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Synthesis of semimetal A_3Bi (A = Na, K) thin films by molecular beam epitaxy

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ABSTRACT

Three-dimensional (3D) Dirac cones are predicted to reside in semimetals A_3Bi (A = Na, K). By using molecular beam epitaxy (MBE) and scanning tunneling microscopy (STM), we have successfully established the growth conditions for Na_3Bi thin films on Si(1 1 1)-7 × 7, and determined that the lattice of Na_3Bi is rotated by 30 degree with respect to that of Si(1 1 1)-7 × 7. The Na_3Bi/Si(1 1 1)-7 × 7 thin film was further used as the substrate for the growth of K_3Bi. The 3D Dirac-cone-like electronic band structures of Na_3Bi and K_3Bi have been clearly revealed by angle resolved photoelectron spectroscopy (ARPES).

1. Introduction

The discovery of Dirac-like band structure in graphene has led to significant attention partially due to its potential to simulate high energy physics with condensed matter [1–5]. In the presence of spin–orbit coupling as well as time-reversal symmetry, the Dirac-cone structure in momentum space can also be found in topological insulators [6–8,3,9–15], such as Bi_2Se_3, Bi_2Te_3, and Sb_2Te_3 [16–20]. Although with a different origin, their surface states mimic the band structure of graphene to a large extent. In addition, the surface states are protected by time-reversal symmetry and are immune to backscattering. The search for new generation of Dirac-cone-like band structure in other systems can provide us with new physics and potential applications. Recently, it has been proposed that a new kind of topological material called topological semimetal, such as Na_3Bi and K_3Bi, may also harbor a Dirac-cone-like structure, which is directly linked to the presence of crystal symmetry [21–23]. The Dirac cones in these materials are three-dimensional, unlike the two-dimensional surface states in topological insulators. The three-dimensional Dirac cone allows for novel realization of high-energy phenomena in condensed matter physics as well as possible applications in spintronics. In this paper, we report the growth of Na_3Bi and K_3Bi by MBE and their electronic band structures revealed by ARPES.

2. Experimental methods

The bulk crystals of Na_3Bi and K_3Bi are difficult to handle because of their high chemical reactivity in air. Therefore we attempt to grow thin films in ultra-high vacuum and measure their electronic structures *in situ*. The experiments were carried out on an Omicron MBE-STM-ARPES combined system in ultra-high vacuum with a base pressure better than 1×10^{-10} mbar. Si(1 1 1)-7 × 7 substrates were cleaned by a standard multi-cycle flashing process. Sodium was bought from Alfa Aesar with a purity of 99.95% and bismuth was from NILACO Co. with a purity of 99.999%. The growth dynamics of Na_3Bi is similar to that of Bi_2Se_3 and Bi_2Te_3 [20,26–29]. Sodium and bismuth from two Knudsen cells held at 190° and 495°, respectively, were evaporated onto the Si(1 1 1)-7 × 7 substrate, which is maintained at 250–300°. The growth proceeds under Na-rich condition (Na/Bi flux ratio = 10–20) and the growth rate only depends on the Bi flux. The extra Na on the surface can quickly desorb under the above growth condition and does not incorporate into the film. Imaging of the samples was performed *in situ*

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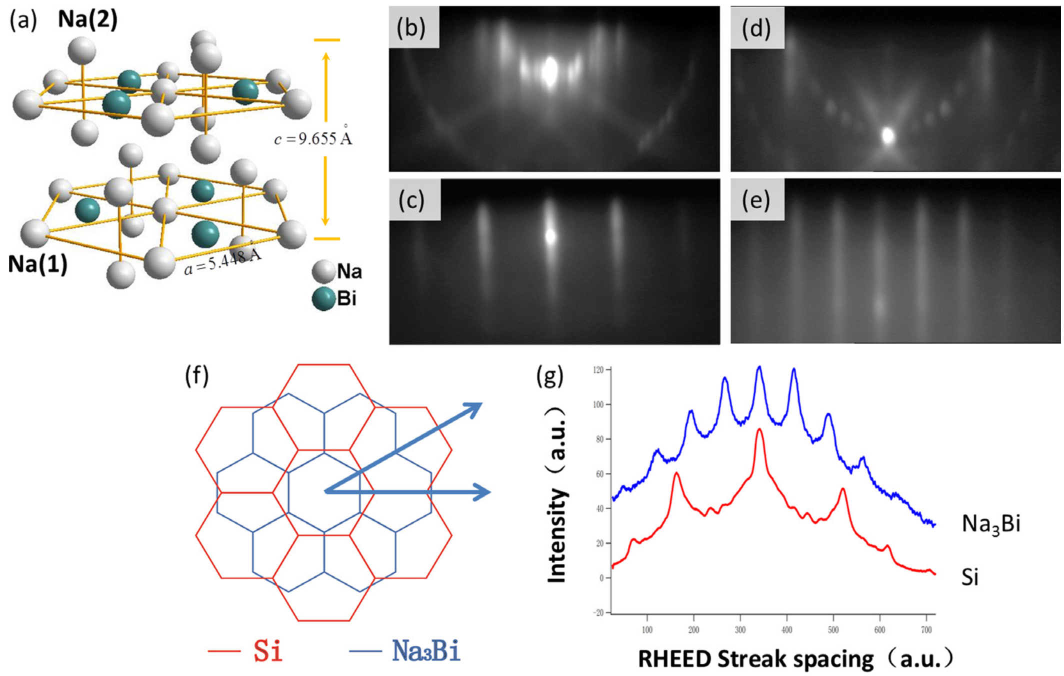

Fig. 1. (a) Crystal structure of Na_3Bi with $P6_3/mmc$ symmetry and two nonequivalent Na sites (Na(1), Na(2)). (b) RHEED pattern of the Si(1 1 1)-7 × 7 substrate along the $\langle 1 1 \bar{2} \rangle$ direction of Si(1 1 1) before growth. (c) RHEED pattern of Na_3Bi along the ⟨1 1 0⟩ direction of Na_3Bi(1 0 0) after growth. (d) RHEED pattern of Si(1 1 1)-7 × 7 along the ⟨1 1 0⟩ direction of Si(1 1 1) before growth. (e) RHEED pattern of Na_3Bi(1 0 0) along the $\langle 1 1 \bar{2} \rangle$ direction of Na_3Bi after growth. (f) Illustration of 30-degree rotation of reciprocal lattice of Na_3Bi and Si. (g) RHEED streak spacing of Na_3Bi(1 0 0) and Si(1 1 1).

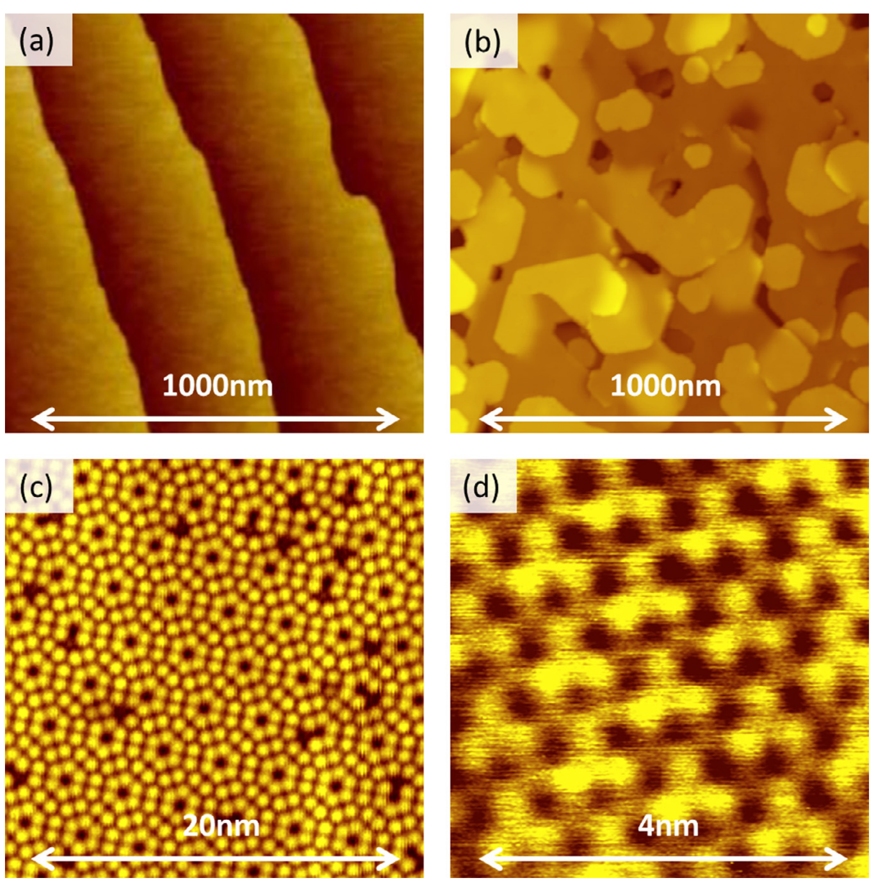

Fig. 2. STM images (1000 nm × 1000 nm), acquired from (a) the Si(1 1 1)-7 × 7 substrate and (b) the 20 nm-thick Na_3Bi(1 0 0) film. High-resolution images are (c) the Si(1 1 1)-7 × 7 substrate and (d) Na_3Bi(1 0 0).