Analytical solutions for the surface states of $Bi_{1-x}Sb_x$

Yuki Fuseya[1], Hidetoshi Fukuyama[2]

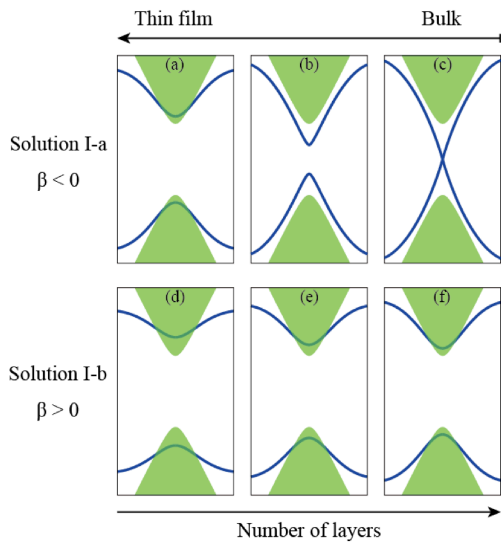
[1]Department of Engineering Science, University of Electro-Communications, Chofu, Tokyo 182-8585, Japan

[2]Research Institute for Science and Technology, Tokyo University of Science, Kagurazaka, Shinjuku, Tokyo 162-8601, Japan

fuseya@uec.ac.jp

From the viewpoint of the spin-orbit coupling (SOC) originated surface state (SS), bismuth is one of the most fascinating materials [1,2], because it has the largest SOC among the radioactively safe elements. Moreover, following the proposal of the existence of a three-dimensional topological insulator in $Bi_{1-x}Sb_x$, the SS of $Bi_{1-x}Sb_x$ (especially for $0 \leq x < 0.1$) has attracted considerable attention in solid-state physics. While it has been widely accepted that pure Bi is topologically trivial, it has been proposed that $Bi_{1-x}Sb_x$ becomes topologically nontrivial for $x>0.04$ due to band inversion at the L point in a bulk Brillouin zone. A drastic change in the SS is therefore expected due to this topological transition. Nevertheless, the SS does not exhibit a qualitative change with respect to the Sb substitution even though the bulk conduction and valence band are inverted at $x \sim 0.04$. This has been a mystery discussed lively in the fields of both topological physics and surface science.

In this paper, analytical solutions for the SS of an extended Wolff Hamiltonian, which is a common Hamiltonian for strongly spin-orbit coupled systems, are obtained both for semi-infinite and finite-thickness boundary conditions [3]. For the semi-infinite system, there are two types of Solutions: (I-a) linearly crossing SSs in the direct bulk band gap, and (I-b) SSs with linear dispersions entering the bulk conduction or valence bands away from the band edge. For the finite-thickness system, a gap opens in the SS of solution I-a. Numerical solutions for the SS are also obtained based on the tight-binding model of Liu and Allen [4] for $Bi_{1-x}Sb_x$. A perfect correspondence between the analytic and numerical solutions is obtained including their thickness dependence. This is the first time that the character of the SS numerically obtained is identified with the help of analytical solutions. The size of the gap for I-a SS can be larger than that of bulk band gap even for "thick" films (<200 bilayers ~ 80 nm) of pure bismuth. Consequently, in such a film of $Bi_{1-x}Sb_x$, there is no apparent change in the SSs through the band inversion at $x \sim 0.04$, even though the nature of the SS is changed from solution I-a to I-b. Based on our theoretical results, the experimental results on the SS of $Bi_{1-x}Sb_x$ are discussed.



Schematic summary of the present analytical solutions. The right panels correspond to the semi-infinite system. The shaded regions express the bulk band, the extremum of which correponds to the M point in the surface Brillouin zone of $Bi_{1-x}Sb_x$.

References:
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