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Generation of valley polarized current in graphene using quantum adiabatic pumping

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Abstract. We study a device structure which can be used to generate pure valley current and valley polarized current using quantum adiabatic pumping. The design of the structure allows the flexibility of changing the structure from one for pure valley current generation to one for valley polarized current generation by changing the applied electric potentials through changing the symmetry of the structure. The device is useful for the development of valleytronic devices.

Keywords: nano-physics; nano-devices; nano-science; nano-tech; nano-carbon

1. Introduction

Graphene is a two dimensional material composed of carbon atoms, which have a hexagonal lattice structure and, since its discovery, has attracted a lot of research interest owing to its special properties. Geim (2007) For example, the energy dispersion is linear around the K and K' points of the Brillouin zone, resembling the dispersion of a Dirac Fermion. Castro Neto *et al.* (2009) Apart from the interest in the fundamental physics of graphene, researchers also have interest in using graphene in electronic and spintronic applications owing to its special characteristics. Liu and Chan (2011), Zhang *et al.* (2011, 2012) In electronic applications, the charge transport characteristics are exploited, while in spintronic applications, the special characteristics of the electron spin in graphene is exploited. This strong interest in studying and exploiting the physical characteristics of electron spin is stimulated by the possibility of using the electronic spin to make devices with lower power consumption, faster processing speed as well as devices for quantum computing. Zutic *et al.* (2004) Stimulated by the developments in spintronics, there is also a considerable interest in using the valley degree of freedom in graphene as it can be regarded as a kind of pseudo spin degree of freedom. The key issues in the exploitation of the valley degree of freedom is the generation and detection of valley polarized current. Pereira Jr. *et al.* (2008), Xiao *et al.* (2007). There are already studies of valley filters and generation of pure valley current. Rycerz *et al.* (2006), Gunlycke and White (2011), Zhai *et al.* (2011), Jiang *et al.* (2013) However,

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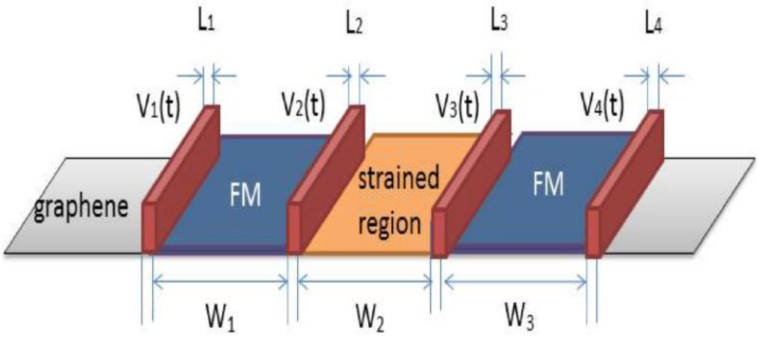

Fig. 1 Schematic illustration of the proposed structure. Two ferromagnetic stripes with opposite magnetizations are deposited on a sheet of monolayer graphene, which is strained in the middle section. The ferromagnetic and the strained regions are separated by four metal gates

there is still a need of a source of valley polarized current which can have tunable valley polarization. In this paper, we study a graphene structure which can be used to generate valley polarized current with tunable polarizability using quantum adiabatic pumping. It can be tuned to get pure valley current or highly valley polarized current by changing the some electric potentials.

Quantum adiabatic pumping is a technique which can be used to generate a d.c. current without an applied bias. Thouless (1983), Switkes *et al.* (1999), Tiwari and Blaauboer (2010) Zhu and Chen (2009) The technique uses two a.c. signals to modify the electronic structure of a nanostructure and thus modify the scattering characteristics of the structure. When the two a.c. signals are not in phase, a d.c. current is generated. There are already many examples of using two a.c. voltages as the pumping signals because it is easy to modify the electronic properties of a nanostructure using applied voltages. The quantum adiabatic technique is shown to be a versatile technique for generation of charge and spin currents, which prompts us to study in details how it can be used to generate tunable valley polarized current. Zhang *et al.* (2011, 2012)

The structure we propose here, which is shown schematically in Fig. 1, consists of a single layer graphene on which four electrodes are deposited, which can be used to induce 4 electrical potential barriers (d.c. plus a.c.) in the graphene layer. Between the electrical potential barriers, are strained and ferromagnetic graphene regions. The strained graphene is generated by inducing strain in the substrate on which the graphene is grown and the ferromagnetic region is induced by the proximity effect when a layer of ferromagnetic material is deposited on the graphene layer. The in-plane strain in the graphene layer causes a change in the hopping coupling between neighbouring atoms , which appears as a gauge potential term in the Hamiltonian. Since the system has time reversal symmetry, the strain induced gauge potentials have opposite signs in the two valleys. When the time reversal symmetry is broken by a magnetic field, the valley degeneracy is broken too and valley polarization can be readily generated in the structure.

2. Model

The Dirac Hamiltonian for an electron with wave vectors close to the K (or K') point is given by $H_\xi = v_F\boldsymbol{\sigma}\cdot\left(\boldsymbol{p} + e\boldsymbol{A_{FM}} + \xi\boldsymbol{A_s}/v_f\right) + V\sigma_0$, where $\xi = \pm 1$ denotes the K and K' valleys, v_F is the Fermi velocity, $\boldsymbol{\sigma} = (\sigma_x, \sigma_y)$ are the Pauli matrices, σ_0 is a unit matrix, $\boldsymbol{p} = (p_x, p_y)$ are the momentum operators, $\boldsymbol{A_{FM}}$ and $\boldsymbol{A_s}$ are the Landau gauge potentials of the magnetic field and the strain respectively, which are non-zero in the magnetic and strained regions. $V = V(x)$ is the one dimensional electrical potential, which is zero between the electrodes and has the following potentials in the 4 electrode regions

$$V_i(t) = V_i + v_i \sin(\omega t + \phi_i), \quad i = 1, 2, 3, 4 \tag{1}$$

where V_i denotes the static potentials and v_i and ϕ_i denote respectively the amplitudes and phases of the a.c. voltages. By controlling the 4 amplitudes and phases, various configurations of the applied a.c. voltages can be obtained. Usually only two a.c. signals are applied in quantum pumping and thus we need to restrict to those combinations which have two a.c. signals. For example, we put V_1=V_4 and V_2=V_3 to obtain two applied a.c. voltages.

The current generated by quantum adiabatic pumping can be obtained from the emissitivities of the structure caused by the changes in the two applied voltages $\frac{dn(m)}{dV_1}$ and $\frac{dn(m)}{dV_2}$ using the expression $\delta Q = \frac{dn(m)}{dV_1}\delta V_1 + \frac{dn(m)}{dV_2}\delta V_2$, where m denotes the left or the right lead. The emissitivity can be obtained from the scattering matrix S by using

$$\frac{dn(m)}{dV_i} = \frac{1}{2\pi}\sum_{\beta}\sum_{\alpha\in m} \mathrm{Im}\frac{\partial S_{\alpha\beta}}{\partial V_i} S^*_{\alpha\beta} \tag{2}$$

Since the applied voltages are periodic with an angular frequency ω, we can obtain an expression for the pumped current by averaging the charge emitted in a cycle, which is done by integrating δQ with respect to time over a complete period. The expression for the current is $I = \frac{e\omega}{2\pi}\int_0^{\tau} dt \int_{-k_f}^{k_f} \frac{dn}{dV_1}\frac{dV_1}{dt} + \frac{dn}{dV_2}\frac{dV_2}{dt} dk_y$ (Brouwer 1998). The integration with respect to k_y is necessary for including the contribution of all the transverse modes, which are denoted by the wave vector k_y because the structure has translation symmetry along the y direction.

The scattering matrix elements for the structure can be found from the amplitudes of the reflected wave and transmitted wave of the scattering wave function of the structure in the required lead. As the structure consists of sections of constant electrical and the gauge potentials with analytical eigen-solutions, it is convenient to use the transfer matrix method to find the necessary wave amplitudes. Wang and Zhu (2010) The transfer matrix relates the wave amplitudes of two neighbouring sections and is obtained by matching the wavefunctions of the two sections at the boundary according to the following equations, where A and B denote respectively the right going (the +*x* direction) and the left going wave amplitudes in section 1 and C and D denote respectively the right and the left going wave amplitudes of section 2.

$$Ae^{ik_1 a}\begin{bmatrix} f_{1+} \\ g_{1+} \end{bmatrix} + Be^{-ik_1 a}\begin{bmatrix} f_{1-} \\ g_{1-} \end{bmatrix} = Ce^{ik_2 a}\begin{bmatrix} f_{2+} \\ g_{2+} \end{bmatrix} + De^{-ik_2 a}\begin{bmatrix} f_{2-} \\ g_{2-} \end{bmatrix} \tag{3}$$

$$\begin{bmatrix} e^{ik_1a}f_{1+} & e^{-ik_1a}f_{1-} \\ e^{ik_1a}g_{1+} & e^{-ik_1a}g_{1-} \end{bmatrix}\begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} e^{ik_2a}f_{2+} & e^{-ik_2a}f_{2-} \\ e^{ik_2a}g_{2+} & e^{-ik_2a}g_{2-} \end{bmatrix}\begin{bmatrix} C \\ D \end{bmatrix} \tag{4}$$

$$\begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} e^{ik_1a}f_{1+} & e^{-ik_1a}f_{1-} \\ e^{ik_1a}g_{1+} & e^{-ik_1a}g_{1-} \end{bmatrix}^{-1}\begin{bmatrix} e^{ik_2a}f_{2+} & e^{-ik_2a}f_{2-} \\ e^{ik_2a}g_{2+} & e^{-ik_2a}g_{2-} \end{bmatrix}\begin{bmatrix} C \\ D \end{bmatrix}$$

$$\begin{bmatrix} A \\ B \end{bmatrix} = \widetilde{M}\begin{bmatrix} C \\ D \end{bmatrix} \tag{5}$$

For an eigenfunction with the form

$$e^{i(k_x x + k_y y)}\begin{bmatrix} f \\ g \end{bmatrix} \tag{6}$$

The eigenvalue is $E = U + v_F\hbar\left(k_x{}^2 + \left(k_y + A_\xi\right)^2\right)^{1/2}$ where A_ξ is used to denote the gauge potentials in the present structure given by $\hbar A_{\xi} = eA_{FM} + \xi A_s / v_F$ which are considered to vary along the x direction and the eigenfunction is

$$\Psi = Ne^{i(k_x x + k_y y)}\begin{bmatrix} \dfrac{v_F\hbar(k_x - i(k_y + A_\xi)}{E-U} \\ 1 \end{bmatrix}$$

where N is the normalization constant

Combining the transfer matrix of the five sections in the structure, we can find a relation between the wave amplitudes of the right and left leads using the following expression

$$\begin{bmatrix} A_L \\ B_L \end{bmatrix} = \widetilde{M}_1\widetilde{M}_2\widetilde{M}_3\widetilde{M}_4\widetilde{M}_5\widetilde{M}_6\begin{bmatrix} A_R \\ B_R \end{bmatrix} = \widetilde{M}_t\begin{bmatrix} A_R \\ B_R \end{bmatrix} \tag{8}$$

By putting A_L=1, A_R=t, B_R=0 and B_L=r, we can easily find the transmission coefficient t and reflection coefficient r from the equation. Putting A_R=r', B_R=1, A_L=0, B_L=t', we can obtain another set of transmission and reflection coefficient t' and r'. When the transmission and reflection coefficients on one lead are found, the pumped current can be obtained from the expression given above.

3. Results

In our calculation we use the following parameters in the symmetrical structure. The widths of

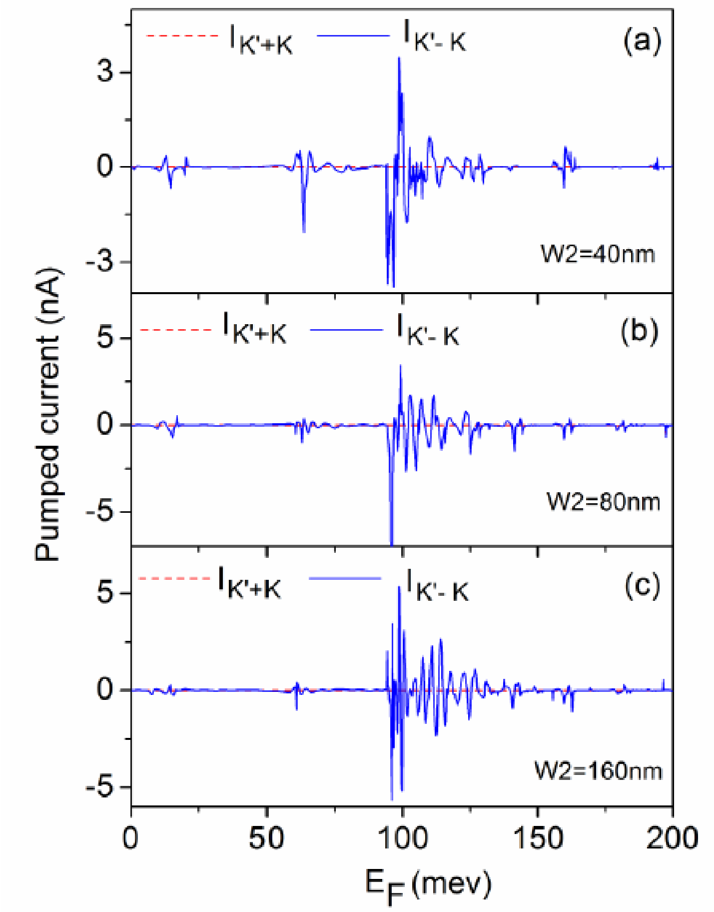

Fig. 2 The pumped currents vs Fermi energy. The width of the strained regions are (a)40nm, (b) 80 nm and (c) 160 nm. The other parameters are L_1=L_2=L_3=L_4=30 nm, W_1=W_3=80 nm. The vector potential due to strain is 5 meV. The vector potentials of the FMs are 5 meV and -5 meV. V_1=V_2=210 meV

the barriers are set to be L_1=L_2=L_3=L_4=30 nm and the distances between the barriers are W_1=W_2=W_3=80 nm. The strength of FM is $v_F e A_{FM}$=5 meV and the strength of strain is A_s=5 meV. To obtain a pure valley current, the electrical potential in the structure has to be symmetrical and the magnetic fields in the two FM regions are parallel and identical in magnitude (the magnetic vector potential is antisymmetrical). The heights of the electrical potential barriers are 210 meV and the amplitude of the a.c. oscillation is 1 meV. For the asymmetrical structures, we consider the following cases: W_3=40 nm, $A_{FM(\text{right})} = -2A_{\text{FM(left)}}$ and V_1=V_2 and V_3=V_4 (the two groups of a.c. potentials have different a.c. phases). We consider a structure with a transverse dimension of 10 μm and the frequency ω of 5GHz. The pumped current obtained are expressed in units of nA in the figures. We first consider the pumped currents in the two valleys when the structure is symmetrical with respect to the center line of the middle section (a mirror symmetry). The structure is made symmetrical by setting V_1=V_4, V_2=V_3. In all considered situation the phase difference of the two kinds of a.c. potentials is $\pi/2$. In Fig. 2, we present the total charge current $I_{K'+K}$=$I_{K'}$+I_K and the pure valley current $I_{K'-K}$=$I_{K'}$−I_K as a function of the Fermi energy for three different widths of the strained region W_2. The charge current remains zero for all the Fermi energies, which means $I_K=-I_{K'}$ and the two currents in the two valleys are equal and opposite and have an oscillatory dependence on the Fermi energy with the most prominent current found at Fermi energies between 100 meV and 120 meV. When the width of the central strained section is increased, the number of oscillations increases without significant changes in the current amplitude.

When the structure is asymmetrical, the charge current is not zero. In Fig. 3, we plot the pumped current for two asymmetrical configurations: W_3 is different (30 nm) and different right and left magnetizations. The charge currents generated in the two valleys in these structures exhibit different oscillations, which can be used to generate valley currents with tunable valley polarization controlled by the Fermi energy. We can change the magnitudes of the two charge currents by changing the Fermi energy in the structure. As a result, the ratio of the K (or K') valley current to the charge current, $I_{K'(K)}/I_{K+K'}=(I_{K+K'}+(-)I_{K'-K})/2I_{K+K'}=1/2+(-)I_{K'-K}/2I_{K+K'}$, which is a measure of the degree of polarization, is changed.

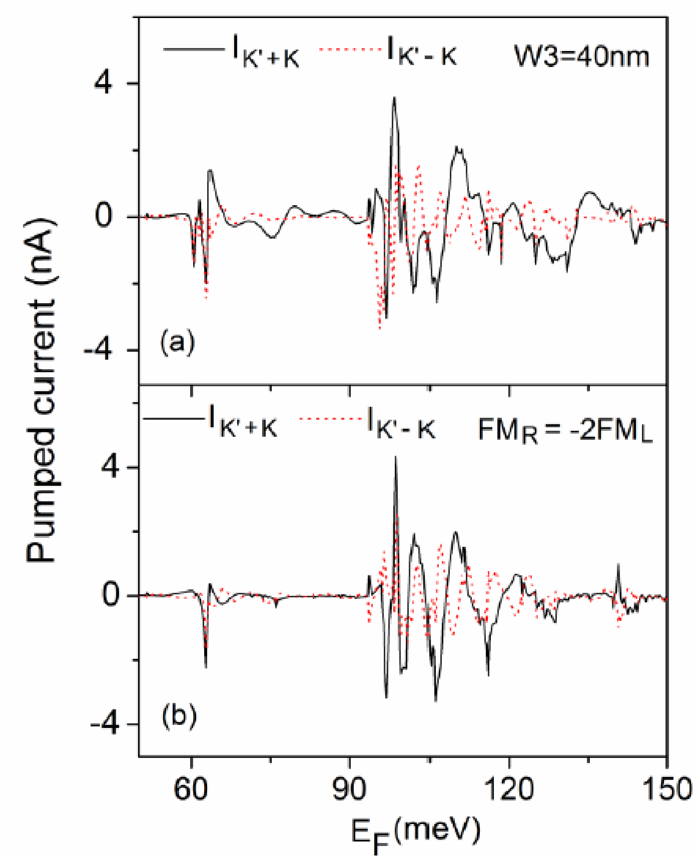

Fig. 3 The pumped current vs Fermi energy. The structure is not symmetrical about the central line. (a) The width of the right ferromagnetic stripe is 40 nm. (b) The magnitude of the right FM vector potential is two times of the magnitude of the left FM vector potential. The other parameters are the same as for Fig. 2

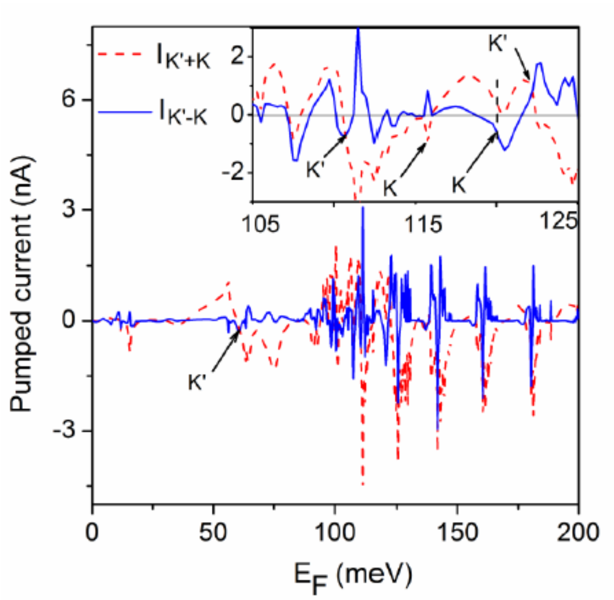

Fig. 4 The pumped current vs Fermi energy. The four applied voltages varies according to V_1=V_2=210 meV+sin(wt) and V_3=V_4=200+sin(wt+$\pi/2$)

The advantage of the present structure is its high tunability which allows us to convert the structure into an asymmetrical one easily by changing the electrical potentials through the applied voltages. Fig. 4 shows the charge and valley currents obtained by using the following configuration of potentials V_1=V_2 and V_3= V_4. In the inset, we show an enlargement of a part of the figure to demonstrate how we can obtain current in either the K or K' valley only. For example, when we have identical valley and charge currents, $I_{K'-K}$=$I_{K+K'}$, we have non-zero current in the K' valley only, i.e., $I_{K'}$≠0, I_K=0. When $I_{K'-K}$=−$I_{K+K'}$ we have pure K valley current, I_K≠0, $I_{K'}$=0.

The pumped current arises from the change of the S matrix, which is more significant at large incident angles when there is a rapid change in the S matrix. Fig. 5 shows the pumped current vs the incident angle at two Fermi energies. The pump current is significant for large incident angle and small for small incident angles. This can be explained by considering the plot of the transmission vs the Fermi energy and incident angle in Fig. 6. Significant changes of the transmission is found for large incident angles where there is a transition from high transmission to low transmission. When the potentials change, the transmission for large incident angles changes significantly. For a fixed incident angle the transmission oscillates with the Fermi energy and the range of incident angles in which significant transmission is found to also oscillate with the Fermi energy. These oscillations come from the Fabry-Perot resonances in the structures and are related to the oscillation of the pumped current. According to the above results, it is easy to get that the symmetry property of the structure plays an important role in obtaining a pure valley in the whole energy region. When the vector potentials and a.c. voltages are symmetric about the central line of the structure, the Hamiltonians of the two valleys satisfy the following relationship $\sigma_z R_x H_K(k_y) R_x^{-1} \sigma_z^{-1} = H_{K'}(-k_y)$, thus $T_K(k_y) = T_{K'}(-k_y)$. If the symmetry property is broken, the K valley Hamiltonian cannot be related to the K' valley Hamiltonian through the operator $\sigma_z R_x$ and $T_K(k_y) \neq T_{K'}(-k_y)$.

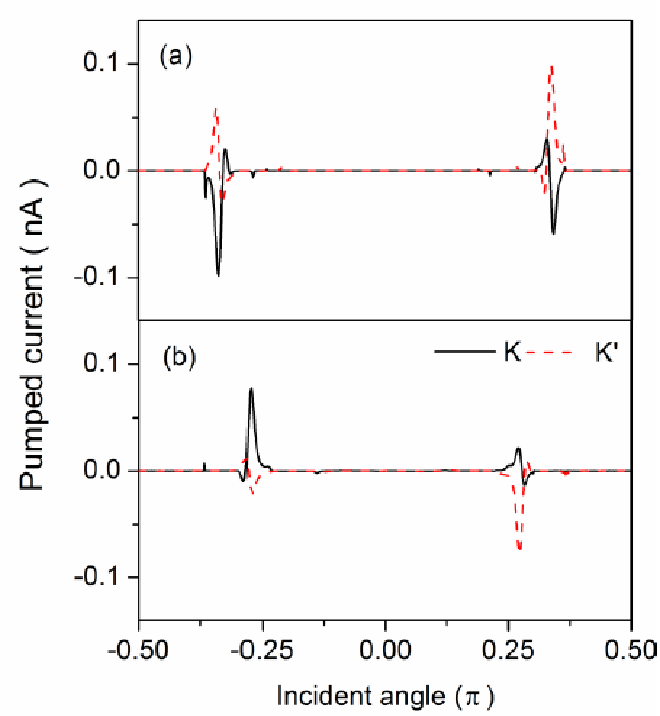

Fig. 5 The pumped current vs incident angle at fixed Fermi energies: (a) 99.75 meV, (b) 105 meV. The other parameters are the same as for Fig. 2(b)

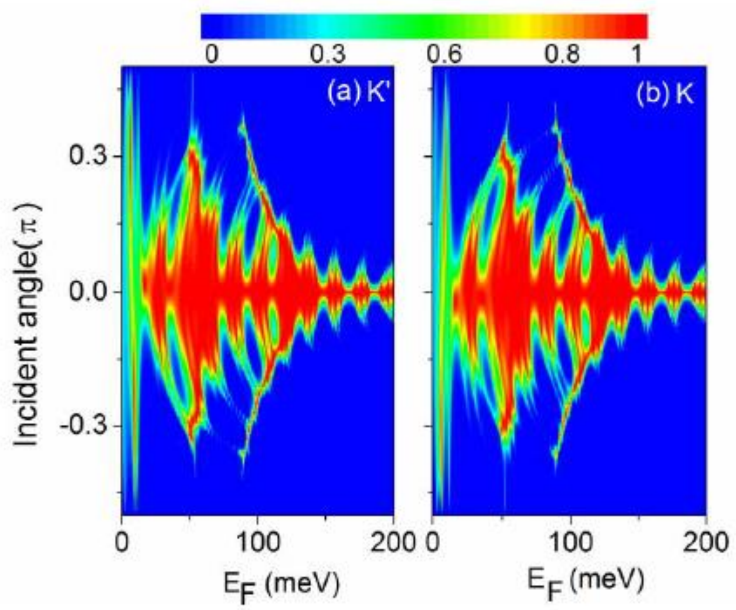

Fig. 6 Contour plot of the transmission probability as a function of Fermi energy and incident angle. (a) *K'* valley and (b) *K* valley. The other parameters are the same to Fig. 2(b)

4. Conclusions

In conclusion, we study the pumped valley and charge currents in a structure with potential barriers, localized strain and magnetic field. Pure valley current and valley polarized current with tunable polarizability can be generated in the structure by modifying the structure parameters such as the electric potential, and the magnetic field strength. The device structure is useful for the development of valleytronic devices.

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