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Electron tunneling in single layer graphene with an energy gap*

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When a single layer graphene is epitaxially grown on silicon carbide, it will exhibit a finite energy gap like a conventional semiconductor, and its energy dispersion is no longer linear in momentum in the low energy regime. In this paper, we have investigated the tunneling characteristics through a two-dimensional barrier in a single layer graphene with an energy gap. It is found that when the electron is at a zero angle of incidence, the transmission probability as a function of incidence energy has a gap. Away from the gap the transmission coefficient oscillates with incidence energy which is analogous to that of a conventional semiconductor. The conductance under zero temperature has a gap. The properties of electron transmission may be useful for developing graphene-based nano-electronics.

Keywords: graphene, transmission

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1. Introduction

Graphene is a one-atom-thick planar sheet of carbon atoms that are densely packed in a honeycomb crystal lattice.[1] It has many novel properties and potential applications. For example, the observation of half-integer quantum hall effect,[2] finite conductivity at zero charge carrier concentration,[3] universal optical conductance,[4,5] ultrahigh carrier mobility,[6] nonlinear optical effect,[7−9] strong terahertz response,[10] etc. One of the novel transport properties is the perfect transmission under normal incidence through an arbitrarily high and wide graphene barrier, a phenomenon that is referred to as Klein tunneling.[11] Since the first research on the tunneling characteristics of Dirac fermions through a single barrier in graphene,[11] the transport properties of massless Dirac fermions, including Klein tunneling and resonance transmission, have been extensively studied in the single[11,12] and double graphene barriers[13,14] and graphene superlattices.[15]

Despite these intriguing properties, one of the biggest difficulties for graphene to be used as an electronic material is its lacking of an energy gap in the electronic spectrum. In experiment, it has been shown that a finite energy gap can be induced due to the role of substrate which is an intrinsic property of epitaxial graphene.[16,17] The induced gap in graphene energy spectrum results in the fact that the charge carrier has a finite mass and the energy dispersion relation is not linear in momentum in the low energy regime. It has been demonstrated that the charge carriers obey two-dimensional (2D) massive Dirac equations and the tunneling characteristic is different from that in the case of massless fermions in graphene.[18]

In the present paper, we consider a 2D square potential barrier in an epitaxially grown graphene with an energy gap. We investigate the transmission of massive Dirac-like electrons and its dependence on incidence energy, angle, energy gap and the width of the barrier region. We further analyse the zero temperature conductance characteristics in such a system. It is shown that at a zero angle of incidence, the transmission probability as a function of incidence energy has a gap which depends strongly on incidence energy. It is shown away from the gap the transmission coef-

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ficient oscillates with incidence energy. Moreover it is shown that the zero temperature conductance also has a gap. These tunneling characteristics are completely different from those in a single layer graphene with no energy gap. The results can be useful for nanoelectronics applications of graphene, such as electron wave filters at the nanoscale level at zero incidence angle with more flexibility and simplicity.[12]

2. Calculation of transmission probability

Now we proceed to calculate the transmission coefficient of massive fermions in graphene with a finite energy gap $2\varDelta$. The hamiltonian of massive Dirac fermions in graphene near the K point of the reciprocal space reads

$$H = \begin{pmatrix} \Delta & \hbar v_{\rm F} k_- \\ \hbar v_{\rm F} k_+ & -\Delta \end{pmatrix}, \tag{1}$$

where $k_\pm = k_x \pm {\rm i}\, k_y$, and $v_{\rm F} \approx c/300$ is the Fermi velocity. The corresponding energy eigenvalue is $E_k = \pm\sqrt{\varDelta^2 + \hbar^2 v_{\rm F}^2 k^2}$, and the wave function can be written as

$$\psi_k(x,y) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ s\sqrt{\dfrac{|E| - s\varDelta}{|E| + s\varDelta}}{\rm e}^{{\rm i}\,\varphi} \end{pmatrix} {\rm e}^{{\rm i}(k_x x + k_y y)}, \tag{2}$$

where $s = {\rm sgn}(E)$, and φ is the incidence angle. In the following, we consider a 2D potential barrier as shown in Fig. 1(a), where V_0 and D are the height and the width of potential barrier, respectively.

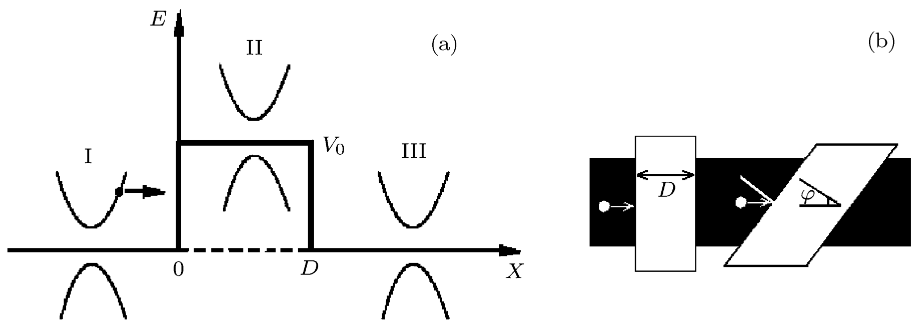

Fig. 1. (a) Schematic diagram for 2D potential barrier in single layer graphene with an energy gap. (b) Schematic diagram of experiment in graphene expectedly grown on SiC. Graphene (black) has two local gates (white) creating potential barrier.

When an electron is incident at angle φ with respective to the x direction, the wave function of the incident electron in regime I is given by Eq. (2). The wave functions in regimes I, II and III can be thus expressed respectively by

$$\begin{aligned}
\varPsi_{\rm I}(x,y) &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ s\sqrt{\dfrac{|E| - s\varDelta}{|E| + s\varDelta}}{\rm e}^{{\rm i}\,\varphi} \end{pmatrix} {\rm e}^{{\rm i}\,k_x x + {\rm i}\,k_y y} + \frac{r}{\sqrt{2}} \begin{pmatrix} 1 \\ -s\sqrt{\dfrac{|E| - s\varDelta}{|E| + s\varDelta}}{\rm e}^{-{\rm i}\,\varphi} \end{pmatrix} {\rm e}^{-{\rm i}\,k_x x + {\rm i}\,k_y y}, \\
\varPsi_{\rm II}(x,y) &= \frac{a}{\sqrt{2}} \begin{pmatrix} 1 \\ s'\sqrt{\dfrac{|E| - s'\varDelta}{|E| + s'\varDelta}}{\rm e}^{{\rm i}\,\theta} \end{pmatrix} {\rm e}^{{\rm i}\,q_x x + {\rm i}\,k_y y} + \frac{b}{\sqrt{2}} \begin{pmatrix} 1 \\ -s'\sqrt{\dfrac{|E| - s'\varDelta}{|E| + s'\varDelta}}{\rm e}^{-{\rm i}\,\theta} \end{pmatrix} {\rm e}^{-{\rm i}\,q_x x + {\rm i}\,k_y y}, \\
\varPsi_{\rm III}(x,y) &= \frac{t}{\sqrt{2}} \begin{pmatrix} 1 \\ s\sqrt{\dfrac{|E| - s\varDelta}{|E| + s\varDelta}}{\rm e}^{{\rm i}\,\varphi} \end{pmatrix} {\rm e}^{{\rm i}(k_x x + k_y y)},
\end{aligned} \tag{3}$$

where $k_x = k\cos\varphi$ and $k_y = k\sin\varphi$ are the perpendicular and the parallel wave vector components outside the barrier with $k = (E^2 - \varDelta^2)^{1/2}/\hbar v_{\rm F}$, but inside the barrier the parallel wave vector $q_x = (k'^2 - k_y^2)^{1/2}$, $s' = {\rm sgn}(E - V_0)$, the refraction angle $\theta = \arctan(k_y/q_x)$ with $k' = [(V_0 - E)^2 - \varDelta^2]^{1/2}/\hbar v_{\rm F}$. According to the boundary conditions, we obtain the following transmission coefficient:

$$t=\frac{2ss'\mathrm{e}^{-\mathrm{i}\,k_xD}\cos\phi\cos\theta}{ss'[\mathrm{e}^{\mathrm{i}\,q_xD}\cos(\varphi-\theta)+\mathrm{e}^{-\mathrm{i}\,q_xD}\cos(\varphi+\theta)]-\mathrm{i}\,F\sin(q_xD)},\tag{4}$$

where $F=2[E|V_0-E|-ss'\varDelta^2]/\hbar^2v_{\mathrm{F}}^2kk'$. There are two different cases: Klein tunneling ($E<V_0$) and classical motion ($E>V_0$), which correspond to $ss'=-1$ and $ss'=1$ respectively. When we consider the influence of k_y which is a conserved quantity, we can see that the transmission can be divided into evanescent and propagating mode. The case of $k'^2>k_y^2$ corresponds to the propagating mode, and the case of $k'^2<k_y^2$ corresponds to the evanescent mode. The transmission probability of the propagating mode $T_{\mathrm{p}}\equiv tt^*$ can be given as follows:

$$T_{\mathrm{p}}=\frac{k_x^2q_x^2}{k_x^2q_x^2\cos^2(q_xD)+(\frac{F}{2}kk'-ss'k_y^2)^2\sin^2(q_xD)}.\tag{5}$$

The transmission probability of the evanescent mode $T_{\mathrm{e}}\equiv tt^*$ can be obtained in the following form:

$$T_{\mathrm{e}}=\frac{k_x^2\kappa^2}{k_x^2\kappa^2\mathrm{ch}^2(\kappa D)+(\frac{F}{2}kk'-ss'k_y^2)^2\mathrm{sh}^2(\kappa D)},\tag{6}$$

where

$$\begin{aligned}\kappa&=(k_y^2-k'^2)^{1/2},\\ \mathrm{ch}(x)&=(\mathrm{e}^x+\mathrm{e}^{-x})/2,\\ \mathrm{sh}(x)&=(\mathrm{e}^x-\mathrm{e}^{-x})/2.\end{aligned}\tag{7}$$

When $\mathrm{e}^{\kappa D}\gg 1$, T_{e} will decay exponentially according to the following form:

$$T_{\mathrm{e}}\doteq\frac{4k_x^2\kappa^2}{k_x^2\kappa^2+(\frac{F}{2}kk'-ss'k_y^2)^2}\mathrm{e}^{-2\kappa D}.\tag{8}$$

We can find that there is a critical incidence angle φ_c separating the propagating and the evanescent modes, which is determined by the condition $k'^2=k_y^2$. It is written as

$$\varphi_c=\sin^{-1}\left(\left|\frac{(V_0-E)^2-\varDelta^2}{E^2-\varDelta^2}\right|^{1/2}\right).\tag{9}$$

With the incidence angle $\varphi>\varphi_{\mathrm{c}}$ the electrons can tunnel through the potential barrier, and with $\varphi<\varphi_{\mathrm{c}}$ the electrons decay exponentially in the potential barrier. When the electrons are in propagating mode, the transmission probability depends periodically on incidence energy. While when the electrons are in evanescent mode, the transmission probability approaches to zero quickly. Obviously due to the evanescent mode, there is a transmission gap determined by the condition $q_x^2<0$. Here we also give the transmission coefficient for a conventional semiconductor with an energy $2\varDelta$,

$$t=\frac{4k_xq_x\mathrm{e}^{-\mathrm{i}\,k_xD}}{\mathrm{e}^{-\mathrm{i}\,q_xD}(k_x+q_x)^2-\mathrm{e}^{\mathrm{i}\,q_xD}(k_x-q_x)^2}.\tag{10}$$

So the transmission probabilities through a square barrier in a conventional semiconductor read

$$T_{\mathrm{p}}=\frac{4k_x^2q_x^2}{(k_x^2-q_x^2)^2\sin^2(q_xD)+4k_x^2q_x^2}$$

for the propagating mode and

$$T_{\mathrm{e}}=\frac{4k_x^2q_x^2}{(k_x^2+q_x^2)^2\mathrm{sh}^2(q_xD)+4k_x^2q_x^2}$$

for the evanescent mode, where the parameters are defined in the same way as that in graphene.

3. Results and discussion

Figure 2(a) shows the dependences of the transmission probability on incidence energy with electrons at a zero angle of incidence for three different gap energies. One can see that when the energy gap is zero, the potential barrier always remains perfectly transparent whatever the incidence energy is. It has been shown that it is the feature unique to massless Dirac fermions and directly related to the Klein paradox in quantum electrodynamics.[9] More significantly, however, when a finite energy gap exists, the transmission probability at a zero angle of incidence has a gap centred at $E=V_0$. The transmission gap increases with the increase of the energy gap. Outside the potential barrier the transmission probability is an oscillation function of tunneling parameters, and under some resonance conditions, $q_xD=N\pi$ ($N=0,1,\ldots$), the transmission probability T equals 1. Actually the parallel wave vector $k_y=0$ at a zero incidence angle, hence $q_x^2=k'^2=(V_0-E)^2-\varDelta^2<0$ will change the electron from propagating mode to evanescent mode. The transmission probability T decays exponentially in the potential barrier when $V_0-\varDelta<E<V_0+\varDelta$, which determines the transmission gap $\varDelta E=2\varDelta$. Because in this regime of incidence energy there is no electronic state in the potential barrier, the transmission probability in this case decays exponentially to form a transmission gap. The transmission probability of graphene with a finite energy gap at a zero incidence angle is different from that in the case of gapless single layer graphene,[9] but analogous to that in the case of conventional 2D material as shown in Fig. 2(b).

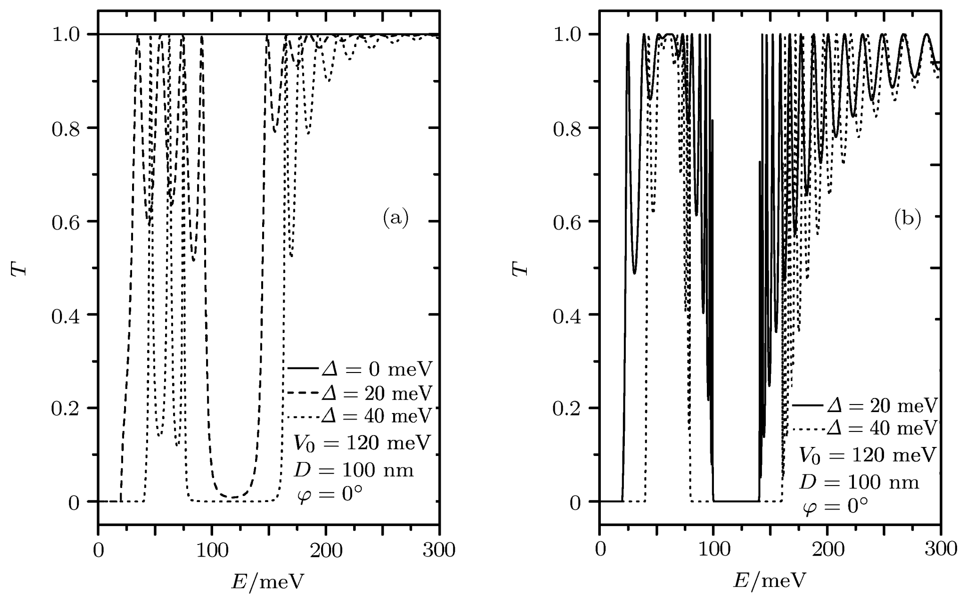

Fig. 2. (a) Transmission probabilities versus incidence energy at zero angle of incidence, where $D = 100$ nm, $V_0 = 120$ meV. Solid, dash and dot curves correspond to $\varDelta = 0$, 20 and 40 meV, respectively. (b) Transmission probabilities versus incidence energy for a conventional semiconductor.

Figure 3(a) shows the dependences of the transmission gap on the width of potential barrier in graphene with an energy gap for three different D values. The transmission gap becomes shallower with the decrease of the barrier width, and these gaps are all centred around V_0. According to Eq. (7), the decay factor $\exp(-2\kappa D)$ increases as the barrier width decreases. As a result, the transmission gap will become shallower. In Fig. 3(b), we also show the case of conventional semiconductor with the same energy gap. We can find that, whatever the width is, the transmission gap does not change and always approaches to zero. Their significant difference is that for a wide potential barrier with a width between 30 nm and 100 nm the electrons can have a finite tunneling probability through the barrier in graphene, but in conventional semiconductor the electron cannot tunnel through the barrier at all.

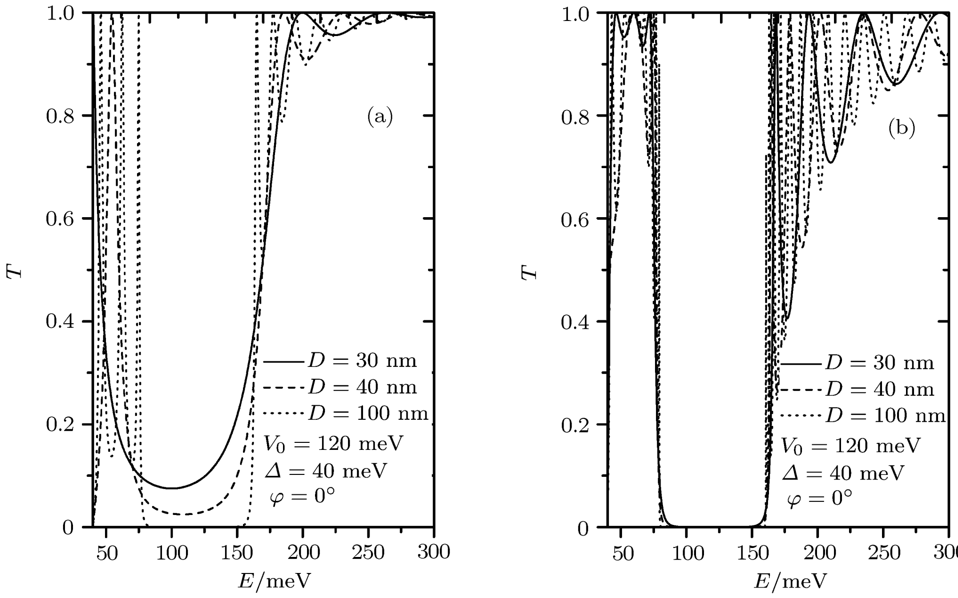

Fig. 3. (a) Transmission probability dependences on incidence energy with different widths of the potential barrier, where $\varDelta = 40$ meV. Solid, dash and dot curves correspond to $D = 20$, 40 and 100 nm, respectively. (b) Transmission probabilities versus incidence energy with different widths of the potential barrier for a conventional semiconductor.

In Fig. 4, we plot the transmission probabilities versus incidence energy with electrons at an oblique incidence. One can see that the gap becomes wider with the increase of the incidence angle due to the increase of $\varDelta E = 2\sqrt{k_y^2 + \varDelta^2}$ with the increase of incidence angle. Moreover, the transmission gap in an actual device structure can be used in various graphene-based electronic devices.

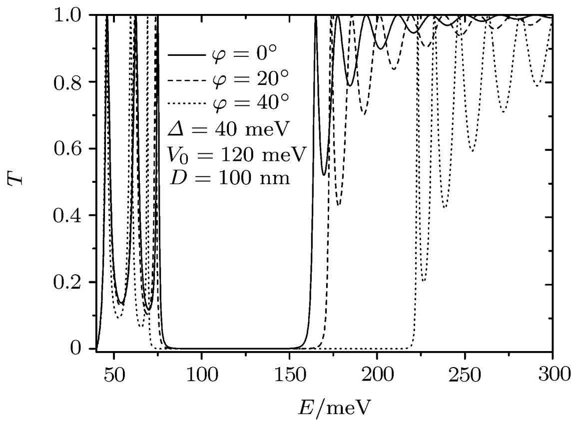

Fig. 4. Transmission probabilities versus incidence energy at an oblique incidence, where $\varDelta = 40$ meV. Solid, dash and dot curves correspond to $\varphi = 0°$, $20°$, and $40°$, respectively.

The ballistic conductance under zero temperature is obtained by averaging electron flux over half the Fermi surface as[12,19]

$$G = G_0 \int_{-\pi/2}^{\pi/2} T(\varphi)\cos\varphi \mathrm{d}\varphi, \tag{11}$$

where

$$G_0 = (2e^2/\hbar)(l/\pi\hbar v_{\mathrm{F}}),$$

and l is the length of the structure along the y direction. Figure 5 depicts the conductances each as a function of incidence energy. It is indicated that there are several kinks of the conductances caused by the transmission resonances, which are related to the quasibound states. More significantly, all conductance curves each have an obvious forbidden region. This is a direct consequence of the gap in transmission probability. The forbidden region of the conductance becomes wider and deeper with the increase of the energy gap.

The above analysis implies that the phenomena can be tested experimentally by using graphene devices. The basic principle behind such experiments admits the using of local gates and collimators similar to those used in electron optics in 2D gases to measure the tunelling in a single layer graphene without SiC substrate, about which one may refer to Ref. [11]. For the experimental realization, we can let graphene expectedly grow on SiC, and then use gate voltage to create potential barrier of a variable height as shown in Fig. 1(b). The gate simply crosses the whole graphene sample at different angles corresponding to different incidence angles with the electron incident along the vertical direction of the gate. The voltage drop across the barrier can be measured by using potential contacts. And by measuring the voltage drop across the barrier as a function of applied gate voltage, their transparencies for different V_0 values can be analysed.

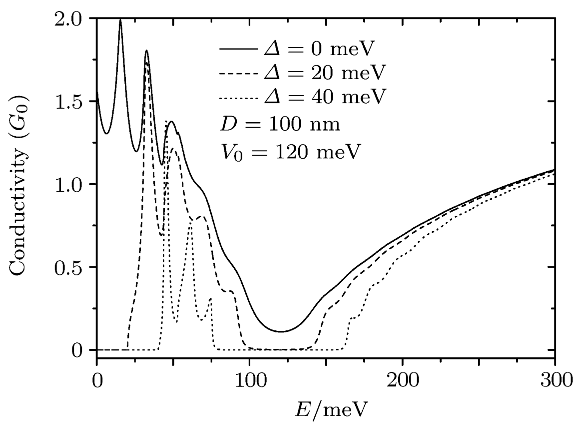

Fig. 5. Conductances versus incidence energy, where $D = 100$ nm, solid, dash and dot curves correspond to $\varDelta = 0$, 20 and 40 meV, respectively.

4. Conclusions

We have investigated the transmission and the conductance of electrons in a single layer graphene with a finite energy gap, which can be accomplished by being epitaxially grown on silicon carbide. It is shown that at a zero angle of incidence, the transmission probability as a function of incidence energy has a gap and away from the gap it is an oscillation function of incidence energy. This leads to a conductance gap at zero temperature. The transmission probability is dependent on the incidence angle and the width of potential barrier. The transmission characteristics reported may have potential applications in actual graphene-based electronic devices.

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