Massless Dirac Fermion in Borophene

Honeycomb structures of group IV elements can host massless Dirac fermions with nontrivial Berry phases. Their potential for electronic applications has attracted great interest and spurred a broad search for new Dirac materials especially in monolayer structures. We present a detailed investigation of the \( \{ \beta \} \) sheet, which is a borophene structure that can form spontaneously on an Ag(111) surface. Our tight-binding analysis revealed that the lattice of the \( \{ \beta \} \) sheet hosts Dirac cones, and each Dirac cone could be split by overlayer-substrate interactions. These unusual electronic structures were confirmed by angle-resolved photoemission spectroscopy and validated by first-principles calculations.

One of the promising routes for realizing novel two-dimensional materials is by tailoring or modifying the honeycomb lattice. An example is a monolayer boron sheet (i.e., borophene), which is realized by introducing periodic boron atoms in a honeycomb-like lattice. As boron has one less electron than carbon, the honeycomb structure is unstable, but the introduction of additional boron atoms in the honeycomb lattice can stabilize the structure by balancing out the two- and multicenter bonds. Depending on the arrangements of the extra boron atoms, various monolayer-boron structures have been experimentally realized on Ag(111) [1-4]. For example, it was reported that there were a stable striped phase and a metastable homogeneous phase [1]. The striped phase was proposed to be a complete triangular lattice with anisotropic, out-of-plane buckling. In another study, a similar striped phase with a different rotation angle was observed [3]. This phase, named \( \{ \beta \} \) sheet (Fig. 1h), has an essentially flat structure and interacts weakly with the Ag(111) substrate [3, 4]. However, there have been few experimental investigations on the electronic properties of monolayer boron.

We synthesized \( \{ \beta \} \) borophene and studied its electronic structure by angle-resolved photoemission spectroscopy at BL-2A [5]. A schematic drawing of the Brillouin Zone (BZ) of Ag(111) with the three domain orientations is shown in Fig. 1a, together with the measured Fermi surface. The band structure from the boron layer shows one Femi pocket centered at the \( \{ \beta \} \) sheet and a pair of Fermi pockets centered at the M point of Ag(111), as indicated by the red and black arrows, respectively. The photoemission bands derived from the boron layer do not disperse with photon energy, which is in agreement with its two-dimensional characteristic.

The pair of Fermi pockets centered at the M point of Ag(111) is associated with Dirac cones. In Fig. 1b, we show constant energy contours (CECs) at different binding energies (\( E_b \)). With increasing binding energies, the Fermi pockets first shrink in size and then become points at \( E_b = -0.25 \text{ eV} \). Further increase of the binding energy leads to a pair of closed contours which touch each other at \( E_b = -0.68 \text{ eV} \). The pair of closed contours merges into one contour at higher binding energies. The measurements of cut 1 using \( \sigma \) polarized light (Fig. 1d) reveal a Dirac cone as well as the bulk sp band of Ag(111). The Dirac point is located at approximately 0.25 eV below the Fermi level, in agreement with the evolution of the CECs in Fig. 1b. The linear dispersing bands extend to as deep as 2 eV. Within the first BZ of the \( \{ \beta \} \) sheet, we observed two pairs of Dirac cones in total, as schematically illustrated in Fig. 1g.

The orbital contribution of the boron bands can be probed by switching the linear polarization of the incident light. The \( s \) polarized light primarily probes the in-plane \( p_x \) and \( p_y \) orbitals, while the \( p \) polarized light probes both the in-plane \( (p_x^s \pm p_y^s) \) and out-of-plane \( (p_z^s) \) orbitals. The band structures along cut 1 measured with \( s \) and \( p \) polarized light are shown in Figs. 1c and 1d, respectively. The Dirac cone was not observed with \( p \) polarized light, leaving only the bulk sp bands of Ag(111). This means that the Dirac cones originate from the \( p_z \) orbital of boron.

Recent successes in graphene science indicate that “borophene”, as revealed by our work, is an interesting new field of research in physics and technology.

REFERENCES

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