

Spin polarization of surface states on (100) $\text{Pb}_{0.73}\text{Sn}_{0.27}\text{Se}$

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We present the experimental evidence for the spin polarization of the surface states on the (100) surface of $\text{Pb}_{0.73}\text{Sn}_{0.27}\text{Se}$ in the TCI phase as well as in the trivial one.

The recent discovery of topological crystalline insulators (TCI) [1-3] (stimulated by theoretical considerations [4,5]) widened the range of solids considered as hosting topologically protected surface states by systems from the family of IV-VI narrow band gap semiconductors. Our experiments aimed at revealing the topologically protected surface states on TCI, were successfully concluded by observation of such states on the (100) surface of $\text{Pb}_{1-x}\text{Sn}_x\text{Se}$ [1]. The properties of this solid solution are turned out to be particularly advantageous for studying the electronic structure of the TCI phase. In $\text{Pb}_{1-x}\text{Sn}_x\text{Se}$ crystals the strong relativistic effects result in a remarkable compositional evolution of their band structure leading to zero gap state for a specific composition $x=x_c$. For lower and higher Sn compositions the energy gap is open, but the parity of electronic states at band edges is reversed. The crystal with inverted parity of the states at the band edges (for $x>x_c$) hosts the topologically protected surface states. Thus, the properties of both TCI and trivial phases can be investigated in a single experiment, while the transition from one phase to another is induced by the change in temperature.

The experimental data were acquired by spin- and angle resolved photoelectron spectroscopy. The measurements were carried out at the I3 and I4 beamlines at the MAX-III synchrotron at MAX-lab, Lund University, Sweden. Since The band-structure inversion in $\text{Pb}_{0.73}\text{Sn}_{0.27}\text{Se}$ occurs at $T \approx 250$ K, the normal insulator phase was studied at $T=300$ K while the TCI phase at $T=80$ K. ARPES measurements confirmed the formation of the TCI phase below, but gapped states above the band-gap-inversion temperature. The spin-resolved experiments provided evidence for the spin polarization of surface states in both cases: TCI phase and normal insulator. The experimental results are coherent with the results of corresponding tight-binding band structure calculations. The spin polarization seems to be inherent to surface states in narrow-gap IV-VI semiconductors with the electronic band structure influenced by very strong spin-orbit interaction. The transition to the TCI phase induced by the band-symmetry inversion is related to the orbital degrees of freedom of electrons and holes but this also results, via spin-orbit interaction, in the spin polarization of electrons occupying both in-gap Dirac-metal surface states as well as the states close to the bottom of the conduction band and the top of the valence band.

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