basis of the tight binding model approximation, the transfer matrix and the overlap matrix obtained can be used as the parameters for calculating the electronic band structure for calculating the energy band structure of the material, and the experimental values and the first principle calculations results are compared. Furthermore, both the perturbation theory using extrapolation and the Slater-Koster method using interpolation can be used to derive the electronic properties of carbon material systems.

5. Deformation Potential (DP)

The concept of deformation potential was proposed by Bardeen and Shockley in 1950 [10]. It describes that the deformation of non-polar semiconductor lattice can lead to the conduction band (CB) and valence band (VB). And the mobility of electrons (e) and holes (h) under longitudinal acoustic phonon (LA) scattering. The carrier mobility is first discussed based on the concept of the effective mass (m^*) introduced into the carrier.

The electronic properties exhibited by semiconductors are often controlled by the electronic properties of the conduction or valence band near the Fermi surface. Therefore, the relationship between $E(k)$ and k in the vicinity of the energy band can be found by using Taylor expansion approximation. Assuming that the value of k near the bottom of the band is very small, expanding $E(k)$ to k^2 at $k = 0$ yields:

$$E(k) = E(0) + \left(\frac{dE}{dk}\right)_{k=0} k + \frac{1}{2} \left(\frac{d^2E}{dk^2}\right)_{k=0} k^2 + \dots, \quad (3)$$

Because when $k=0$, $\left(\frac{dE}{dk}\right)_{k=0} = 0$, so we care about the second term $E(k) - E(0) = \frac{1}{2} \left(\frac{d^2E}{dk^2}\right) k^2$,

from which it can be defined $\frac{1}{\hbar} \left(\frac{d^2E}{dk^2}\right)_{k=0} k^2 = \frac{1}{m_n^*}$. Usually define m_0 as the electronic inertial mass, m_n^* as the effective mass of electrons, which is positive.

Mobility is a manifestation of the semiconductor's behavior in the application of external electric fields. Under the action of an external electric field of intensity \mathcal{E} , the change of electron energy is

$dE = \frac{f}{\hbar} \frac{dE}{dk} dt$, and $dE = \frac{dE}{dk} dk$, so $f = \hbar \frac{dk}{dt}$, the rate of change of electron wave vector k is proportional to the external force. On the other hand, the acceleration of the electrons is

$$a = \frac{dv}{dt} = \frac{f}{\hbar^2} \left(\frac{d^2 E}{dk^2} \right), \text{ which is obtained by taking the expression of the effective mass } m_n^* \text{ into the}$$

$$a = \frac{f}{m_n^*}$$

above equation:

From this it can be seen that in the semiconductor under the action of external electrons, describing the law of its movement is the effective mass m_n^* , rather than inertial mass m_0 . More in-depth, the effective mass can be determined by cyclotron resonance experiment, the introduction of the concept of effective mass is that it summarizes the role of the internal potential field of the semiconductor, when studying the law of the movement of electrons in an external potential field, we may not discuss the potential for internal interaction with other atoms or electrons.

The traditional theory of deformation potential points out that when a uniform strain ε_{ij} is applied to the lattice, the energy band structure near the Fermi surface can be expressed as: $E(\varepsilon_{ij}) = E_0 + E_1 \Delta$, where $\Delta = \varepsilon_{11} + \varepsilon_{22} + \varepsilon_{33}$. In a system with a small momentum P , the energy expression is $E(P, \varepsilon_{ij}) = E_0(P) + E_1 \Delta + O(P^2)$, and the last term reflects the change of the effective mass with strain, which is negligible. Therefore, the movement of the band edge can be described by the deformation potential $E_1 \Delta$, where E_1 is called the traditional deformation potential constant. The deformation potential theory is widely used to study the mobility of semiconductor materials.

6. Conclusion

Recently, the theoretical prediction on carrier mobility of two-dimensional (2D) materials has aroused wide attention. It is particularly important to theoretically design and screen the high-performance 2D layered semiconductor materials with suitable band gap and high carrier mobility. In this paper, we summarized the basic methods and principles of first principles calculations for solid materials. In the meantime, the calculation method of two-dimensional Dirac material mobility around graphene is described in detail. At present, Tight-binding models and Deformation Potential theory are the most mature methods for calculating 2D materials. Of course, there are some approximations between these two methods. The intrinsic mobility of graphene is controlled by the phonon scattering process. The traditional deformation potential theory takes into account the scattering of longitudinal acoustic (LA) phonons. However, the resulting deformation constant is about 20eV, which is nearly four times larger than the 4 eV calculated by the first-principles calculation. Now we realized that among the factors that affect the mobility of graphene, transverse acoustic phonon scattering (TA) and longitudinal acoustic phonon scattering process are very important. Therefore, there are still many problems for the study of two-dimensional material mobility worth exploring and studying in depth.

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