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Investigation of the electron-surface phonon interaction effects in graphene on a substrate made of polar materials

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ABSTRACT

We present a theoretical study of the electron- surface phonon interaction in mono-layer graphene (1LG) on polar substrates such as SiO_2,HfO_2,SiC and hexagonal BN. Thus we have used the eigen energies derived from the tight-binding Hamiltonian in mono-layer graphene. Our results indicate that the electron-surface phonon interaction depends on the polar substrate. Such polar substrates allow for the existence of polar optical phonons localized near the graphene-substrate interface which could be an important scattering source for graphene carriers through the long-range Fröhlich coupling. Likewise, we have investigated the effect of various dielectrics on the SO phonon-limited mobility, the SO phonon-limited resistivity, the SO phonon-limited conductivity and the scattering rate in single layer graphene by considering the effects of the SO optical phonon scattering arising from the polar substrates and by varying the temperature, the charge carrier density and the physical separation between graphene and interface of dielectric substrate.

1. Introduction

Graphene, a two-dimensional (2D) system composed of carbon atoms arranged in a hexagonal, honeycomb lattice continues to attract much attention of scientific interest due to its many important physical properties, such as high mobility and conductivity, high optical transparency, mechanical flexibility, robustness, and environmental stability [1–3]. Thus graphene is a promising material in diverse device applications such as transparent electrodes, solar cells, photodetectors, nanogenerators, and light-emitting diodes [4–8]. This material exhibits extraordinary optoelectronic properties derived from its peculiar band structure of massless charge carriers and relativistic properties of the conduction electrons in a single graphene layer [9]. Graphene is an excellent candidate for the next generation of electronic materials due to its fascinating electrical, mechanical, optical and thermal properties [10–13].

In single layer graphene (1LG) valence and conduction bands touch each other, making it a zero gap semiconductor, i.e. a semimetal, with a conically shaped valence and conduction band reminiscent of relativistic Dirac cones for massless particles [13,14]. In addition the 1LG electronic structure is a linear dispersion around the K point of the Brillouin zone, which makes it different from most materials in condensed matter physics. Consequently the Schrödinger equation is not being sufficient to describe its electronic properties. 1LG is an exception and its charge carriers mimic relativistic particles and are more easily and naturally described by the Dirac equation [15].

In fact, several features make graphene's electronic properties truly unique and different from the other material. The first is that: its electrons can cover submicron distance without scattering. Second, the electron waves propagating through the honeycomb lattice completely lose their effective mass, which results in quasiparticles that are described by a Dirac like equation rather than the Schrödinger equation [9,16,17] Third, due to the massless carriers and little scattering, quantum effects in graphene are robust and can survive even at room temperature. Fourth, electron waves in graphene propagate within a layer that is only one atom thick, which makes them accessible and amenable to various scanning probes.

The coupling of the electronic degrees of freedom to lattice degrees of freedom is crucial to understanding materials properties. This coupling is usually described by interactions between the electronic excitations and phonons, and is responsible for many interesting effects in a crystal, such as the formation of polarons.

The vibrational properties of graphene, shows that the phonon dispersion is shaped by the effects of electron–phonon interaction, which results in the presence of two Kohn anomalies in the highest optical branch. Thus the properties of phonons in graphene have attracted strong attention of the researchers to explain the effect of electron–phonon interaction in optical properties of graphene.

Graphene is a non-polar material, thus the most current available graphene samples uses polar substrate such as SiO_2, SiC, h-BN or HfO_2

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for fundamental studies and certainly for technological applications. Such polar substrates allow for the existence of polar optical phonons localized near the graphene-substrate interface which could be an important scattering source for graphene carriers through the long-range Fröhlich coupling. Thereby the study of electron SO phonon coupling effects is important for understanding the role of this coupling in the change of the electronic properties in graphene using polar substrate such as SiO_2, SiC, h-BN or HfO_2. Thus the electron SO phonon coupling affects the transport properties which allow scientists to develop quantitative theories for many different experimental studies in graphene.

In this paper, we present an overview of our theoretical studies of one specific dynamical optical property, namely electron–phonon (e–ph) interactions in single layer graphene (1LG). This material exhibits a high electronic quality, in which charge carriers can travel thousands of interatomic distances without scattering [18,19]. These interactions between the electronic excitations and phonons are responsible for the formation of polarons in the single layer graphene (1LG).

This paper is organized as follow; first we begin with a description of the crystal structure of monolayer graphene; the real space structure and the reciprocal lattice of graphene, then we present the eigenenergies derived from the tight-binding Hamiltonian in mono-layer graphene. Second, we investigate the electrical transport in graphene by calculating the SO phonon-limited mobility, the SO phonon-limited resistivity, the SO phonon-limited conductivity and the scattering rate in the single layer graphene (1LG) on polar substrates. Third, we study theoretically the electron-surface phonon interaction in monolayer graphene on polar substrates such as SiO_2,HfO_2,SiC and hexagonal BN.

2. Electronic structure of monolayer graphene

Graphene is made out of carbon atoms arranged in hexagonal structure as shown in Fig. 1.

Note that the honeycomb structure is not a Bravais lattice because atomic positions A and B are not equivalent. Taken alone, the A atomic positions (or, the B atomic positions) make up an hexagonal Bravais lattice and, in the following, we will often refer to them as the 'A sublattice' (or, the 'B sublattice'). This structure can be seen as a triangular lattice with a basis of two atoms per unit cell. Where the primitive vectors of the honeycomb lattice are:

$$a_1=a_0\left(\frac{3}{2},\frac{\sqrt{3}}{2}\right)$$

$$a_2=a_0\left(\frac{3}{2},-\frac{\sqrt{3}}{2}\right)$$

The symbol a_0 denotes the carbon-carbon bond length, which is about 1.42 Å. The reciprocal lattice is characterized by the following lattice vectors:

$$b_1=\left(\frac{2\pi}{3a_0},\frac{2\pi}{\sqrt{3}a_0}\right)$$

$$b_2=\left(\frac{2\pi}{3a_0},-\frac{2\pi}{\sqrt{3}a_0}\right)$$

The two points K and K′ at the corners of the graphene Brillouin zone (BZ) have a particular importance for the physics of graphene. Their positions in momentum space are given by:

$$K=\left(\frac{2\pi}{3a_0},\frac{2\pi}{3\sqrt{3}a_0}\right)$$

$$K'=\left(\frac{2\pi}{3a_0},-\frac{2\pi}{3\sqrt{3}a_0}\right)$$

The vectors $\delta_i(i=1,2,3)$ connect the three nearest neighbors vectors in real space and are given bellow:

$$\delta_1=\frac{a_0}{2}(1,\sqrt{3})$$

$$\delta_2=\frac{a_0}{2}(1,-\sqrt{3})$$

$$\delta_3=-a_0(1,0)$$

The primitive cell of graphene contains two atoms, one at R which runs over sublattice A another at $R+\delta_1$ which runs over sublattice B. $R=\delta_1+a_1n_1+a_2n_2$ where $n_{1,2}$ are integers

Throughout this theoretical study, we use a Cartesian coordinate system with x and y axes in the plane of the graphene crystal.

The tight-binding Hamiltonian for electrons in mono-layer graphene considering that electrons can hop both to nearest and next nearest neighbor atoms has the form [20]:

$$H=-t_0\sum_{R\in A}\sum_{i=1,2,3}c_R^*c_{R+\delta_i}+H.\,c.$$

Where "H.c." stands for "Hermitian conjugate" and t_0~3.1 eVis the nearest neighbor hopping energy (hopping between different sublattices) [20].

The energy bands derived from this Hamiltonian are given as follow [20]:

$$E(k)=\varepsilon_{k\pm}=\pm|t_k|=\pm t_0\sqrt{3+F(k)}$$

where

$$t_k=t_0\left[1+2exp\left(-i\frac{3k_xa_0}{2}\right)\cos\left(\frac{\sqrt{3}}{2}k_ya_0\right)\right]$$

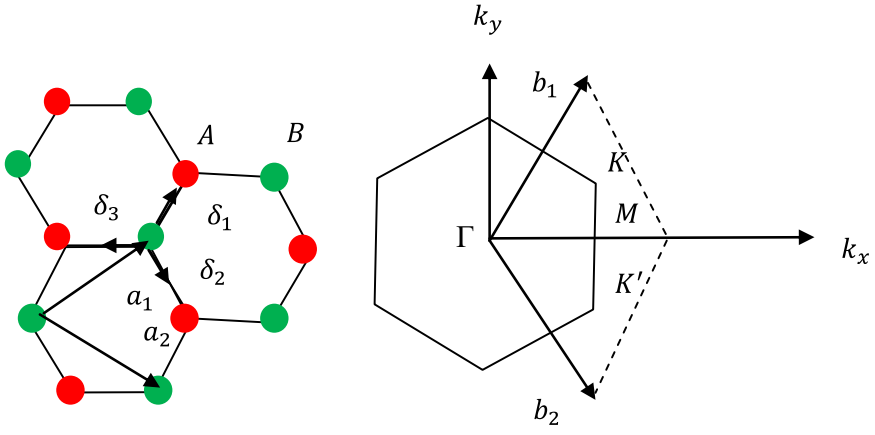

Fig. 1. Left: lattice structure of graphene, made out of two interpenetrating triangular lattices a_1 and a_2 are the lattice unit vectors, and δ_i,i=1, 2, 3 (are the nearest neighbor vectors); right: corresponding Brillouin zone. The Dirac cones are located at the K and K′ points.