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Surface states on topological crystalline insulator $Pb_{1-x}Sn_xSe$ – an ARPES study

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It was recently realized that the concept of topological protection can be extended to other symmetries beyond that of time reversal (crucial for topological insulators). For the case of point-group symmetries, this gives rise to the new class of "topological crystalline insulators" (TCI) in which specific crystalline symmetries warrant the topological protection of metallic surface states [1,2]. A group of IV-VI semiconductors, in particular SnTe, was indicated as possible examples of TCIs [2].

We report on the angle-resolved photoelectron spectroscopy (ARPES) and spin-resolved photoelectron spectroscopy experiments, supported by band structure calculations which have proven existence of topologically protected surface states with the Dirac-like dispersion on the (100) and (111) surfaces of $Pb_{1-x}Sn_xSe$ and have showed that this narrow-gap semiconducting solid solution belongs to the class of topological crystalline insulators (TCI) [3-5].

$Pb_{1-x}Sn_xSe$ offers advantageous conditions for search for surface states of the TCI phase. The increasing Sn content leads to closing the energy gap at some specific crystal composition. For higher Sn contents, the gap opens again but the parity of electronic states at band edges is reversed. Since this transition can also be induced by temperature for properly chosen Sn contents, in these crystals it is possible to study both the open-gap topologically trivial case and open-inverted-gap with topologically nontrivial properties.

The ARPES experiments were performed on the I3 and I4 beam lines at the MAX-III synchrotron facility in Lund (Sweden). The (100) surfaces were obtained by *in situ* cleavage of $Pb_{1-x}Sn_xSe$ crystals grown by self-selecting vapour growth method. $Pb_{1-x}Sn_xSe$ films with (111) surfaces were grown *in situ* on BaF_2 (111) substrates using an open hot wall epitaxy method.

In the ARPES studies for $Pb_{0.77}Sn_{0.23}Se$, the band inversion at T_C=150 K was achieved. Below the inversion temperature we observed the formation of topological states with Dirac-like energy dispersion and the Dirac cones centered in the vicinity of the $\bar{X}$ point of the surface Brillouin zone [3]. Our spin-resolved ARPES experiments enabled us to prove also the existence of spin polarization around the $\bar{X}$ point in the surface Brillouin zone in the TCI phase of $Pb_{0.73}Sn_{0.27}Se$ [5]. In contrast to the (100) face, the Dirac-like surface states on (111) are well separated and noninteracting, located at the time reversal invariant momenta $\bar{\Gamma}$ and $\bar{M}$ in the surface Brillouin zone. Our observations are consistent with the results of tight binding band structure calculations studying surface states on surfaces of topological crystalline insulators.

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