27A/2010G660

Determination of the atomic arrangement at the graphene/α-Al_2O_3(0001) interface by normal incident X-ray standing wave spectroscopy

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1 Introduction

Direct growth of graphene films on insulator substrates is currently one of the most important subjects for graphene-based nanoelectronics and spintronics. Despite the critical role of substrate on the electronic property of graphene, the atomic structure of the graphene/insulator substrate interface is still not clear. Normal incidence X-ray standing wave (NIXSW) spectroscopy is a powerful tool for investigating the interface atomic structure, because the positions of atoms relative to the scattering plane in the substrate can be determined precisely and element-specifically [1]. In this study, the atomic arrangement of single-layer graphene (SLG) directly grown on c-plane sapphire (α-Al_2O_3(0001)) has been studies by NIXSW spectroscopy.

2 Experiment

The graphene growth on α-Al_2O_3(0001) was performed in a vacuum quartz tube furnace with a base pressure of 2 × 10^{-6} Pa. The α-Al_2O_3(0001) substrate was annealed at 1173 K for 60 min in an open air to prepare atomically flat surface. The SLG film was grown by exposing the α-Al_2O_3(0001) surface to methanol vapour in a pressure of ~1000 Pa at the substrate temperature of 1273 K [2]. The NIXSW measurements were conducted at the BL-27A station by scanned-energy technique [3]. The NIXSW profiles were obtained by recording the intensities of the Al 1*s*, O 1*s* and C 1*s* photoelectrons as a function of the photon energy.

3 Results and Discussion

Figures 1 (a), (b) and (c) show SW profiles for the Al, O and C atoms in SLG/α-Al_2O_3(0001). Clear SW profiles are seen in Fig.1, and the Bragg energy can be determined as 2938.5 eV. This energy nearly corresponds to the Bragg diffraction peak from the one-sixth of the c-axis of α-Al_2O_3 unit cell (d = 2.17 Å). The SW profile is written as

$$I(E)/I_0 = 1+R(E)+2F[R(E)]^{1/2}\cdot\cos[2\pi d_H-\delta(E)] \quad (1)$$

where E is the photon energy, $R(E)$ is the reflectivity of the substrate, $\delta(E)$ is the energy-dependent phase modulation caused by the X-ray standing wave, F is the structure factor, and d_H is the coherent position of the atoms measured from the X-ray scatter plane [4]. The d_H of Al, O and C is calculated as -0.1 ± 0.1, 0.5 ± 0.3 and 1.7 ± 0.3, respectively. Thus, the Al, O and C atoms respectively are located at -0.2, 1.1 and 3.7 Å above the scatter plane. From these results, we propose the vertical structure of SLG/α-Al_2O_3(0001) as schematically illustrated in Fig.2. The SLG layer is ~2.6 Å above the α-Al_2O_3(0001) surface, which is comparable with the distance between the SLG layer and the Ni(111) surface (2.14 Å) [5]. This suggests rather strong interaction at the SLG/α-Al_2O_3(0001) interface.

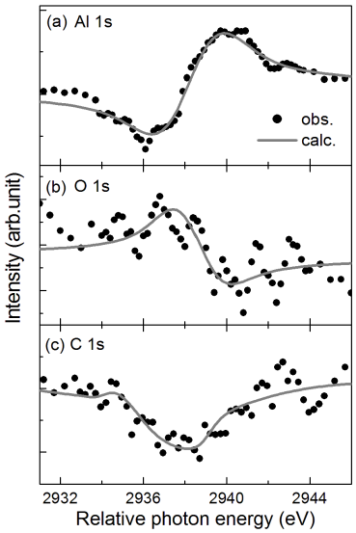

Fig. 1: NIXSW profiles from (a) Al 1*s*, (b) O 1*s* and (c) C 1*s* core level emission. The calculated SW profiles (solid line) are also included in the figure.

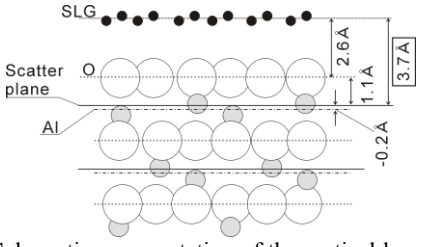

Fig. 2: Schematic representation of the vertical locations of the Al, C and O atoms in SLG/α-Al_2O_3(0001).

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