

## Configuration, composition and orientation of hexagonal BCN films synthesized by radiofrequency plasma enhanced CVD

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### Introduction

Considerable efforts have been given to synthesis of boron carbonitride (BCN) compounds in the last few years since the BCN compounds are predicted as a novel super-hard material with hardness comparable to diamond or a semiconducting material with variable band-gap energy [1,2]. However, most of the reported BCN compounds are the mixture of the hexagonal and cubic or amorphous phases. Single phase of the hexagonal BCN compound (h-BCN) has not been synthesized up to now and the configuration in the films are known little. In this work, we studied on the configuration, composition and orientation of h-BCN films prepared by radiofrequency plasma enhanced CVD (RF-PECVD).

### Experimental

The films were deposited on Si (100) surface at the RF power of 400~800 W at the working pressure of 0.2 ~ 0.4 Torr using tris(dimethylamino) borane (TDMAB) as a precursor. The chemical bonds and the crystallinity of the films were studied by FT-IR and XRD. The chemical composition and the configuration were studied by XPS and NEXAFS at the Beam Line 27A and Beam Line 11A, PF, KEK, using the linearly polarized synchrotron radiation.

### Results and Discussion

When the N<sub>2</sub> carrier gas was used, the C content in the films was low compared with B and N (sample 1: B<sub>44</sub>C<sub>22</sub>N<sub>34</sub>). CH<sub>4</sub>+H<sub>2</sub> carrier gas increased the C content (sample 2: B<sub>36</sub>C<sub>35</sub>N<sub>29</sub>). This may be due to the higher reactivity of the fragments of CH<sub>4</sub> than that of the N<sub>2</sub> fragments in the plasma. The B1s, C1s and N1s XPS spectra were broad, probably because of the formation of sp<sup>2</sup>-B-C-N hybrid bonds with different configurations. As the C content increased (sample 2), the broad B1s peak slightly shifted to the higher energy. This may be due to a distortion of the sp<sup>2</sup>-BCN chemical environment with the incorporated C. Tailing of the C1s peak to the higher energy was clearly observed. The formation of the CN<sub>x</sub> phase can not be excluded. The N1s spectra also suggested the formation of the sp<sup>2</sup>-BCN atomic hybrids with a variety of configurations [1].

The NEXAFS spectra for the sample 1 and 2 are shown in Fig.1. A broad peak (B<sub>2</sub>) was predominantly observed at the photon energy of 191.8 eV at the normal incidence (θ=0°) of the X-ray. The B<sub>2</sub> peak could be ascribed to the π\*resonance of sp<sup>2</sup>-B-C-N bonds, suggesting formation

of the sp<sup>2</sup>-BCN hybrids with a similar configuration to BN<sub>3</sub> in the h-BN. As the incident angle of the X-ray was increased (θ = 55°, 75°), the B<sub>2</sub> peak decreased and some fine structures such as B<sub>1</sub>, B<sub>3</sub> and B<sub>4</sub> appeared evidently. It indicates the formation of various atomic configurations around B atoms with different N vacancies [2]. The decrease of B<sub>2</sub> peak height was not prominent and B<sub>1</sub> and B<sub>3</sub> fine structures were not obvious for sample 1 in comparison with those of sample 2. This implies the predominant existence of the h-BCN configuration in sample 1. The notable decrease in the B<sub>2</sub> peak height and increase in σ\* resonance peak (denoted by B<sub>5</sub>) with the incident angle of the X-ray suggests that the h-BCN layers may orient in the direction perpendicular to the silicon substrate.

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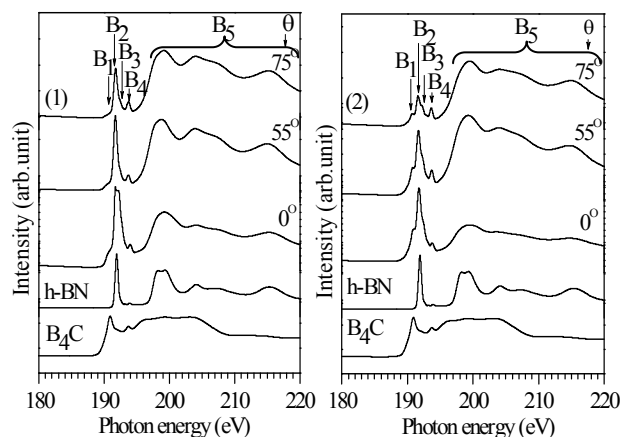


Fig.1 NEXAFS spectra of the samples 1 and 2 at various incident angle (θ) of X-ray.

### References

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