Determination of the atomic arrangement at the graphene/α-Al₂O₃(0001) interface by normal incident X-ray standing wave spectroscopy

Shiro Entani1,*, Manabu Ohtomo1, Yoshihiro Matsumoto1, Yuji Baba2, Ayumi Narita2, Norie Hirao2, Iwao Shimoyama2, Tetsuhiro Sekiguchi2, Pavel V. Avramov1, Naramoto Hiroshi1 and Seiji Sakai1
1Advanced Science Research Center, Japan Atomic Energy Agency, Tokai 319-1195, Japan
2Quantum Beam Science Directorate, Japan Atomic Energy Agency, Tokai 319-1195, Japan

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-Al₂O₃(0001)) has been studied by NIXSW spectroscopy.

2 Experiment

The graphene growth on α-Al₂O₃(0001) was performed in a vacuum quartz tube furnace with a base pressure of 2 × 10⁻⁶ Pa. The α-Al₂O₃(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-Al₂O₃(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 1s, O 1s and C 1s 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-Al₂O₃(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-Al₂O₃ unit cell (d = 2.17 Å). The SW profile is written as

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

(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 substrate, as illustrated in Fig.2. The SLG layer is ~2.6 Å above the α-Al₂O₃(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-Al₂O₃(0001) interface.

References

* entani.shiro@jaea.go.jp