DFT simulations of Sb(111) surface states.

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Antimony is a Pierls semimetal. I.e. electronic and atomic structure is a consequence of Pierls transition. Atomic structure can be described in terms of Pierls distortion of a simple cubic structure of praphase. As a result a lattice period of Sb in [111] direction exceeds twice one of the praphase. Doubling of period leads to creation of covalent bods between double atomic plains while the double plains are connected by Van der Waals forces. Dispersion of bulk electrons reveals a small gap in a vicinity of Γ point. Surface states spectrum is a resulted from surface crystal lattice symmetry [1]. Non degenerated Dirac massless cone of surface states in a vicinity Γ point with a Dirac point at 270 mev below the Fermi level is due to strong spin orbit coupling.

In this work we present the results of our simulations of Sb(111) crystal structure and surface states in a frame of DFT approximation. The simulations were performed for Sb(111) cleaved both by Van der Waals and covalent bonds. Crystal structure of Sb(111) cleaved by Van der Waals bonds can be described in terms of bulk like structure with a small distortion of atomic interplane distance (about 1%) in the vicinity of the surface. In contrast, structure of the crystal cleaved by covalent bonds reveals break of Pierls distortion in a top 8 atomic layers. Dirac cone is robust to a way of cleavage while a local break of a Pierls transition in a vicinity to the surface leads to deformation of electron spectrum of a bulk electrons. As a result electron subbands appears of in an energy gap close to the Fermi level. Dirac cone of surface states was found to be robust on adsorption of Pb at the surface. The results of simulations were confirmed in ARPES, STM, STS experiments.

1. Molotkov S.N, Ryzhkin M.I., JETP Lett (Sov) 102, 216, 2015