Topological states on uneven PbSnSe surfaces

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The solid solution $Pb_{1-x}Sn_xSe$ is known to belong to the topological crystalline insulator (TCI) class, under the condition that its bulk band gap is inverted. At room temperature this is satisfied for $0.3 < x < 0.4$. High symmetry surfaces of such crystal – e.g., (001), (110), (111) – host metallic states dispersing linearly around Dirac points, whose degeneracy is protected by mirror symmetries of the rock-salt type lattice [1, 2].

As the bulk band gap is located at four L points, four Dirac cones are expected to appear on the surface. However, at the (001) cleavage plane, two L valleys project onto the same $\bar{X}$ point in the surface Brillouin zone, causing the two associated cones to hybridize through valley mixing. Thus, a "double Dirac cone structure" (DDCS) is formed, in which the degeneracy at $\bar{X}$ is split by tens of meV, while the two protected crossings are shifted away from $\bar{X}$ along the $\bar{X} - \bar{\Gamma}$ line [3]. Recently, it has been shown that such valley splitting is extremely sensitive to morphology of the surface, e.g., in presence of densely spaced odd-height atomic ridges collapses completely to a doubly-degenerate cone [4]. Also the 1D states along sparsely distributed odd-height atomic step edges have been shown to originate from the DDCS [5].

In this communication a systematic theoretical study of the structure of electronic surface states on a (001) $Pb_{1-x}Sn_xSe$ plane with atomic-height terraces, of varying width and number of atomic layers, is presented. Using a realistic tight-binding model we show that in the regime of vast terraces the odd-height step edges act effectively as domain-walls for the surface states. As a result, each separate terrace has its own size-quantized ladder of states. When the width of the terraces decreases, the quantized states of each terrace begin to hybridize with the exponentially-localized 1D step-edge states as well as with states on adjacent terraces. This destroys the domain structure and causes the collapse of the DDCS. Such evolution can be explained using a simple effective mass model in which the mismatch of atomic structure at a step-edge translates to a phase shift between states belonging to the surface Dirac cones on adjacent terraces.

This work was supported by the Polish National Science Centre under projects 2014/15/B/ST3/03833 and 2016/23/B/ST3/03725.

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