Surface states of the topological crystalline insulator $Pb_{0.4}Sn_{0.6}Te$

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Lately, it has been shown by angle-resolved photoelectron spectroscopy (ARPES) studies, that IV-VI substitutional alloys, $Pb_{(1-x)}Sn_xTe$ and $Pb_{(1-x)}Sn_xSe$ with Sn content *x* higher than a critical value, are topological crystalline insulators (TCIs) [1,2]. Very recently, spin-resolved photoelectron spectroscopy (SRPES) allowed the observation of chiral spin textures of (001) surface states in the TCI phase of these alloys [1, 3].

Here, using a tight-binding approach, we study theoretically the nature of surface states in $Pb_{(1-x)}Sn_xTe$. The Sn content x=0.6 assures the band inversion and, thus, the newly discovered TCI phase in the (Pb,Sn)Te material. In this rock-salt TCI, the surface states with nontrivial Dirac-like energy spectrum can form at any surface of the crystal. The number of Dirac points in the surface Brillouin zone corresponds to four L-points. At least two of these Dirac points are topologically protected only at crystal surfaces symmetric about any of {110} mirror planes. These are {n n m} surfaces. We study thus, apart from the (001)-oriented surface, the surface states for the two other surface families, {011} and {111}, in which the mirror symmetry of the crystal's rock-salt structure plays the same role.

For {n n m} surfaces the four L-points in the 3-dimensional Brillouin zone project to four different points in the 2-dimensional Brillouin zone, but only when n and m have the same parity (it means of course that they are both odd numbers). When the parities of n and m are different, the L-points are projected in pairs. In this case, two protected Dirac points appear on the mirror symmetry line in the vicinity of the L-projection. Only for (001) surface there are two such lines and four Dirac points are topologically protected. Indeed, our calculations show that while in (111) $Pb_{0.4}Sn_{0.6}Te$ four single topologically protected Dirac-cones should appear, for the (011) surface states the protection is lifted for two L points projections. In this case, instead of the Dirac points energy gaps for the surface states occur, due to the interaction between the two L valleys.

The spin polarization of metallic surface states in the TCI phase of $Pb_{0.4}Sn_{0.6}Te$ has been studied by calculating the in-plane spin texture along the constant-energy lines of the surface states. For all studied surfaces, (001), (011) and (111), chiral spin textures have been obtained.

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