Formation of Defects in Cubic Boron Nitride by Low Energy Ion Bombardment

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Formation of defects in cubic boron nitride (*c*-BN) under low-energy argon or nitrogen ion-bombardment has been studied by near-edge X-ray absorption fine structure (NEXAFS) around boron K-edge.

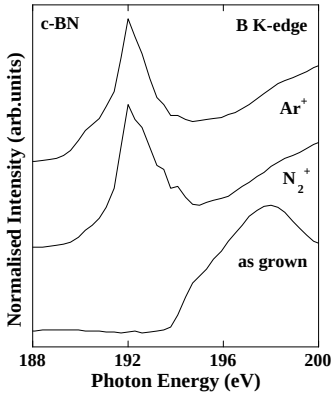

Fig. 1: NEXAFS spectra around B K-edge from an as grown *c*-BN sample and samples bombarded with 2 keV Ar^+ or N_2^+ ions for 5 min.

The samples used in this study were prepared by attaching the commercially available crystalline *c*-BN powder (Gem Diamond Products, ~40㎛m grains) to the conductive carbon tape.

In general, the low-energy ion bombardment creates quite efficiently different point defects in semiconductors, such as interstitials, vacancies, and antisites, within the collision cascade by displacing matrix atoms from their original lattice sites. All these defects may form some unoccupied or empty energy levels within the bandgap of semiconductors and can be, in principle, identified directly by NEXAFS measurements. In the case of *c*-BN, boron and nitrogen interstitials and vacancies (N_i, B_i, V_N and V_B) form some unoccupied levels within the bandgap [1], accessible for NEXAFS transitions.

In Fig. 1 we show some characteristic B K-edge NEXAFS spectra from as-grown and ion-bombarded *c*-BN samples. In contrast to hexagonal phase of BN (*h*-BN), the cubic phase of as-grown BN samples does not show the characteristic π* resonance at around 192 eV [2]. However, a new, strong peak at around 192 eV has been observed in all NEXAFS spectra of ion-bombarded *c*-BN samples, as shown in Fig. 1.

In Fig. 2 we show the structure of this new feature in more detail. For both argon and nitrogen bombardment, there is a dominant peak at 192.0 eV (peak 1 in Fig. 2), followed by several less intensive peaks at both high- and low-energy side of 1. The peak 1 is typical for *h*-BN structure and has been interpreted as a core exciton with a π-like final state wave function. The three new resonances at the high-energy side of 1, labelled 2, 3 and 4 in Fig. 2 have been observed previously in *h*-BN samples bombarded with argon or nitrogen ions and attributed to the different coordination of the excited B atom [3]. While the resonance 1 corresponds to the core exciton of $[BN_3]$ configuration, with B bonded to thee N atoms, resonances 2 and 3 correspond to the transition in $[BN_2]$ and [BN] bonding configuration, respectively, with B bonded to two N atoms or a single N atom, respectively. The resonance 4 simply represents the elemental boron. In other words, resonances 2, 3 and 4 are effectively created by one, two or three nitrogen vacancies, N_V, respectively, around the excited B atom, following the breaking of B-N bonds under argon or nitrogen bombardment.

We further note that the energy levels involved in transitions 5-7 in Fig. 2 are placed below the absorption edge, i.e. within the energy gap of BN. Theoretical calculations predict several half-occupied or empty states within the energy gap of BN for the neutral and charged B_i defects [1], in qualitative agreement with our experimental data.

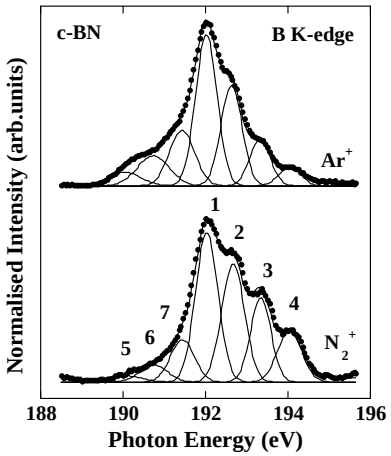

Fig. 2: High-resolution B K-edge NEXAFS spectra of ion-bombarded samples from Fig. 1 around 192 eV.

Our NEXAFS measurements have provided the direct evidence for the creation of V_N and B_i, in *c*-BN bombarded by low-energy Ar^+ or N_2^+ ions, in agreement with theoretical predictions. Breaking of B-N bonds is responsible for the creation of one, two or three V_N, observed directly around excited boron atoms by NEXAFS measurements around the B K-edge. Boron atoms displaced to interlayer positions, B_i, may bond with neighbouring boron atoms, forming small boron clusters. Finally, our measurements fully support the possibility for a bombardment-induced phase transformation in *c*-BN to a phase similar to the damaged hexagonal phase [2].

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