SPF-A3/2014S2-004

Structure Determination of Graphene on Metal Substrates using Total-Reflection High-Energy Positron Diffraction (TRHEPD)

Yuki Fukaya[1,*], Shiro Entani[1], Seiji Sakai[1], Izumi Mochizuki[2], Ken Wada[2], Toshio Hyodo[2], and Shin-ichi Shamoto[1]
[1]JAEA, Ibaraki 319-1195, Japan
[2]KEK-IMSS, Tsukuba 305-0801, Japan

1 Introduction

Graphene, a two-dimensional atomic sheet of carbon, has attracted much attention because of its high electron mobility and other promising properties such as high thermal conductivity and high rigidity. The synthesis of graphene has been successfully performed on various metal substrates. The theoretical calculations demonstrate that the electronic band structure of the graphene, so-called Dirac cone, is modified by the interaction with the substrate materials [1]. The magnitude of the interaction is closely related to the spacing between the graphene and the metal substrate. Thus, the spacing between graphene and metal substrate is the key factor to determine the electronic property of graphene adsorbed on the substrate. In this study, we determined the spacing between the graphene and the Cu(111) and the Co(0001) substrates using total-reflection high-energy positron diffraction (TRHEPD).

TRHEPD is a surface-sensitive tool owing to the positive charge of the positron [2]. When the positron beam is incident on a crystal surface at a grazing angle, the total reflection takes place on the surface. The penetration depth of the positron beam under the total reflection condition is less than approximately 2 Å, which corresponds to the thickness of 1-2 atomic layers. Therefore, the TRHEPD is suitable for the determination of the atomic configurations of graphene adsorbed on the substrate.

2 Experiment

Experiments were carried out at the Slow Positron Facility, KEK. The incident positron beam was accelerated to 10 keV. The diffraction pattern was observed with a microchannel plate with a phosphor screen and a CCD camera. In order to measure the rocking curve, the glancing angle of the incident positron beam was varied by rotating the sample at a step of 0.1°. All the measurements were conducted at room temperature.

Cu atoms were deposited on a α-Al_2O_3(0001) substrate at room temperature, followed by annealing up to 1270 K in H_2 atmosphere to form a Cu(111) thin film. Then a single layer of graphene was grown on the the film by exposing it to the gas mixture (Ar, H_2, CH_4) at 1270 K. Co atoms were deposited on a α-Al_2O_3(0001) substrate at 620 K to form Co(0001) thin film. A single layer of graphene was grown on the film by an exposure to acetylene at 870 K.

3 Results and Discussion

The obtained TRHEPD rocking curves for the graphenes on the Cu(111) and the Co(0001) substrates exhibit different shapes, as shown by the open circles in Fig. 1. We determined the spacing between the graphene and the substrate by minimizing the difference between the measured and calculated curves. From the analysis based on the dynamical diffraction theory, the spacings between the graphenes and the Cu(111) substrate and the Co(0001) substrate were estimated to be 3.32 Å and 2.24 Å, respectively. The results are consistent with the theoretical calculations based on the density functional theory [1]. The value of 3.32 Å for the Cu(111) substrate is very close to the interlayer distance in graphite (3.35 Å). The spacing for Co(0001) substrate is much lower than this. Therefore, the graphene on the Co(0001) substrate interacts strongly with the substrate as compared with that on the Cu(111) substrate.

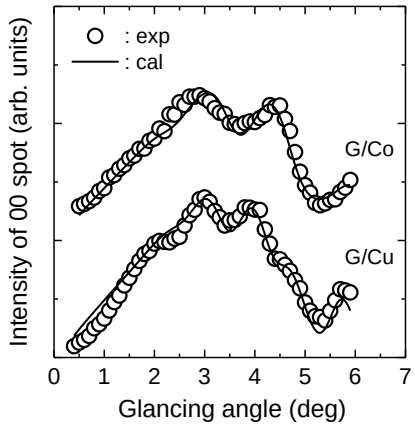

Fig. 1: TRHEPD rocking curves for the graphene on the Cu(111) (lower) and the Co(0001) (upper) substrates. Open circles and solid lines denote the experiment and calculation, respectively.

References

[1] G. Giovannetti *et al*., *Phys. Rev. Lett.* **101**, 026803 (2008).
[2] Y. Fukaya *et al*., Appl. Phys. Express **7**, 056601 (2014).

* fukaya.yuki99@jaea.go.jp