Physics Letters A ••• (••••) •••–•••

Contents lists available at ScienceDirect

Physics Letters A

www.elsevier.com/locate/pla

Valleytronics and phase transition in silicene

Tayyaba Aftab

Department of Physics, Quaid-I-Azam University, Islamabad 45320, Pakistan

ARTICLE INFO

Article history:
Received 9 July 2016
Received in revised form 29 December 2016
Accepted 18 January 2017
Available online xxxx
Communicated by M. Wu

Keywords:
Two dimensional materials
Silicene
Quantum phase transition
Valley polarization
Valley magnetic moment
Valleytronics and spintronics

ABSTRACT

Magnetic and transport properties of silicene in the presence of perpendicular electromagnetic fields and a ferromagnetic material are studied. It is shown that for small exchange field, the magnetic moment associated with each valley is opposite for the other and it gives a shift in band energy, by a Zeeman-like coupling term. Thus opening a new horizon for valley–orbit coupling. Magnetic proximity effect is seen to adjust the spintronics of each valley. Valley polarization is calculated using the semi classical formulation of electron dynamics. It can be modified and measured due to its contribution in Hall conductivity. Quantum phase transitions are observed in silicene, providing a tool to control the topological state experimentally. The strong dependence of the physical properties on valley degree of freedom is an important step towards valleytronics.

1. Introduction

Silicene is a monolayer of silicon atoms that forms a two dimensional honeycomb lattice. Due to its unique properties, silicene has attracted much attention both theoretically and experimentally [1–5]. Though fabrication and synthesis of silicene was a challenge because of its air stability issue, but researchers fabricated it using a growth transfer process and made transistors working at room temperature. This approach is proposed to be effective for other two dimensional materials like germanene and phosphorene [40]. There is Dirac like electron dispersion at K points of the Brillouin zone in silicene as well. This and many other similarities are observed because they all come from the same column on the periodic table. But silicene possesses stronger SOC than graphene, which can be increased under strain. Silicene is a model system for studying the spin and valley physics not prominent in graphene due to the smaller SOC. The band gap is tunable with external electric field. The sites on the sub-lattices are in different vertical planes with separation, causing silicene to be buckled. When electric field perpendicular to the plane is applied, then on site potential difference Δ_z arises [6,7].

Over the past few years, it was examined that Berry curvature has a major role on the physical properties of materials and a range of phenomena, such as orbital magnetism, Hall effects (charge and spin) and polarization of electrons. It is an intrinsic property of bands as it depends on the wave function only. It is non-zero in crystals with broken inversion or time-reversal symmetry [8]. Previously valley contrasting properties were studied in graphene [9]. In silicene it was discussed with electric field applied to the system [10] and in the presence of magnetic field [11]. It was observed that graphene [9] and TMD [12] show valley contrasting behavior in the presence of substrate potential only. For TMD there is an extra contribution from spin splitting and that leads to asymmetric Landau levels [13]. For graphene valley-dependent physics, generation and experimental evaluation of valley polarization, were explored [14–17]. Creating valley polarization is rather less straightforward but has been shown for AlAs Bismuth, graphene and MoS_2 [18]. Valley degree of freedom is controlled using circularly polarized light which gives the possibility of the use of valley excitons for the applications in quantum information and ultrafast devices. With optical light, they are proposed to open up the possibility of coherent manipulation of the valley polarization in TMD [32,41–43].

The Quantum Hall effect is an important area of condensed matter physics from 1980s to date. From two dimensional electron gas to silicene, charge and spin responses have been studied in the presence of electromagnetic fields [19–24]. Similar to spin, valleys give another degree of freedom, to study valleytronics [9,25]. In graphene, valley polarization has been proposed to be detected with broken inversion symmetry. Each valley is characterized by opposite Hall transport i.e. the carriers flow in different transverse edges when electric field is applied perpendicular to the system [9]. The valley polarized quantum anomalous Hall state in silicene has been predicted. In the presence of exchange field with intrinsic and extrinsic Rashba coupling, quantum anomalous Hall effect has

E-mail address: tayyaba.agha@gmail.com.

http://dx.doi.org/10.1016/j.physleta.2017.01.020
0375-9601/

List of abbreviations

SOC	Spin Orbit Coupling	BI	Band Insulator
TRS	Time Reversal Symmetry	TMD	Transition Metal Dichalcogenides
TI	Topological Insulator	QSHE	Quantum Spin Hall Effect
QHE	Quantum Hall Effect		

shown non-zero Chern numbers [26]. Valleytronics is an emergent field which deals with valley based electronic applications and it needs valley degree of freedom to be treated separately to evaluate the contrasting physics of two valleys effectively [33–37].

The phase transition occurs in silicine from topologically trivial to a band insulating state and further to a semi metallic state under inhomogeneous perpendicular electric field [10,27]. The combination of an electric and magnetic fields with intrinsic SOC also leads to topological phase transition [11]. Silicene has not been discussed with proximity effect by studying the physical phenomenon as studied in this article.

In present article it is shown that silicene, in the presence of electric and magnetic fields taken in proximity with a magnetic material, has opposite Berry curvature for the valleys, thus different magnetic moments resulting in net magnetization, for low exchange field. It is interesting to notice such magnetic moment relying strictly on valley degree of freedom, which is similar to the properties of spin and a Zeeman like interaction. Moreover, this magnetic momentum can be tuned by the buckled silicene structure, external electric field and exchange term. In addition to this, proximity effect has caused the suppression of one type of spin and favored the other in the calculation of valley magnetic moments; which is proposed to define a new phenomenon named valley–spin coupling which is one of the uniqueness of the article. Exchange field due to proximity with ferromagnetic material is seen to shift the degeneracy point of opposite valleys from zero. The magnetization and valley Hall effect provides a way to experimentally observe the phenomenon. Valley polarization has also been calculated and plotted, showing tuning of polarization with external electric field and chemical potential. Thus an important aspect of spin i.e. its accumulation or polarization is also being proposed to appear for valleys in silicene. The quantum phase transition in silicene in the presence of electromagnetic fields and ferromagnetic proximity is clear from Hall conductivity plots. The exchange field due to proximity effect causes a transition in spin Hall conductivity of each valley while net spin conductivity remains unchanged. The physical properties discussed here for two dimensional physical system under these external parameters have never been studied before.

2. Valley dependent Berry curvature and magnetic moment

Silicene sheet in proximity with a magnetic material is taken in xy-plane, with electric and magnetic fields perpendicular to it. The effective Hamiltonian is given [26,31] as:

$$H_{s_z}^{\tau_z} = \hbar v\left[k_x(1_s\otimes\tau_z\otimes\sigma_x) + k_y(1_s\otimes 1_\tau\otimes\sigma_y)\right] - \Delta_{so}[s_z\otimes\tau_z\otimes\sigma_z] + \Delta_z[1_s\otimes 1_\tau\otimes\sigma_z] + h[s_z\otimes 1_\tau\otimes 1_\sigma] \quad (1)$$

The first term is graphene like for Dirac fermions in buckled silicene with $v = 5\times 10^5$ m/s, s_z is the spin index and $\tau_z = \pm 1$ is a symbol used to indicate valley K and K', the second term is SOC term as described by Kane and Mele [24], where Δ_{so} is the spin orbit coupling gap induced by this term; taken to be 7.9 meV [29]. From density functional theory calculations $\Delta_{so} = 1.55$ meV [6,7,44] and tight binding calculations $\Delta_{so} = 7.9$ meV [44]. The next term is associated with electric field with $\Delta_z = a_0 E_z$, where E_z is an electric field which is applied perpendicular to the silicene sheet and $a_0 = 0.23A^0$. h is an exchange field in the last term due to proximity effect, $h = 1.1$ meV [31], $h = 9$ meV [39], σ_i are the Pauli matrices acting in the pseudospin space which differentiate A and B sub-lattices. Valley physics arises because of the inversion symmetry breaking and here electric field plays the role.

In the presence of perpendicular magnetic field B, the vector potential is taken to be $(0, Bx, 0)$. The Hamiltonian defined in Eq. (1) after Peierls substitution becomes:

$$H_{s_z}^{\tau_z} = \hbar v\left[\left(\left(k_x + \frac{eA_x}{\hbar}\right)(1_s\otimes\tau_z\otimes\sigma_x) + \left(k_y + \frac{eA_y}{\hbar}\right)(1_s\otimes 1_\tau\otimes\sigma_y)\right] - \Delta_{so}[s_z\otimes\tau_z\otimes\sigma_z] + \Delta_z[1_s\otimes 1_\tau\otimes\sigma_z] + h[s_z\otimes 1_\tau\otimes 1_\sigma] \quad (2)$$

Taking $\pi = k + \frac{eA}{\hbar}$, $\omega = v\sqrt{\frac{2eB}{\hbar}} = \frac{v}{l_B}$, l_B being the magnetic length. Let $a = \frac{l_B}{\sqrt{2}}[\pi_x - i\pi_y]$, $a^\dagger = \frac{l_B}{\sqrt{2}}[\pi_x + i\pi_y]$ be the annihilation and creation operators respectively.

The energy after diagonalizing the Hamiltonian in Eq. (2) is:

$$E_{s_z}^{\tau_z}(n,\lambda) = hs_z + \lambda\sqrt{n\hbar^2 w^2 + (\Delta_{so}s_z - \Delta_z\tau_z)^2}, \quad (3)$$

where $\lambda = +/-$ showing the electron/hole band and n is an integer showing Landau level.

The zero mode energy is:

$$E_{s_z}^{\tau_z}(0,\lambda) = hs_z + \lambda(\Delta_{so}s_z - \Delta_z\tau_z). \quad (4)$$

The interplay between Δ_{so} and Δ_z play a major role in tuning the energy. The zero modes show a phase transition from TI to BI for zero exchange field due to band inversion [29] but with non-zero exchange field degeneracy points are shifted.

The corresponding wave functions are calculated to be:

$$\Psi_{s_z}^{\tau_z}(n) = \begin{pmatrix} t_1\Phi_{n-1} \\ t_2\Phi_n \end{pmatrix}, \quad (5)$$

$$\Psi_{s_z}^{\tau_z}(n') = \begin{pmatrix} t_1\Phi_{n'} \\ t_2\Phi_{n'-1} \end{pmatrix}, \quad (6)$$

where Φ_n is Hermite Polynomial, $t_1 = \sin(\frac{\theta_n}{2})$, $t_2 = \cos(\frac{\theta_n}{2})$ with $\theta_n = \tan^{-1}(\frac{\sqrt{n}\hbar w}{(\Delta_{so}s_z - \Delta_z\tau_z)})$.

With exchange field of 9 meV dispersion relation exhibits shift in Dirac point from 0 eV to 0.01 eV as depicted in Figs. 1(a) and 2(a). Interestingly Dirac point for spin up of both valleys is shifted to the conduction band and spin down to the valence band. Thus the polarization of spins is possible, which is an important step for spintronics. Exchange field is coupled to spin that is the reason of its role in spin dependent devices.

Similar to gauge field tensor in electrodynamics, Berry curvature is a gauge-field tensor. It is a gauge invariant and thus observable. In addition to the electron dynamics, Berry curvature has a major role on transport properties, the density of states of electrons defined in the phase space and thermodynamic behavior of crystals.