11A/2001G107

Electronic Structure of hexagonal boron nitride thin film on Ni(111) substrate

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Introduction

Hexagonal boron nitride (*h*-BN) is known as an analogue to graphite, the lattice constant of *h*-BN is different from that of graphite by only 1.6 % in *c* plane. Whereas, the electric property of *h*-BN is quite different from that of graphite. Graphite is a semimetal and *h*-BN is an insulator. Due to the two-dimensional anisotropy and insulating property, *h*-BN has gained an increasing interest as thin-film material [1]. Recently, Nagashima *et al*. [2] succeeded in synthesis of epitaxial *h*-BN thin film on various single crystal surfaces (Ni, Pd, Pt, and TaC(111)) by CVD method using borazine ($B_3N_3H_6$). According to their report, coherent *h*-BN grows on Ni(111) surface taking the lattice constant which is consistent with that of Ni(111). Then, *h*-BN/Ni(111) has unique electronic structure. To clarify the electronic structure of *h*-BN/Ni(111), we studied the NEXAFS of this system.

Experimental

Thermal CVD method was devoted to synthesize *h*-BN film. 100 L borazine gas was exposed to heated (~800 °C) Ni(111) substrate in a vacuum chamber. The typical pressure of the borazine was about 10^{-4} Pa. Composition ratio and thickness of the film were estimated from XPS spectra. We measured B K-edge NEXAFS spectra of the film by total electron yield method. All the NEXAFS spectra were obtained by subtracting background spectra of Ni(111) from the spectra of *h*-BN/Ni(111). XPS and NEXAFS experiments were performed at BL-11A. All the experiments were carried out *in situ* to avoid the effect of contamination.

Results and Discussion

Thickness and Composition

The thickness of the film was estimated to be 6.5 Å from the intensity ratio of B 1s and Ni 3s photoelectron peaks. This thickness corresponds to about 2.4 layers of BN. The composition ratio of [B]/[N] is close to unity. Each B and N 1s photoelectron peak consists of one component. The binding energies of the B and N 1s states are 190.6 and 397.9 eV, respectively. These energies are similar to those of bulk *h*-BN. Therefore, it is concluded that homogeneous *h*-BN film was formed on Ni(111).

NEXAFS of h-BN/ Ni(111)

Figure 1 shows B K-edge NEXAFS spectra of *h*-BN/ Ni(111). The clear polarization dependence observed in the NEXAFS spectra strongly supports this film has graphite-like two-dimensional orientation on Ni(111).

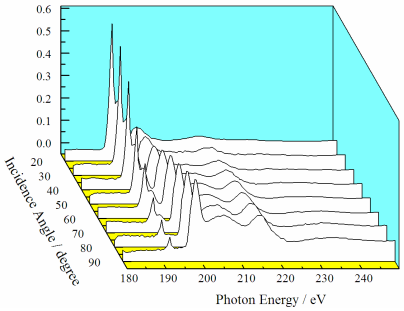

Figure 1. Polarization dependence of B K-edge NEXAFS spectra of *h*-BN/Ni(111). Incidence angle of x-ray is defined as the angle between surface normal and electric vector ***E*** of linear polarized x-ray.

Though the NEXAFS of *h*-BN/Ni(111) is similar to that of bulk *h*-BN, some differences are observed as shown in figure 2. The most noteworthy difference is the new π^* peak appearance which is indicated by red arrow in the figure. To study the origin of the new peak, we calculated the electronic structure of model clusters using DV-Xa method. In figure 3, we show the PDOS of the model clusters. $(B_7N_{12})^{-15}$ cluster has dominant π^*_A state and minor π^*_B state (Fig. 3-(a)). On the other hands, new π^*_A' state emerges in the PDOS of $(B_7N_{12})^{-15}/Ni_6$ cluster (Fig. 3-(b)). By comparing the PDOS of B with that of Ni, we found this new π^*_A' state has antibonding character between π^*_A molecular orbital of *h*-BN and Ni 4p orbital. This result indicates that orbital mixing occurs between *h*-BN and Ni substrate.

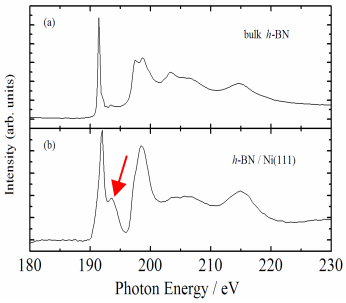

Figure 2. B K-edge NEXAFS spectra of bulk *h*-BN (curve a) and *h*-BN/Ni(111) at 55° incidence (curve b).

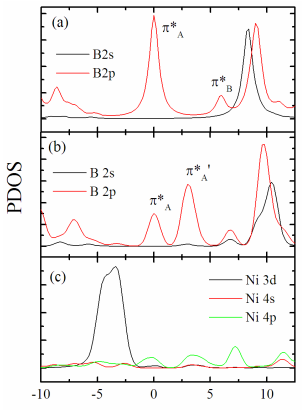

Figure 3-(a). PDOS of B 2s and 2p states for $(B_7N_{12})^{-15}$ cluster. 3-(b). PDOS of B 2s and 2p states for $(B_7N_{12})^{-15}/Ni_6$ cluster. 3-(c). PDOS of Ni 3d, 4s, and 4p states for $(B_7N_{12})^{-15}/Ni_6$ clusters.

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References

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[2] Nagashima, *et al*., Phys. Rev. B 51, 4606 (1995)