**Structure of the Boron Atomic Wire on Cu(111) and its Unique Relationships to the Carbon Chain Molecules**

We investigated atomic structure and electron states of 2D ordered phase, \( ^{73} \text{B}/\text{Cu}(111) \) by a concerting usage of postion diffusion and photoemission spectroscopy. The surface overlayer is 2D copper boride with a periodic arrangement of the boron atomic chains that are isoelectronic to cumulene. The unique chemical character of the 1D boron molecule may allow us to call it "Bumulene". Though it has been known that the B and Cu phases are completely separated in three-dimensional (3D) materials, the present study intriguingly revealed that a compound is formed in two-dimensional (2D) at the surface. The 2D Cu-B compound on Cu(111) likely becomes an ideal B/Cu interface to develop surface science and boron chemistry.

Recently, there have been growing interests in chemistry and physics of boron polymorphs or metal borides on surfaces due to unique multi-center bonding between boron atoms [1]. On the well-known Cu(111) substrate, the 2D ordered phase, \( ^{73} \text{B}/\text{Cu}(111) \), is prepared by boron deposition where the surface structure has not been known. In the present research, we made the structure analysis by total-reflection high-energy positron diffraction (TRHEPD) experiment at SPF, with a measurement setup illustrated in Fig. 1(a). The positron beam is totally reflected at a glancing angle \( \theta \) below the critical angle and the probe has the highest surface beam intensity at the (00) spot taken at 10 keV under the surface at a glancing angle [2].

The surface structure is described by the 2D Cu boride model with the alternate arrangement of Cu and boron atomic chains. Evaluations of the chemical states were made by measurements of the Cu and B core-level spectra as shown in Fig. 2(a, b). In the 2D Cu boride, there appear two Cu components that can be ascribed to the surface layer (L) and in the bulk (Bu), while the B 1s spectrum has only a single component. The B 1s binding energy at 187.8 eV means that the boron atoms were negatively charged, and the electrons are likely transferred to the boron atoms from the surrounding copper atoms.

A combination of TRHEPD and XPS results evidences a correlation between the surface structure and the negative charge at the boron atom. Taking the building blocks of the boron atom chain as linear molecules with two triangular terminals, Figures 2 (c, d) show the cis- and trans-configurations, respectively. In the cis-type (trans-type), the LUMO and HOMO energy levels were \(-5.15\text{eV} (-5.32\text{eV})\) and \(-5.63\text{eV} (-5.45\text{eV})\) with reference to the vacuum level, respectively. In a free space, an optimized structure of the molecule takes the trans-configuration. On the other hand, the 2D Cu boride model (Fig. 1c) has the triangle groups lying on the surface, taking the cis-configuration. The difference can be understood by considering the charge state between the two structures. We first recall that boron atoms are negatively charged, as unveiled by XPS measurements of the Cu and B core-level spectra as shown in Figs. 2(a, b). In the 2D Cu boride, there appear two Cu components that can be ascribed to the surface layer (L) and in the bulk (Bu), while the B 1s spectrum has only a single component. The B 1s binding energy at 187.8 eV means that the boron atoms were negatively charged, and the electrons are likely transferred to the boron atoms from the surrounding copper atoms.

A combination of TRHEPD and XPS results evidences a correlation between the surface structure and the negative charge at the boron atom. Taking the building blocks of the boron atom chain as linear molecules with two triangular terminals, Figures 2 (c, d) show the cis- and trans-configurations, respectively. In the cis-type (trans-type), the LUMO and HOMO energy levels were \(-5.15\text{eV} (-5.32\text{eV})\) and \(-5.63\text{eV} (-5.45\text{eV})\) with reference to the vacuum level, respectively. In a free space, an optimized structure of the molecule takes the trans-configuration. On the other hand, the 2D Cu boride model (Fig. 1c) has the triangle groups lying on the surface, taking the cis-configuration. The difference can be understood by considering the charge state between the two structures. We first recall that boron atoms are negatively charged, as unveiled by XPS measurements of the Cu and B core-level spectra as shown in Figs. 2(a, b). In the 2D Cu boride, there appear two Cu components that can be ascribed to the surface layer (L) and in the bulk (Bu), while the B 1s spectrum has only a single component. The B 1s binding energy at 187.8 eV means that the boron atoms were negatively charged, and the electrons are likely transferred to the boron atoms from the surrounding copper atoms.

**REFERENCES**


**BEAMLINE**

SPF-A3

Y. Tsujikawa and I. Matsuda (The Univ. of Tokyo)