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Surface optical phonon-assisted cyclotron resonance in graphene on polar substrates

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HIGHLIGHTS

- PACR in graphene on polar substrates has been investigated.
- The two-photon absorption process has been included.
- The combined effect on MOAC and half-width has been discussed.
- A significantly quantitative picture for SO phonons interaction has been provided.

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ABSTRACT

We theoretically study the influence of surface optical (SO) phonons on the phonon-assisted cyclotron resonance (PACR) effect in a single-layer graphene on different polar substrates via both one- and two-photon absorption processes. The two-photon absorption process gives a significant contribution to magneto-optical absorption coefficient (MOAC) compared to one-photon process. The shifts of the absorption peaks are larger for polar substrates than those in graphene on nonpolar substrates, where only the intrinsic optical phonons of graphene with higher energy contribute. Effects of temperature, graphene-substrate separation, and magnetic field on the magneto-optical absorption coefficient and the half-width are discussed. Our results provide a significantly quantitative picture for SO phonons interaction induced magneto-optical absorption in graphene on polar substrates.

1. Introduction

Single-layer graphene exhibits an outstanding physical properties, including fascinating transport and optical properties [1–6]. One of its significant physical properties results from the unusual Landau levels (LLs) in a perpendicular quantized magnetic field. In contrast to conventional 2D systems where LLs are proportional to a non-negative integer and equally spaced, the LLs of graphene are not equally spaced in energy but proportional to both the square root of the magnetic field and the LL index [7–11]. This unusual LL structure of graphene has been observed indirectly by the use of cyclotron resonance [12–16]. One more of the main reasons for the enormous interest shown in graphene in a magnetic field is its peculiar optical properties, which is conveniently described by the so-called magneto-optical absorption coefficient. In contrast to traditional 2D electron gases, which only show one obvious absorption peaks centered around the cyclotron resonance energy, in single-layer graphene a series of distinct optical absorption peaks can be experimentally observed [8,13,17–21].

It is evident that the phonon-assisted electron transitions between different LLs involving the absorption or emission of a phonon can be displayed via a series of peaks in the density of states [22]. Although these transitions have involved optical phonons, the electron–phonon interaction has not been described clearly. It is known that in graphene, the electron – optical phonon interaction plays an important role for understanding of electron transitions between different LLs [23,24], of the absorption or emission of optical phonons by electrons [25], and of the absorption of photon [26]. Meanwhile, based on the theory of the fine structure of PACR in graphene, Zhu et al. [27] have discovered that even for small electron–phonon coupling, the PACR is governed by the peaks resulting from the electron–phonon interaction, which established an asymmetric doublet around the optical phonon

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frequency. However, this result has been obtained only with the one-photon absorption while the two-photon one has not been done. In one of our previous work [28], we investigated the PACR effect in a single-layer suspended graphene sheet via two-photon absorption. The result demonstrated that the PACR effect is a useful tool for examining magneto-optical properties of graphene material. However, a detailed consideration of this effect in graphene on polar substrates is still lacking.

When graphene is situated on a polar substrate, electrons couple with two different types of phonons: intrinsic graphene optical phonons [29–31] and SO phonons of polar substrates [32–35]. These SO phonons interact with the electrons in graphene via their electric fields [36,37], and can have a profound impact on current saturation in graphene [32,38–41], on the carrier mobility [42,43], on the optical absorption [37,44], on magneto-phonon resonance [45], and on magneto-optical conductivity [46]. Hence, it stands to reason that the magneto-optical properties of graphene on polar substrates, including PACR effect, would be affected by SO phonons. Therefore, a detailed investigation of SO phonons in graphene on different polar substrates and the related MOAC can provide important information for graphene-electronic devices. With increasing reports on the observation of SO phonon modes in graphene, it is therefore believed that the influence of SO phonons on PACR effect in graphene is especially important and should be taken into account. The main goal of this work is to study the PACR effect generated from SO phonons in a single-layer graphene on polar substrates in both one- and two-photon absorption processes. To do this in Section 2, we derive an expression for the MOAC. The evaluation for single-layer graphene on different substrates is presented in Section 3. The conclusion is shown in Section 4. Our results show that the substrates strongly influence on the magneto-optical absorption spectra not only in the magnitude but also in the position of the resonant peaks due to electron − SO phonons scattering.

2. Theory

In this work, we mainly consider a single-layer graphene situated on the polar substrates. In the presence of magnetic field of magnitude B and perpendicular to the graphene sheet, the Hamiltonian of the carrier − SO phonon systems is given by

$$\mathscr{H} = \sum_{n,k,\nu} \varepsilon_n a^{\dagger}_{n,k,\nu} a_{n,k,\nu} + \sum_{\mathbf{q},\nu} \hbar\omega^{\nu}_{SO} b^{\dagger}_{\mathbf{q},\nu} b_{\mathbf{q},\nu} + \mathscr{H}_{int}, \tag{1}$$

where $\varepsilon_n = S_n\hbar\omega_c\sqrt{n}$ is the energy spectrum for a carrier with the effective magnetic energy $\hbar\omega_c = \gamma\sqrt{2}/a_c$, $a_c = (\hbar/eB)^{1/2}$ the magnetic length, and γ the band parameter [9–11], $S_n = +1$ and -1 stand for the conduction and valance bands, respectively. Here, n is an integer denoting a LL in the conduction ($n > 0$) or valence bands ($n < 0$). The LL with $n = 0$ is at both the bottom of the conduction and the top of the valence bands. The wave function associated with the energy spectrum ε_n has been presented in Refs. [9,11,47]. Also $a^{\dagger}_{n,k,\nu}(a_{n,k,\nu})$ is the carrier creation (annihilation) operator with the valley and momentum quantum numbers ν and k. The second term of Eq. (1) is the phononic Hamiltonian, where $\hbar\omega^{\nu}_{SO}$ is the SO phonon energy and $b^{\dagger}_{\mathbf{q},\nu}(b_{\mathbf{q},\nu})$ represents the surface phonon creation (annihilation) operator for the ν-th mode. The last term of Eq. (1) is the carrier − phonon interaction part of the Hamiltonian, which is given by [36].

$$\mathscr{H}_{int} = e\mathscr{F}_{\nu}\sum_{\mathbf{q}} \frac{e^{-qd}}{\sqrt{q}}\left(e^{i\mathbf{q}\cdot\mathbf{r}} b^{\dagger}_{\mathbf{q},\nu} + e^{-i\mathbf{q}\cdot\mathbf{r}} b_{\mathbf{q},\nu}\right), \tag{2}$$

where e is the absolute value of the electron charge, $\mathbf{q}$ and $\mathbf{r}$ are the two-dimensional wave vector and spatial vector in the graphene plane, respectively, and d is the equilibrium distance between the graphene sheet from the substrate. The carrier − phonon coupling parameter $\mathscr{F}_{\nu}$ is given by [36,48–50].

$$\mathscr{F}^2_{\nu} = \frac{\hbar\omega^{\nu}_{SO}}{2\mathscr{A}\varepsilon_0}\left(\frac{1}{\chi_{\infty}+1} - \frac{1}{\chi_0+1}\right), \tag{3}$$

where $\chi_{\infty}(\chi_0)$ is the high (low) frequency dielectric constant, $\mathscr{A}$ is the area of graphene, and ε_0 the permittivity of vacuum. In the following, we will treat this interaction term to calculate the optical absorption coefficient due to the carrier − SO phonons scattering.

To obtain the optical absorption intensity, we calculate the magneto-optical absorption coefficient $K(\Omega)$. When an electromagnetic field with frequency Ω is applied to the system, the MOAC of a Dirac fermion due to scattering from the potential of the ν-th SO phonon in graphene on a substrate is given by [51].

$$K^{\nu}(\Omega) = \frac{\sqrt{\varepsilon}}{n_r c}\sum_{\alpha} \mathscr{W}^{\pm,\nu}_{\alpha,\alpha'} f_{\alpha}, \tag{4}$$

where ε is the average dielectric constant of the system. For example, for graphene between SiC ($\chi_{SiC} = 9.7$) and air ($\chi = 1$), $\varepsilon = (9.7+1)/2 = 5.35$, n_r is the refractive index, c is the speed of light in free space. The electronic states for a carrier are specified by the set of quantum numbers $\alpha = (n,k,\nu)$, the Fermi-Dirac function $f_{\alpha} \equiv f_n$ is associated with the energy spectrum $\varepsilon_{\alpha} \equiv \varepsilon_n$. The transition probability due to carrier − photon−phonon interaction, $\mathscr{W}^{\pm,\nu}_{\alpha,\alpha'}$, of the 2D carrier can be written with the use of Fermi's golden rule [28,52–54] and taking into account the properties of the graphene LL wave functions

$$\mathscr{W}^{\pm,\nu}_{\alpha,\alpha'} = \frac{2\pi}{\hbar}\sum_{\alpha',\mathbf{q}}\sum_{\ell=1}^{\infty}\frac{(a_0 q)^{2\ell}}{(\ell!)^2 2^{2\ell}}\left|\mathscr{M}^{\pm,\nu}_{\alpha',\alpha}\right|^2 (1-f_{\alpha'})\delta\left(\varepsilon_{\alpha'} - \varepsilon_{\alpha} \pm \hbar\omega^{\nu}_{SO} \pm \ell\hbar\Omega\right), \tag{5}$$

where the upper (+) and lower signs (−) refer to the emission and absorption processes of phonons and photons, respectively, a_0 is the dressing parameter. The transition matrix element of the carrier − SO phonons interaction $\mathscr{M}^{\pm,\nu}_{\alpha',\alpha}$ is given by

$$\left|\mathscr{M}^{\pm,\nu}_{\alpha',\alpha}\right|^2 = g_{\nu}g_s e^2 \mathscr{F}^2_{\nu}\frac{e^{-2qd}}{q}\cos^2\left(\frac{\theta}{2}\right)\left|\mathscr{J}_{nn'}(x)\right|^2\left(N^{\nu}_q + \frac{1}{2}\pm\frac{1}{2}\right)\delta_{|n|,|n'|\pm 1}, \tag{6}$$

where $g_{\nu} = 2$ and $g_s = 2$ are the valley and spin degeneracy, respectively; θ is the scattering angle; the Bose factor N^{ν}_q presenting the number of $(\nu,\mathbf{q})$ phonon; and the function $\mathscr{J}_{nn'}(x)$ is defined as follows [11].

$$\left|\mathscr{J}_{nn\nu}(x)\right|^2 = C_n^2 C_{n'}^2 \frac{m!}{(m+j)!}e^{-x}x^j\left[L^j_m(x) + S_n S_{n'}\sqrt{\frac{m+j}{m}}L^j_{m-1}(x)\right]^2, \tag{7}$$

where $C_n = ((1+\delta_{n,0})/2)^{1/2}$, $x = a_c^2 q^2/2$, $m = \min(|n|,|n'|)$, $j = ||n'| - |n||$; and $L^j_m(x)$ is the associated Laguerre polynomials.

The transition probability in Eq. (5) contains a contribution of the absorption process of ℓ−photon. In this work, we only restrict ourselves to consider the two-photon absorption, i.e. $\ell = 1,2$. Substituting Eq. (5) into Eq. (4) and straightforwardly calculating, we have the following expression for the MOAC of a Dirac fermion due to scattering from the potential of the ν-th SO phonon via two-