Rashba splitting in (111)-oriented PbSnTe:Bi topological crystalline insulators films

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Exploiting the spin degree of freedom of the electrons is one of the primary goals in the rapidly growing field of spintronics. A promising candidate to achieve this goal is so-called Rashba effect observed in the inversion non-symmetric systems and with strong high spin-orbit interaction.

In the present work we show the results of theoretical modeling of Rashba splitting in (111)-oriented topological crystalline insulator PbSnTe films doped with Bi atoms which compared to experimentally obtained angle resolved photoemission spectra (ARPES) of epilayers grown by molecular beam epitaxy. The presence of Bi atoms affects the carrier concentration in the crystal and modifies the effective potential at the surface. The latter effect was simulated in the calculations by applying a potential described by Thomas-Fermi screening model. Using the tight-binding method we have calculated the surface spectral density of states in the normal and in topological crystalline insulator phases of the material. Sufficiently high surface potential leads to large Rashba splitting of states. Our theoretical results suggest however, that spin split surface states should be observed even without any additional potential due to the lack of the inversion symmetry at the surface. These states are much better visible in the case of anion terminated surface than in the case of the cation terminated one. The additional potential due to the Bi doping modifies the surface states increasing the Rashba splitting. By choice of appropriate band bending parameters a good agreement with the ARPES measurements of MBE grown PbSnTe:Bi films for various Sn content and temperatures is achieved.

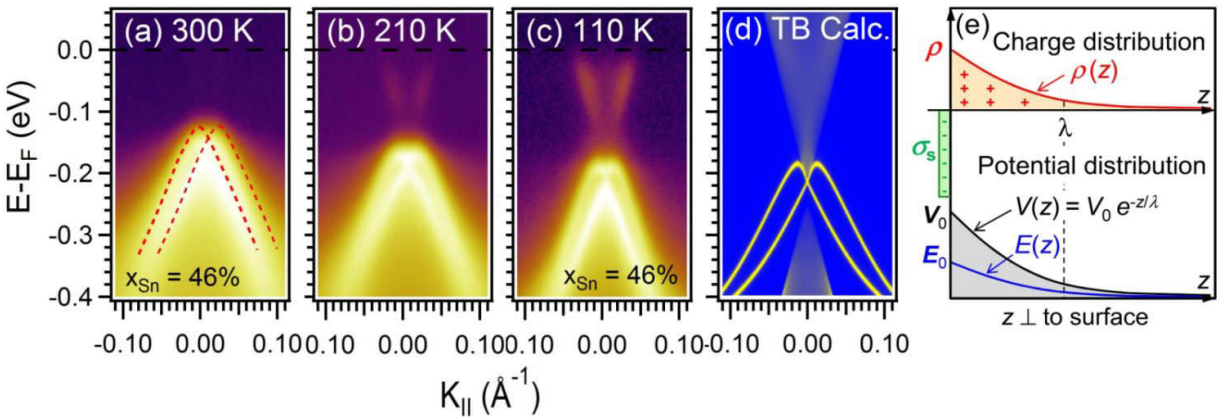

Figure 1: (a) - (c) Temperature dependent ARPES maps of a PbSnTe (111) epilayer with Bi doping of 0.25% at. measured with a photon energy of 18 eV around the Γ point of the surface Brillouin zone compared to tight binding calculations (d) performed for a surface band bending potential $V(z)=V_0e^{-z/\lambda}$ with V_0 = 0.3 V and λ = 2.5 nm. The corresponding charge, potential and electric field distribution is shown schematically in (e).