



Energy band nonparabolicity and density of states of graphene

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ABSTRACT

Energy band nonparabolicity is present in the materials such as graphene, GaAs, HgCdTe, InSb, wurtzite GaN etc. The energy levels for the nonparabolic subbands are different from parabolic subbands. In this work we discuss about nonparabolicity factor and find its numerical value in monolayer, bilayer and multilayer graphene. We also discuss how the nonparabolicity affects the density of states of graphene. The density of states function tells us how many quantum states are available in the band per unit energy level. The nonparabolic effects are more pronounced in two-dimensional system because carriers in subbands are always away from the band edge. Here, we use a dispersion relation that can be used to describe nonparabolicity in a variety of materials and device structures. This dispersion relation is based on Kane's k.p model and is suitable for both narrow and widegap nonparabolic materials.

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KEYWORDS

Nonparabolicity;
Density of states;
Graphene;
Kane's k.p model.

INTRODUCTION

The effect of nonparabolicity in energy band on semiconductor device has been noticed in the case of bulk material^[1-3], inversion layer^[4], heterojunction interfaces^[5], quantum wells^[6-8] and superlattices^[9,10]. The nonparabolicity is well established in narrow gap devices. Some examples of non-parabolic solid state materials are HgCdTe, GaAs and graphene. The situation is complicated in wide gap materials such as GaAs and graphene when spin orbit interaction is taken into account.

Graphene^[11] is the recently discovered thinnest and strongest ever measured material in the universe. Its charge carrier exhibit intrinsic mobility and can travel micrometer long distance without scattering at room temperature. This is a monolayer of carbon atoms^[12,13].

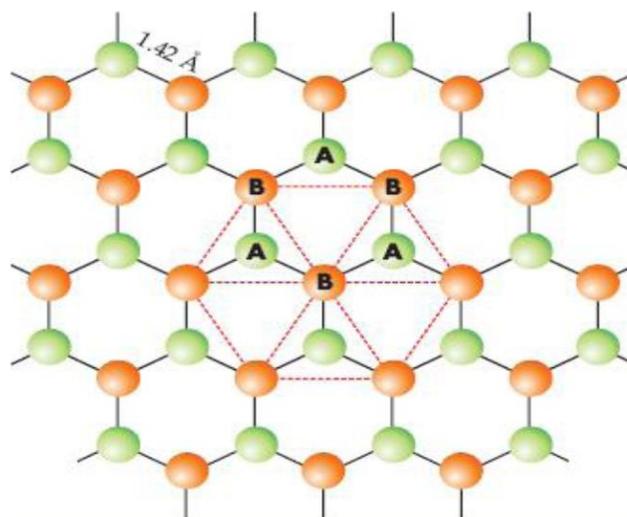


Figure 1 : Honeycomb structure of graphene^[12]

They are packed into a dense honeycomb crystal structure. Carbon atoms are arranged in hexagonal struc-

ture and have two atoms per unit cell. The carbon-carbon bond length is 1.42\AA (Figure 1)^[12].

This paper is organized as follows: In section 2, we discuss about band structure of monolayer graphene. In section 3, we discuss band structure of bilayer graphene. In section 4, we evaluate the nonparabolicity

factor of graphene and discuss the dependence of density of states on it.

BAND STRUCTURE OF MONOLAYER GRAPHENE

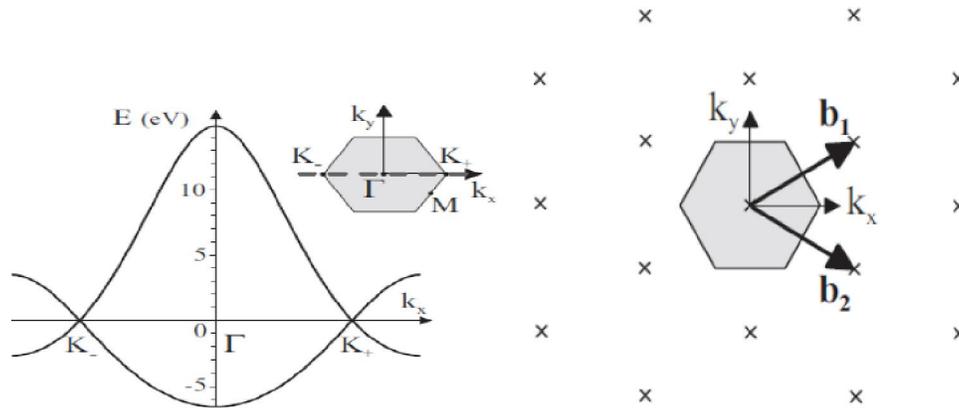


Figure 2 : Band structure of monolayer graphene^[14,15]

The electronic band structure of monolayer graphene is gapless with crossing of the bands at two points K_+ and K_- located at the corners of the Brillouin zone. Although the first Brillouin zone has six corners only two of them are non equivalent pair. It is possible to connect two of the other corners to K_+ using a reciprocal lattice vector (Hence the other two are equivalent to K_+) and it is possible to connect K_+ and K_- with a reciprocal lattice vector. To distinguish between K_+ and K_- an index $\hat{a} = \pm 1$ is used. Using this values of primitive lattice vector b_1 and b_2 it can be seen that the wave vector corresponding to point $K_{\hat{a}}$ is given by $K_{\hat{a}} = \hat{a} (4\delta/3a, 0)$. The K points are called ‘valley’s using nomenclature from semiconductor physics. Exactly at the

$k_{\hat{a}}$ point, $k = K_{\hat{a}}$. This indicates that there is no coupling between the A and B sublattices exactly at the $K_{\hat{a}}$ point. The two sublattices are both hexagonal Bravais lattices of carbon atoms.

BAND STRUCTURE OF BILAYER GRAPHENE

Bilayer graphene consists of two weakly Vander Waals coupled honeycomb sheets of covalent bond carbon atoms. The system can be described in terms of four sublattices. There are four energy bands, two conduction bands and two valence bands. Overall, the band structure is similar to that of monolayer graphene, with

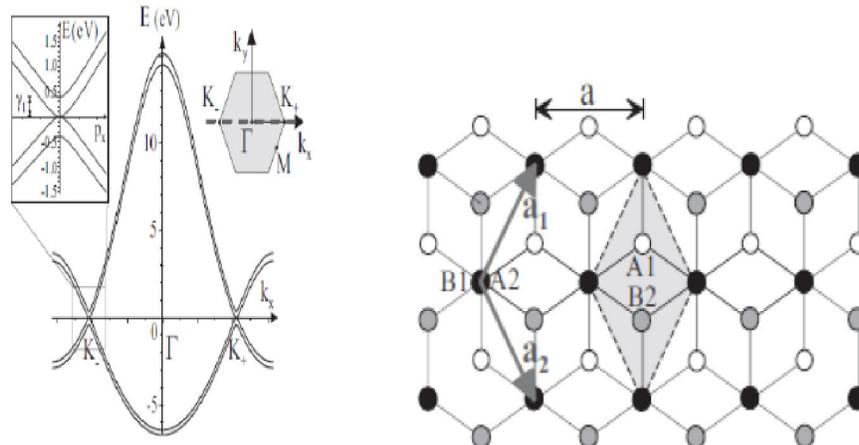


Figure 3 : Band structure of bilayer graphene^[14,15]

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each monolayer band split into two by an energy. The most interesting part of the band structure is in the vicinity of the K points, as shown in the left inset of Figure 3 which focuses on the bands around K_+ .

NONPARABOLICITY FACTOR OF GRAPHENE

For energies above $k = 0$ of the order of a fraction of the band gap the conduction band becomes nonparabolic. At this point straight forward perturbation theory breaks down because of the small band gap the nonparabolic nature of the conduction band will be important at high temperature or high electron concentration.

Kane considered both $k.p$ interaction^[1,2] and spin orbit coupling as perturbations to the classical Hamiltonian in isotropic material. The resulting Hamiltonian can be diagonalized exactly and does not in principle require the carrier kinetic energy E to be small. However Kane's solution is accurate only if the interaction with the other bands can be neglected which does imply a small E . We define E_g as the prime bandgap and E as the split of splitting which can be written^[8,9] as:

$$E'(E'+E_g)(E'+E_g+E_\Delta)=k^2P^2(E'+E_g+2E_\Delta/3) \quad (1)$$

where $E'=E-(\hbar^2k^2/2m_0^2)$ and P is Kane's momentum. At the band extremum $E \approx 0$.

We can approximate (1) taking upto second order terms (E^2)^[16,17]

$$\hbar^2k^2/2m_1 \approx E + \alpha E^2 \quad (2)$$

where m_1 is the electron effective mass at the band minimum and α is the nonparabolicity factor. eq.(2) represents dispersion relation which is based on Kane's $k.p$ model. The nonparabolicity factors can be determined from (1) and (2)

$$\frac{1}{m_1} = \frac{1}{m_0} + \frac{2p^2}{\hbar^2 E_g} \frac{E_g + \frac{2\Delta}{3}}{E_g + \Delta}, \quad \alpha = \frac{1}{E_g} \left(1 - \frac{m_1}{m_0}\right)^2 \quad (3)$$

Using eq.(3) we can determine the numerical value of nonparabolicity factor for different materials.

In the case of GaAs, $m_1 = 0.067m_0$

$$\alpha = 1/E_g (1-0.067)^2 = 0.87/E_g \quad (4)$$

In the case of graphene nonparabolicity factor depends on electron effective mass

So the nonparabolicity factor of monolayer graphene

	Structure	m_1/m_0 ^[18]
a)	Monolayer grapheme	0.0
b)	Bilayer grapheme	0.022
c)	Multilayer grapheme	0.031

$$\alpha = 1/E_g (1-0)^2 = 1/E_g \quad (5)$$

In case of bilayer graphene, the nonparabolicity factor

$$\alpha = 1/E_g (1-0.022)^2 = 0.956484/E_g \quad (6)$$

In case of multilayer graphene,

$$\alpha = 1/E_g (1-0.031)^2 = 0.4761/E_g \quad (7)$$

DENSITY OF STATES OF GRAPHENE

The states in the bands and their dependence on energy are described by density of states. In semiconductor heterostructures, the free motion of carriers is restricted to two, one or zero

spatial dimension. Here, we use the following relations to determine density of states of graphene^[19]:

$$E(k) = \pm \hbar V_f \sqrt{k_x^2 + k_y^2} \quad V(k) = \frac{1}{\hbar} \frac{\partial E}{\partial K} = V_f, \quad (8)$$

where the Fermi velocity $V_f = 1 \times 10^8$ cm/s.

The density of states of graphene can be evaluated as

$$D_{2D}(E) = \frac{1}{A} \sum \delta(E - E_k) = \frac{1}{A} \frac{A}{(2\pi)^2} \times 2 \int_0^\infty \delta(E - E_k) 2\pi k dk \quad (9)$$

$$E_k = \hbar V_f k \quad dE_k = \hbar V_f dk \quad k dk = E_k dE_k / \hbar^2 V_f^2$$

Here, the factor 2 is due to valley degeneracy (g_v) of graphene.

Putting the above values in eq. (9) we get

$$D_{2D}(E) = \frac{g_v}{\pi v_f^2 \hbar^2} \int_0^\infty \delta(E - E_k) E_k dE_k \quad (10)$$

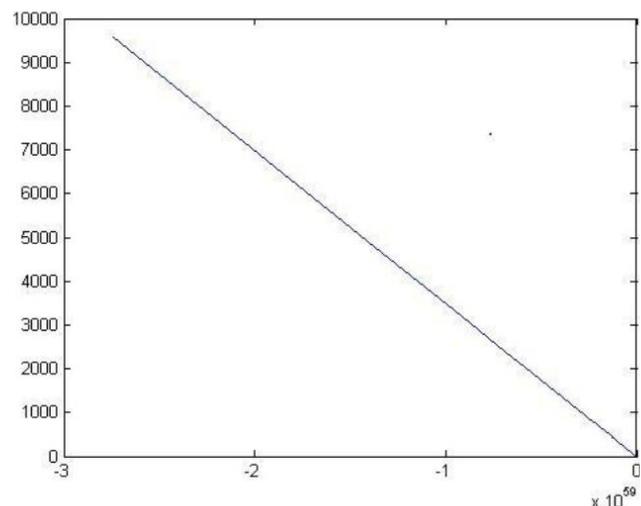


Figure 4 : Dependence of density of states of graphene on nonparabolicity factor. In X- axis nonparabolicity factor and along Y axis density of states have been plotted.

$$D_{2D}(E) = \frac{2E}{\pi v_f^2 \hbar^2} \quad (11)$$

Taking the help of eq. (2), equation (11) can be written as

$$D_{2D} = 2 \left(\frac{\hbar^2 k^2 - 2\alpha E^2 m_1}{2m_1} \right) \times \frac{1}{\pi \hbar^2 v_f^2} \quad (12)$$

Eq. (12) represents the dependence of density of states of graphene on nonparabolicity factor. It is shown in Figure 4.

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