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Near edge X-ray absorption fine structure studies of defected hexagonal boron nitride monolayer on Ni(111).

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1 Introduction

Hexagonal boron nitride (h-BN) is now becoming the focus of attention once again as an insulating material for graphene spintronics[1, 2]. In order to enhance spin injection efficiency, we have to elucidate the spintronic structure at h-BN/magnetic electrode interface.

Using extremely-surface-sensitive spin-polarized metastable helium de-excitation spectroscopy (SPMDS), we revealed that π-3*d* orbital mixing at h-BN/Ni(111) interface induce spin polarization on h-BN. We also revealed that the spin polarization of h-BN around the Fermi level was quenched when the growth temperature was 800˚C. In this study, we report the NEXAFS study of h-BN/Ni(111) to elucidate the nanostructure change at high growth temperature which affect the spin polarization of h-BN.

2 Experiment

Ni(111) film with 20 nm thickness was epitaxially grown on the *c*-plane of α-Al_2O_3 followed by post-annealing at 873 K. Monolayer h-BN was prepared by Ultra high vacuum chemical vapor deposition (UHV-CVD) method with borazine ($B_3N_3H_6$) as a precursor. The Ni(111) surface was exposed to borazine vapor at substrate temperature of 873-1073 K. All fabrication processes were performed in a vacuum chamber with base pressure of 1.0×10^{-7} Pa. The NEXAFS studies were carried out in KEK-PF BL-7A with total electron yield (TEY) conditions.

3 Results and Discussion

The B and N K-edge NEXAFS spectra of monolayer h-BN/Ni(111) are shown in Fig. 1. The spectrum at the substrate temperature of 600˚C basically agreed well with the previous report[3]. The peak assignment is as follows: the two prominent peaks appearing at 192 eV in B K-edge and 402 eV in N K-edge are excitation of 1s electron to empty π^* states, while 1s to σ^* peaks appear at 197-201 eV and 406-420 eV in B and N K-edge, respectively. The π-d orbital mixing produces additional shoulder peaks at 399 eV in N K-edge and minor feature around 191 eV in B K-edge. As the growth temperature increase from 600 to 800˚C, two small peaks appeared on high photon energy side of 1s to π^* absorption at B K-edge. In N K-edge NEXAFS, prominent shoulder peak appeared in the pre-edge region. In analogy to free-standing h-BN, the features (A and B) appearing in B K-edge absorption can be assigned to N defects[4]. Small peak A in boron K-edge absorption is that of boron atoms surrounding nitrogen point defect (labeled with "X" in fig. 1(c)). The possible origin of peak B is X-ray absorption of boron atoms with two adjacent nitrogen atoms defected ("Y" in fig. 1(c)). The pre-edge shoulder in N K-edge, on the other hand, can be assigned to N atoms in interstitial region. Therefore, the mechanism of N defects formation at higher substrate temperature can be estimated as migration of N atoms into Ni bulk as diffusion coefficient increase at higher temperatures.

As nitrogen defects are formed at higher temperature, the work function of the system will be reduced, because defected h-BN will be positively charged, which was confirmed by UPS measurement. The reduction of the work function, together with defect spin polarization, can be the reason for the quench of h-BN spin polarization.

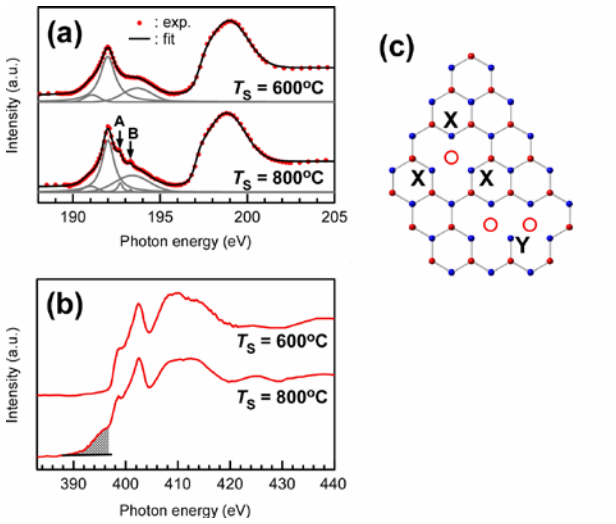

Fig. 1 (a) B and (b) N K-edge NEXAFS spectra of monolayer h-BN/Ni(111). The incidence angle of X-ray was 60˚ and 30˚ from sample normal, respectively. (c) The schematic diagram of h-BN with defects. Red and blue particle represent nitrogen and boron atoms, respectively.

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