Topological phase transition in silicene in the presence of the non-magnetic impurities and the extrinsic Rashba coupling

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Abstract We start with single-particle silicene Hamiltonian, in low-buckled honey-combed lattice structure, comprising of the Dirac kinetic energy, a buckling induced staggered sub-lattice potential between silicon atoms at *A* sites and *B* sites for an applied electric field E_z perpendicular to its plane, the intrinsic spin-orbit coupling (ISOC) t_{so}(~ *4* meV) stronger than that in graphene, and the intrinsic Rashba spin-orbit coupling(IRSOC).The second term breaks the sub-lattice symmetry of the system's honey-comb structure and the SOCs give rise to spin-split band gap. The single-valley(flavor) Dirac physics, determined by two independent Dirac-like cones at ***K*** and ***K'*** points, dominates as long as there is no valley mixing. The silicene system attains a critical value, by tuning E_z , at which the system at the topological insulating phase goes to a semi-metallic state where the 'spin down' upon the 'spin-up' band gap ratio(*r*) << *1* for the valley ***K**,* and *r* >> *1* for the valley ***K'*****.** This state is termed as the 'valley-spin-locked-metal' (VSLM) due to the opposite spin-polarization of the *K* and *K'* valleys. The VSLM crossover is referred to as the topological phase transition(TPT). Upon increasing E_z further, the system turns into a trivial insulator. This is associated with the valley magnetic moment reversal. Our investigation have shown that, as long as the (non-magnetic) impurity strength parameter V_0 is moderate , i.e. V_0 is of the same order as t_{so}, the 'VSLM' phase is protected. For $V_0 \gg t_{so}$, however, one sees the disappearance of this phase due to accentuated intra- and inter-valley scattering processes. In fact, we utilize a model for screened scattering centers (SSC)of the Gaussian shape, with the screening length (*L*) spanning the range varying smoothly on the scale of the lattice constant(*a*), as the facilitator of the former (requires non-local SSC with ,say, $L \sim 10a$) as well as the latter (local SSC with, say, $L \sim a$). The local potentials, due to the lifting of the prohibition on the inter-valley scattering, allow us to go beyond the scope of the single-valley scattering problem. Since the gap-closing is not associated with the intrinsic Rashba coupling, this does not cause the disappearance of the quantum spin Hall effect(QSHE).. The VSLM phase is also found to be robust against this coupling. The inclusion of the extrinsic Rashba spin-orbit coupling(ERSOC) (~ *20* μeV) and the exchange coupling leads to control of spin and valley. This, in turn, indicates the possibility of TPT based spintronic / valleytronic devices.