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Probing Defects in Epitaxially Grown Cubic Boron Nitride on Diamond

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Demand for devices with greater efficiency comes in many forms. Wide-band gap materials (E_g > 3.3 eV) like gallium nitride have succeeded in offering advantages over conventional devices by offering higher breakdown voltages, operating frequencies, and thermal conductivity. Ultrawide-band gap materials promise even greater performance benefits. Among the group-III nitrides, cubic boron nitride (c-BN) is a promising candidate material due to its large band gap (E_g > 6.1eV), high thermal conductivity, and ability to be doped either *p*- or *n*-type. In spite of many efforts, c-BN is still the least mature of the ultrawide-band gap materials [1]. This is primarily due to the difficulties in synthesizing high-quality phase pure c-BN crystals and the large amount of unintentional defects present in grown crystals. Aberration-corrected scanning transmission electron microscopy (STEM) is ideally suited to examine the local structural morphologic, defect, phase/growth relationships, and dopant integration in c-BN epitaxial growth.

In this study, we examine c-BN films grown on diamond via molecular beam epitaxy with post-growth cross-sectional STEM. After confirming the presence of c-BN with Fourier transform infrared spectroscopy samples were analyzed in a Nion UltraSTEM 200X, with a convergence angle of 27 mrad. Electron energy-loss spectroscopy (EELS) was performed at 60 kV while imaging was done at both 60 and 200 kV. Annular bright-field imaging, figure 1, reveal the presence of a high density of stacking faults, which appear in the image as diagonal features inclined 55° to the growth plane. The c-BN/diamond interface is abrupt, with occasional misfit dislocations, further analysis of the EEL near edge structure of the B K-edge identifies a small pre-peak feature ~191.3 eV. This edge feature has previously been attributed to a bound exciton originating from the π* orbital, and in h-BN this is a strong feature equal in intensity to the main edge feature at ~197 eV [2, 3]. π* states are absent in the cubic phase due to bond hybridization, therefore the weak presence of this feature indicates the that the nucleating BN layer contains h-BN like bonding while still maintaining the cubic phase. Atomic resolution imaging, shown in figure 2, finds that the diagonal defects throughout the film are bound by c-BN inversion domains, flipping the c-BN structure along the (001)-direction on opposite sides of the defect. EELS analysis reveals a subtle shift of the edge feature at 208eV to higher energy, the source of which is not entirely clear yet and is a focus of continuing work. Future work will further explore the defect structure and examine dopant integration within the c-BN lattice using high-resolution STEM imaging.

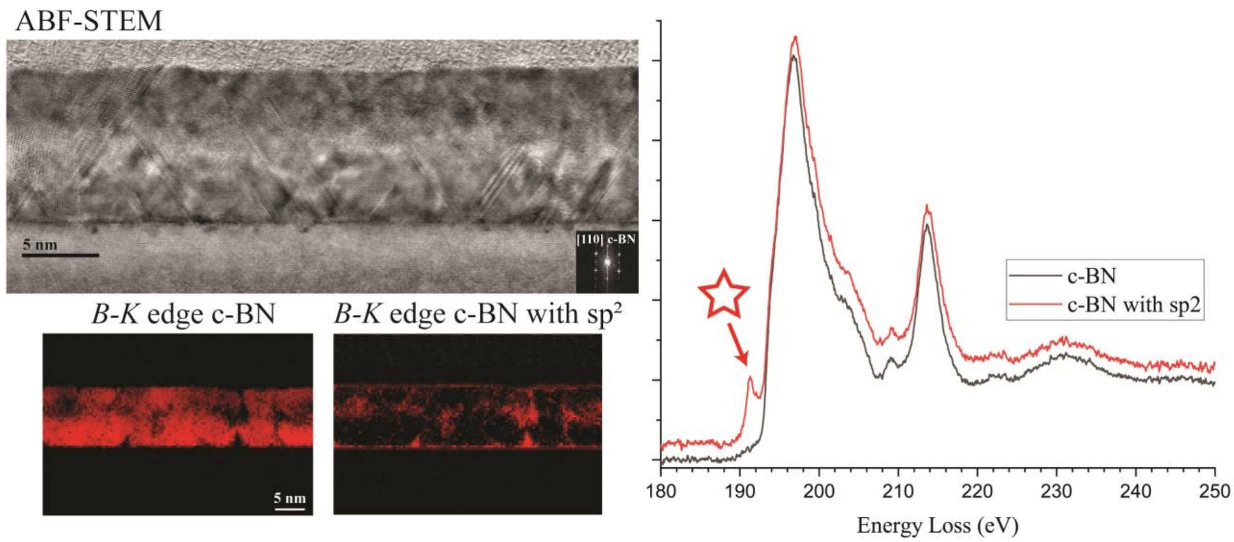

Figure 1. Cross-sectional STEM analysis of c-BN. Top: Annular bright-field STEM image of the c-BN thin film. Bottom: EELS maps showing where individual spectra features of the B K-edge are observed; left, typical c-BN spectra; right, c-BN spectra with a pre-peak feature at 191eV, indicative of the presence of small amounts of sp^2 bonding in the BN. The EEL spectra shown on the right were processed with a power law background subtraction and slightly offset for visual clarity.

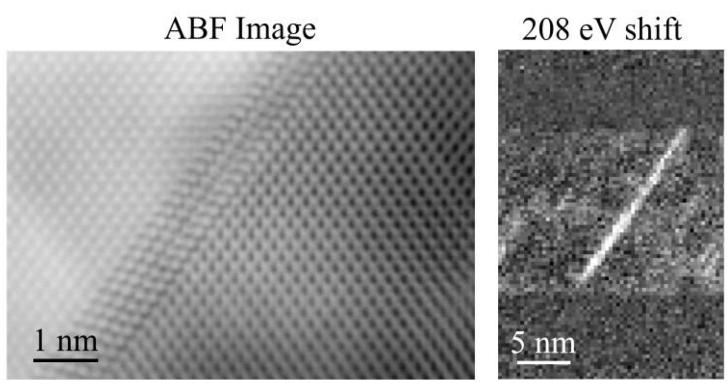

Figure 2. Left: Annular bright-field image across diagonal defect in c-BN. Right: Highlighted area showing the area in the film where the 208eV feature in the B K edge shifts to higher energy.

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