Influence of surface deformation on the topological surface states in $Pb_{1-x}Sn_xTe$

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In topological crystalline insulators (TCI) $Pb_{1-x}Sn_xTe$ or $Pb_{1-x}Sn_xSe$, the mirror symmetry with respect to the (110) crystallographic planes is responsible for the presence of gapless Dirac-like electronic surface states on the (001) facets of rock–salt bulk crystals. Recently, the STM experiments demonstrated that the (001) surface of the topologically nontrivial cubic $Pb_{1-x}Sn_xSe$ crystals is deformed relative to the ideal rock salt geometry due to the relative shift of the anion and cation sublattices along the [110] direction. As a consequence of this distortion, the energy dispersion relation of the surface states along the [110] direction remains gapless because the mirror symmetry with respect to (110) is preserved, while in the $[1\bar{1}0]$ direction, for which this symmetry is broken, the gap opens in the spectrum [1, 2].

In the present work we analyze this this problem numerically by first principles calculations, separating the effect of surface distortion from that of the chemical disorder. To this end, we first study a slab of pure PbTe. The lattice constant $a_0 = 6.2$ Å is assumed, thus, according to the previous studies [3], the bulk crystal has an inverted band ordering and is in the topologically nontrivial phase. In the first monolayer of the slab we introduce the experimentally observed distortion described above, namely we displace the anion sublattice with respect to cation sublattice by a vector $a_0\tau(1,1,0)$, where $0 \leq \tau \leq 0.1$. We show that even small distortions of the single monolayer have significant influence on the surface states dispersion. For example, for $\tau = 0.005$ the gap equals 15 meV, for $\tau = 0.01$ it equals 25 meV, thus it is comparable with the experimental values [1, 2].

Second, we discuss the influence of chemical disorder on the dispersion of the surface states. We consider a thick slab of $Pb_{1-x}Sn_xTe$ with such a distribution of cations that the mirror symmetry with respect to the (110) plane is broken. We show that the chemical disorder also opens the gap, however the calculated 0.1 meV gap is practically vanishing, i.e., it is much smaller than the gap caused by distortion, and is not accessible to ARPES measurements.

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