Selective adsorption of atomic hydrogen on boron nitride thin film

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Boron nitride (BN) have attracted much research attention as a promising candidate for hydrogen storage and it has been reported that BN nanotubes are superior to carbon nanotubes for storing hydrogen. Despite the great attention, it is not clear yet how the adsorption mechanism works on BN materials. One of the most basic arguments is the site dependence of atomic hydrogen adsorption. However, there are a number of theoretical reports that contradict each other. In this work, we investigated the site dependence of atomic deuterium adsorption on a thin film of BN, using near-edge X-ray absorption fine structure (NEXAFS), X-ray photoelectron spectroscopy (XPS), and photo stimulated ion desorption (PSID) in order to verify the theoretical models.

All experiments were performed with linearly-polarized synchrotron radiation at the BL-11A beam line. A BN thin film was formed on Ni(111) by chemical vapor deposition with borazine ($B_3N_3H_6$) gas. Then the film was exposed to an atomic deuterium beam produced by a tungsten hot filament in an ultra high vacuum chamber. NEXAFS and XPS spectra were measured before and after the exposure to atomic deuterium. A clear spectral change was observed in the B K-edge region after deuteration and only slight change was observed in the N K-edge region as shown in Fig.1. The XPS spectrum of B 1s showed a prominent shoulder on the low binding energy side of the main peak after deuteration, while the N 1s spectrum showed only peak broadening at the high binding energy side. After deuteration, D^+ ion yield was measured as a function of the incident photon energy at the B and N K-edges in the PSID measurements. It was observed that there was a clear enhancement of D^+ signal at the B K-edge but there was no enhancement at the N K-edge. The experimental results of NEXAFS and XPS were analyzed by the DV-Xα molecular orbital calculation method with core-hole effect. Finally, we conclude that hydrogen atoms are preferentially adsorbed on the B sites of BN materials, *via* a single hydrogen adsorption model.

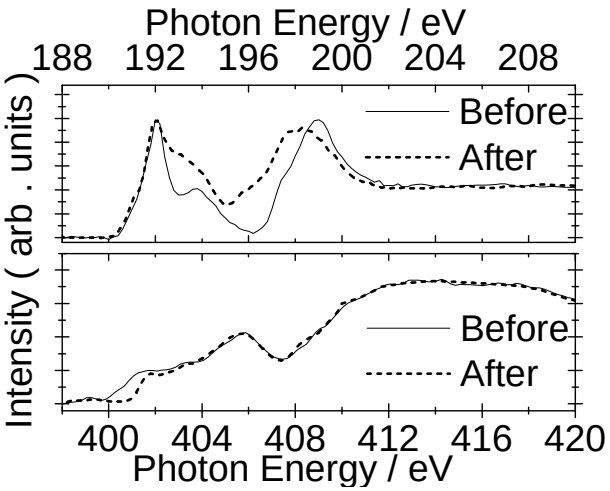

Fig.1. NEXAFS spectra of BN/Ni(111) in B (top) and N (bottom) K-edge regions before (solid line) and after (dotted line) atomic deuterium exposure.