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Optical conductivity of semiconductor crystals with a screw dislocation

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ABSTRACT

We study ac electronic transport in semiconductor crystals with a screw dislocation. The screw dislocation in the crystal results in an effective potential field that has a pronounced effect on the quantum mechanical electronic transport of the system. Alternating current conductivity at a frequency around 100 GHz has been calculated, showing upward shift in the peak position with increasing the Fermi energy. The result is in contrast to the persistency in the peak position observed in a dislocation-free crystal penetrated by magnetic flux, despite the apparent similarity between the two crystalline systems.

1. Introduction

Screw dislocations in crystalline media have attracted a growing interest from both theoretical and experimental viewpoints. From a technological view, screw dislocations are known to be considerably detrimental to device performance because they result in low breakdown voltage and high current linkage. This explains the accumulation of experimental measurements of their characteristics such as density [1,2], spatial distribution [3], amplitude [4,5], and mobility under strain and thermal conditions [6].

In addition to their importance in device development, screw dislocations have profound influences on the electronic [7–9] and optical [10] properties of the host materials; dislocations are also known to yield the polarization plane rotation of light [11] and interference of elastic [12] or classical spin waves [13]. These physical consequences are partly attributed to the dislocation-induced gauge field [14,15]. It was indeed theoretically suggested [16] that, in the continuum limit, a single screw dislocation plays a role similar to that of an isolated magnetic flux tube. More precisely, the Schrödinger equation for electrons moving around a screw dislocation is endowed with an effective vector potential that may cause Aharonov–Bohm (AB) interference phenomena [16–18]. Hence, the resulting field is thought to affect static [19] and dynamic properties of electrons in the realm of quantum mechanics. For instance, the energy spectrum of electrons in a screw-dislocated system was suggested to show a profile similar to that of the AB system [17]. On the other hand, very little work is available to date on the dislocation effect on quantum transport. To address the latter issue, optical conductivity measurement is useful because it provides information on both the degree of electron transport throughout the host medium and on the configurational change in the eigenenergy spectra induced by the effective potential.

In this study, we theoretically calculate the optical conductivity of crystals having a screw dislocation. Referring to the material parameters of silicon carbide (SiC), which is a typical semiconductor containing many screw dislocations, we found that the conductivity shows a peak within the 100 GHz frequency region. In screw-dislocated systems, the peak positions gradually shift to higher frequencies with increasing the Fermi energy. Such the peak-position shift disappears in the three dimensional crystal with an isolated magnetic flux tube but free from screw dislocations. These two contrasting results in optical conductivity indicate that different mechanisms are contributing to dynamic electron transport in crystals having a screw dislocation and those having a magnetic flux tube, contrary to the apparent similarity in their contributions to the *static* electron eigenstates.

2. Continuum approximation

We consider electrons moving in a three-dimensional crystalline medium with a single screw dislocation along the z-axis with

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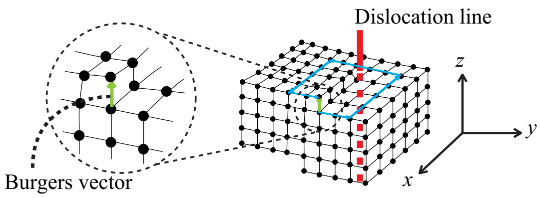

Fig. 1. (Color online) Three-dimensional lattice structure with a single screw dislocation. The dislocation line and Burgers vector, which are both parallel to the z-axis, are illustrated.

Burgers vector $\boldsymbol{b}=b\boldsymbol{e}_z$ (see Fig. 1) [17]. The concept of the effective vector potential associated with dislocation was initially derived from the continuum limit approximation for the tight-binding model of a dislocation-embedding discrete lattice. By assuming that the electron transfer is limited only between nearest neighbour sites, the tight-binding Hamiltonian is given by [17]

$$H=-\frac{1}{2}\sum_{\boldsymbol{n},\boldsymbol{a}(\boldsymbol{n})} t[\boldsymbol{a}(\boldsymbol{n})] \times\left\{c^{\dagger}[\boldsymbol{n}+\boldsymbol{a}(\boldsymbol{n})]c(\boldsymbol{n})+c^{\dagger}(\boldsymbol{n})c[\boldsymbol{n}+\boldsymbol{a}(\boldsymbol{n})]\right\}, \tag{1}$$

where $\boldsymbol{n}$ is the position vector at a lattice site, and $\boldsymbol{a}(\boldsymbol{n})$ is the bond vector pointing from $\boldsymbol{n}$ to the nearest-neighbour sites; $t[\boldsymbol{a}(\boldsymbol{n})]$ is the transfer energy along the bond $\boldsymbol{a}(\boldsymbol{n})$, and $c^{\dagger}$ (or c) is the creation (annihilation) operator satisfying the anticommutation relation:

$$[c(\boldsymbol{n}),c^{\dagger}(\boldsymbol{m})]=\frac{1}{|\boldsymbol{a}|^3}\delta_{\boldsymbol{n},\boldsymbol{m}}. \tag{2}$$

To obtain the continuum approximation of the Hamiltonian given in Eq. (1), we expand $c(\boldsymbol{n}+\boldsymbol{a}(\boldsymbol{n}))$ to the second order in the undistorted lattice constant a and take into account the modulation in $t(\boldsymbol{a}(\boldsymbol{n}))$ caused by the local lattice distortion. As a result, the Schrödinger equation in terms of cylindrical coordinates is given by [17]

$$-\frac{\hbar^2}{2m^*}\left\{\frac{\partial^2}{\partial r^2}+\frac{1}{r}\frac{\partial}{\partial r}+\frac{1}{r^2}\left(\frac{\partial}{\partial\theta}+\frac{b}{2\pi}\frac{\partial}{\partial z}\right)^2+\frac{\partial^2}{\partial z^2} +\frac{b^2}{2\pi^2a^2r^2}\left[1+\frac{1}{2}\left(a\frac{\partial}{\partial z}\right)^2\right]\right\}\phi(r,\theta,z)=E\phi(r,\theta,z). \tag{3}$$

It follows from Eq. (3) that the presence of a screw dislocation causes an effective vector potential $\boldsymbol{A}^{\text{eff}}$ defined by

$$\boldsymbol{A}^{\text{eff}}=\boldsymbol{e}_\theta\frac{\hbar b}{2\pi r}\frac{\partial}{\partial z}, \tag{4}$$

where $\boldsymbol{e}_\theta$ is the unit vector parallel to the θ direction. It clearly has mathematical properties of $\nabla\times\boldsymbol{A}^{\text{eff}}=\boldsymbol{0}$ and $\boldsymbol{A}^{\text{eff}}\propto\boldsymbol{e}_\theta/r$. These facts are reminiscent of the AB system, in which the vector potential associated with a magnetic flux Φ is given by $\boldsymbol{A}=\Phi\boldsymbol{e}_\theta/(2\pi r)\propto\boldsymbol{e}_\theta/r$. The analogy between $\boldsymbol{A}^{\text{eff}}$ and $\boldsymbol{A}$ implies that the magnitude of screw dislocation, b, plays a similar role to Φ in the AB system. However, it should be emphasized that $\boldsymbol{A}^{\text{eff}}$ is a differential operator while $\boldsymbol{A}$ is not. This difference is pronounced particularly in calculating the dynamic conductivity of the two systems as will be demonstrated later.

Substituting separation variables of the form $\phi(r,\theta,z)=R(r)e^{im\theta}e^{ik_zz}$ into Eq. (3) reduces it to the one-dimensional Schrödinger equation:

$$\left(\frac{d^2}{dr^2}+\frac{1}{r}\frac{d}{dr}+k^2-\frac{\nu^2}{r^2}\right)R(r)=ER(r), \tag{5}$$

where

$$k^2=\frac{2m^*E}{\hbar^2}-k_z^2, \tag{6}$$

$$\nu^2=\left(m+\frac{k_zb}{2\pi}\right)^2-\frac{b^2}{2\pi^2a^2}\left(1-\frac{k_z^2a^2}{2}\right). \tag{7}$$

After discarding an unphysical solution, the remaining solution is a Bessel function $J_{|\nu|}(kr)$. Then, we finally obtain the three-dimensional eigenfunction:

$$\phi(r,\theta,k_z)=J_{|\nu|}(kr)e^{im\theta}e^{ik_zz}. \tag{8}$$

3. Alternating current conductivity

We devote ourselves to calculating the ac conductivity by using the Kubo formula [20]. To extract the essential effect of the screw dislocation, we assume that the temperature is absolute zero, at which neither electron–phonon interactions nor electron–electron interactions should be relevant. Thus, the real part of the conductivity is given by

$$\sigma_{\mu\nu}(\omega)=\frac{\pi}{V\omega}\sum_{\alpha,\alpha'}\langle\alpha|j_\mu|\alpha'\rangle\langle\alpha'|j_\nu|\alpha\rangle\delta(E_\alpha-E_{\alpha'}-\hbar\omega), \tag{9}$$

where $\hbar$ is Planck's constant, ω is the angular frequency of the external electric field, V is the volume of the system, and j_μ and j_ν are the current operators with μ,ν components, respectively. $|\alpha\rangle$ and $|\alpha'\rangle$ satisfy relations $H|\alpha\rangle=E_\alpha|\alpha\rangle$ and $H|\alpha'\rangle=E_{\alpha'}|\alpha'\rangle$, respectively. We add all contributions of the quantum numbers α,α' that satisfy the condition $E_\alpha>E_F$ and $E_{\alpha'}<E_F$, where E_F is the Fermi energy of the system.

We calculate $\sigma_{xx}(\omega)=\sigma_{yy}(\omega)\equiv\sigma(\omega)$ to take into account the effect of $\boldsymbol{A}^{\text{eff}}$ in the z direction. In our system, $|\alpha\rangle$ corresponds to $\phi(r,\theta,z)$ given in Eq. (8), and

$$j_x=\frac{e}{m^*}\left(-i\hbar\frac{\partial}{\partial x}-A_x^{\text{eff}}\right), \tag{10}$$

with A_x^{eff} being the x-component of $\boldsymbol{A}^{\text{eff}}$. Substituting them into Eq. (9), we have $\sigma(\omega)=\sigma_{\nu_+}(\omega)+\sigma_{\nu_-}(\omega)$, where

$$\sigma_{\nu_\pm}(\omega)=\frac{e^2\pi^3\hbar^2}{V\omega m^{*2}}\sum_{m,k,k_z,k'}\left|\int_0^R dr\left[\frac{kr}{2}\left(\Gamma^{-1}-\Gamma^{1}\right) -\left(\pm m\mp\frac{bk_z}{2\pi}\right)\Gamma^0\right]\right|^2\times\delta(E_{\nu,k,k_z}-E_{\nu_\pm,k',k_z}-\hbar\omega), \tag{11}$$

here we defined $\Gamma^i\equiv J_{\nu_\pm}(k'r)J_{\nu+i}(kr)$ and

$$\nu_\pm=\sqrt{\left(m\pm1+\frac{k_zb}{2\pi}\right)^2-\frac{b^2}{2\pi^2a^2}\left(1-\frac{k_z^2a^2}{2}\right)} \tag{12}$$

with a double sign in the same order.

Fig. 2 shows a contour plot of $\sigma(\omega)$ as a function of $\omega$and E_F. To verify the experimental feasibility, we set parameters by referring to SiC, an attractive material for high-voltage power devices [21,22]. Note that SiC typically contains a high density of screw dislocations [23], which impair device performance [24–26] and thus warrant consideration in the relevant fields. In the actual calculation, we set the lattice constant as $a=4.4$ Å and the effective mass as $m^*=0.68m_0$, where m_0 is the mass of a free electron. The values of b are set as $b/a=1$, motivated by technological applications [27]. Conductivity values on the order of μS/m are large enough to be measured [27–29] by four terminal experiments [30]. We see from Fig. 2 that the peak positions of $\sigma(\omega)$ tend to move upward with increasing E_F, as highlighted by the dotted line.