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

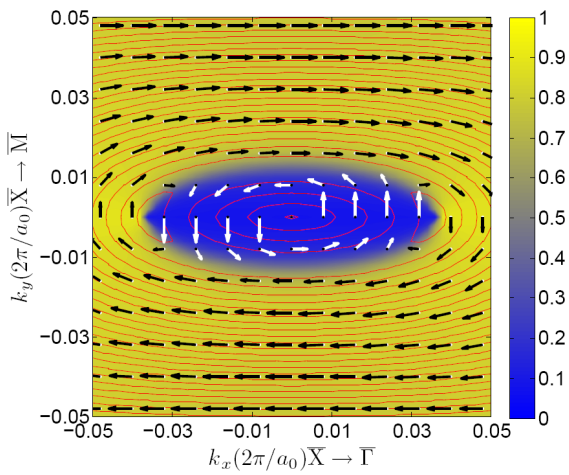
S. Safaei, P. Kacman, R. Buczko
Institute of Physics PAS, al. Lotników 32/46, 02-668 Warsaw, Poland

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. In the Figure this is shown for the (001) surface, as an example. The blue to yellow color coding indicates the contributions of the cation (yellow) and anion (blue) p orbitals to the wavefunctions.



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References

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