13C, 11A/2008G156

Site selective adsorption of atomic deuterium on boron nitride thin film

Kaveenga Rasika KOSWATTAGE[1,2)], Iwao SHIMOYAMA[1)], Tetsuhiro SEKIGUCHI[1)], Yuji BABA[1)], and Kazumichi NAKAGAWA[2)]

[1]Japan Atomic Energy Agency, Tokai-mura, Naka-gun, Ibaraki-ken 319-1195, Japan

[2]Kobe Univ., Tsurukabuto 3-11, Nada-ku, Kobe 657-8501, Japan

Introduction

Boron nitride (BN) is an attractive material for hydrogen storage because it forms nanotubes structure as well as carbon nanotubes (CNT). It is expected that BN nanotubes is superior to CNT because of dipole interaction induced by polarization between B-N bonding. Since an experimental work reported large hydrogen uptake for BN nanomaterials that included many defects [1], chemisorption of hydrogen was supposed for the high uptake. However, detail of the interaction between hydrogen and BN materials has not been clarified well. One of the most basic arguments is site dependence of atomic hydrogen adsorption. Two opposite ideas have been theoretically proposed; One is that hydrogen preferentially adsorbs on B site, and the other is that hydrogen adsorbs both on B and N sites [2,3]. In this work, we investigated site dependence of atomic deuterium adsorption on BN thin film using near-edge X-ray absorption fine structure (NEXAFS) and X-ray photoelectron spectroscopy (XPS).

Experimental

Experiments were performed at the BL13C and BL11A stations. In the experiment at the BL13C, we used APECS apparatus developed by Kakiuchi *et al.* [4]. In the experiments at the BL11A, we used sector-type electron analyzer (VG, CLAM2). BN thin film was formed on Ni(111) by chemical vapor deposition with borazine ($B_3N_3H_6$) gas. After preparation of the BN thin film with a thickness of 7.6 Å, the film was exposed to atomic deuterium beam produced by W hot filament in an ultra high vacuum chamber. We measured NEXAFS and XPS spectra before and after the exposure of atomic deuterium. NEXAFS spectra were measured by total electron yield for various incidence angles θ which is defined as the angle between surface normal and polarization vector of X-ray.

Result and Discussion

Fig. 1 and 2 show B and N K-edge NEXAFS spectra measured at θ = 35°, respectively. Black and red curves correspond to the spectra obtained before and after exposure of atomic deuterium, respectively. Clear spectral change was observed in the B K-edge region as shown in Fig.1. On the other hand, only slight change was observed in Fig.2. Polarization dependence of NEXAFS spectra clarified that the spectral features changed in the low energy region are assigned to out-of plane transitions. These results suggest that deuterium atoms preferentially adsorbed on B sites than N sites with upright standing configuration. XPS measurements also supported this interpretation. B1s peak showed additional discrete component at low binding energy side for the BN film exposed by atomic deuterium. On the other hand, N 1s peak showed only peak broadening after the exposure. In summary, we first clarified site selective adsorption of atomic deuterium on BN thin film.

References

[1] C. Tang, Y. Bando, X. Ding, S. Qi, and D. Golberg, J. Am. Chem. Soc., 124, 14550 (2002).

[2] B. Mårlid and J.-O. Carlsson J. Phys. Chem. B 103, 7637 (1999).

[3] X. Wu, J. Yang, J. G. Hou, and Q. Zhu, J. Chem. Phys. 121, 8481 (2004).

[4] T. Kakiuchi, E. Kobayashi, N. Okada, K. Oyamada, M. Okusawa, K. K. Okudaira, K. Mase, J. Electron. Spectrosc. Relat. Phenom. 161, 164 (2007).

shimoyama.iwao@jaea.go.jp

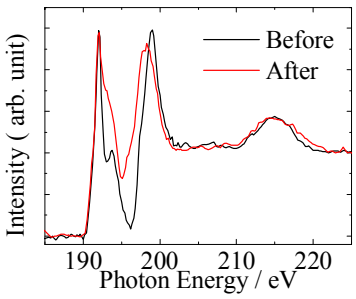

Fig. 1. B K-edge NEXAFS spectra of BN film before and after exposure of atomic deuterium.

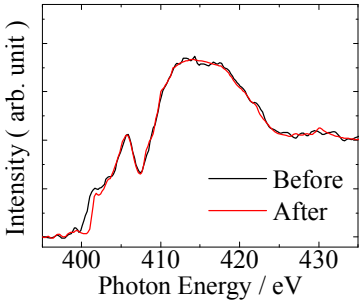

Fig. 2. N K-edge NEXAFS spectra of BN film before and after exposure of atomic deuterium.