Topological crystalline insulator transition in $Pb_{1-x-y}Sn_xMn_ySe$

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$Pb_{1-x}Sn_xSe$ IV-VI semiconductor substitutional alloys are topological crystalline insulators (TCIs) - quantum materials with topologically protected Dirac-like, helical surface states observed at (001) and (111) surfaces of both bulk crystals [1,2] and thin layers [3]. In the TCIs the inverted band ordering results from relativistic effects and the topological protection is warranted by crystalline symmetry. In $Pb_{1-x}Sn_xSe$ the band inversion and the topological transition is observed at a specific Sn content and temperature. TCIs provide ways of controlling topological state by perturbations lowering the symmetry of crystal potential [4,5] as well as controlling topological transition temperature by band gap engineering effects that could be achieved, e.g. by applying hydrostatic pressure or by alloying with similar material of wider energy gap. The aim of this work is to demonstrate tuning of the topological transition temperature by increasing the energy gap of $Pb_{1-x-y}Sn_xMn_ySe$ with Mn incorporation (at the rate of about dE_g/dy=3 eV). Using the topological transition we also aim at experimental determination of the effect of Mn on the band structure of $Pb_{1-x}Sn_xSe$ in the TCI phase with inverted band ordering.

Bulk monocrystals of $Pb_{0.65}Sn_{0.33}Mn_{0.02}Se$ were grown by the Bridgman method and characterized by X-ray diffraction, magnetotransport, thermoelectric, and magnetization measurements. To experimentally examine the topological transition for the (001) surface of bulk $Pb_{1-x-y}Sn_xMn_ySe$ and reference $Pb_{1-x}Sn_xSe$ monocrystals we applied angle-resolved photoemission (ARPES) technique. At low temperatures (in the inverted band structure regime) we found Dirac-like in-gap states close to the X point of the surface Brillouin zone, thus confirming the basic original observations [1]. We found in $Pb_{0.65}Sn_{0.33}Mn_{0.02}Se$ the TCI transition close to 60 K, i.e. strongly shifted to lower temperatures as compared to the reference $Pb_{0.67}Sn_{0.33}Se$ crystal, in which a clear evidence for the TCI states is observed already at 200 K [6]. This large shift of transition temperature well corresponds to about 60 meV increase of the band gap in the $Pb_{1-x-y}Sn_xMn_ySe$ crystal and the rate of the energy gap decrease with the decreasing temperature (about dE_g/dT=0.5 meV/K) in $Pb_{1-x}Sn_xSe$ in the temperature range 50-300 K [6].

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