$Pb_{1-x}Sn_xSe$ topological crystalline insulator: a new kind of quantum material

A synchrotron-based Polish-Swedish collaboration results in experimental evidences for recent theoretical predictions

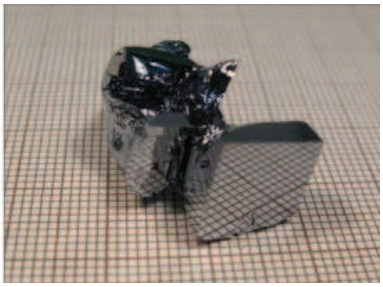

Figure 1. A monocrystal of $Pb_{0.77}Sn_{0.23}Se$ obtained by the self-selecting vapour growth method.

The existence of topologically protected surface states with the Dirac-like dispersion on the (100) surface of $Pb_{1-x}Sn_xSe$ monocrystals has been recently proven by the angle-resolved photoelectron spectroscopy (ARPES) experiments [1].

The discovery of new quantum materials – topological insulators (TI) (one of the most important recent developments in condensed-matter physics) showed that time-reversal symmetry and strong relativistic (spin-orbit) effects led to presence of metallic helical Dirac-like electronic states on surfaces of some particular crystals, like Bi_2Te_3 or Bi_2Se_3.The further theoretical developments in analysis of conditions necessary for occurrence of particular properties characteristic of TI led to widening the class of suitable materials by topological crystalline insulators (TCI), in which specific crystalline symmetries warrant the topological protection of metallic surface states [2,3]. A group of IV-VI semiconductors, in particular SnTe, was indicated as possible examples of TCIs [3]. $Pb_{1-x}Sn_xSe$ monocrystals (Fig. 1) grown in the Institute of Physics, Polish Academy of Sciences, and chosen for the experiments reported in [1], offer 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 x_c. For higher Sn contents, the gap opens again but the parity of electronic states at band edges is reversed. Therefore, the idea was developed in the Institute of Physics, Polish Academy of Sciences to perform thorough investigations of the band structure evolution in these materials. As the topological phase transition can also be easily tuned by temperature, in these crystals it is possible to study in one ARPES experiment both the open-gap topologically trivial case (Fig. 2a) and open-inverted-gap with topologically nontrivial properties (Fig. 2b).

In the ARPES studies carried out for crystals with Sn composition of x=0.23 in the synchrotron laboratory MAX-lab, Lund, Sweden and in the photoelectron spectroscopy laboratory of KTH, Kista, Sweden the band inversion was achieved at T_C = 150 K. Below the inversion temperature one observed the formation of topological states with Dirac-like energy dispersion and the Dirac cone centered in the vicinity of the X point of the surface Brillouin zone [3]. Thus, the presence of the gapless Dirac-like states on the surface of $Pb_{1-x}Sn_xSe$ proved that this narrow-gap semiconducting solid solution belongs to the new class of TCI.

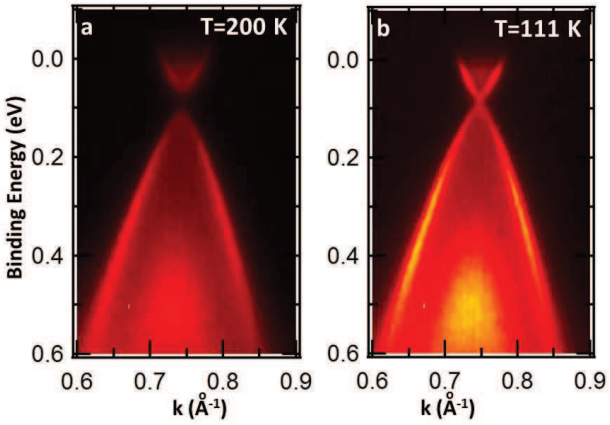

Figure 2.

(a) ARPES spectrum of the surface states taken for the gapped semiconductor phase of $Pb_{0.77}Sn_{0.23}Se$ across the point at which the topologically protected surface states of TCI (with the Dirac-like dispersion) occur in the vicinity of the X point of the surface Brillouin zone (see (b)).

(b) ARPES spectrum across the topologically protected surface states of TCI $Pb_{0.77}Sn_{0.23}Se$ observed in the vicinity of the X point.

The subsequent spin-resolved ARPES experiments allowed to show also the existence of spin polarization around the X point in the surface Brillouin zone in the TCI phase of $Pb_{0.73}Sn_{0.27}Se$. The results were consistent with the results of tight binding band structure calculations [4].

B.J. Kowalski, R. Buczko, and T. Story
Institute of Physics PAS

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