Spin-polarized band structure of a Sn atomic layer at graphene/SiC(0001) interface

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Spin-polarized bands at solid surfaces have been extensively studied not only because of fundamental interests but also spintronic applications. Here, symmetry of the surface plays an important role in characterizing the spin splitting and the spin texture of a two-dimensional band [1]. Peculiar Zeeman-type spin splitting with out-of-plane spin polarization appears at the K point with C_3 symmetry in surface Brillouin zone (SBZ) of Tl/Si(111)-(1×1), where the surface structure belongs to the plane group of *p*3*m*1 [2]. On the other hand, in the case of Bi/Si(111)-($\sqrt{3}\times\sqrt{3}$)R30° that belongs to the plane group of *p*31*m*, Rashba-type spin-splitting was found at the K point having C_{3v} symmetry regardless of time reversal [3]. The difference of the symmetry at the K point in the SBZ determines the type of the spin splitting of the band. Here, we report the both types.

Recently, we synthesized a new two-dimensional material: a triangular lattice atomic layer (TLAL) consisting of Sn [4]. The Sn TLAL is formed by intercalation into the interface between graphene and SiC(0001) substrate. In this material, there is graphene in the topmost layer, and the intercalated Sn atoms are located at T_1 sites on the SiC(0001) surface. The Sn TLAL shows a (1×1) periodicity with respect to the SiC(0001) substrate.

In the present study, we investigated the spin-polarized electronic band structure of the Sn TLAL by (spin-) and angle-resolved photoelectron spectroscopy at the Institute for Solid State Physics, the University of Tokyo [5]. We find that different types of spin splitting appear at a K point of the Sn TLAL: one is Zeeman-type spin splitting and another one is Rashba-type band crossing. Here, the K point has C_3 symmetry with taking the crystal structure into account. Thus, the Zeeman-type is consistent with the symmetry of the lattice while the Rashba-type band crossing is inconsistent. To understand this experimental results, we examined the charge density distribution analysis of the Sn-derived bands by density functional theory calculations. The analysis reveals that the charge density distribution of the Rashba-type band at the K point belongs to the plane group of *p*31*m*, meaning that the electronic state at the K point has C_{3v} symmetry. Therefore, the symmetry of the charge density distribution agrees with the Rashba-type band crossing at the K point. We conclude that the symmetry of the charge density distribution governs the type of the spin splitting of the band beyond the symmetry of the lattice.

References:
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