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Structure characterization and strain relief analysis in CVD growth of boron phosphide on silicon carbide

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ABSTRACT

Boron phosphide (BP) is a material of interest for development of a high-efficiency solid-state thermal neutron detector. For a thick film-based device, microstructure evolution is key to the engineering of material synthesis. Here, we report epitaxial BP films grown on silicon carbide with vicinal steps and provide a detailed analysis of the microstructure evolution and strain relief. The BP film is epitaxial in the near-interface region but deviates from epitaxial growth as the film develops. Defects such as coherent and incoherent twin boundaries, dislocation loops, stacking faults concentrate in the near-interface region and segment this region into small domains. The formation of defects in this region do not fully release the strain originated from the lattice mismatch. Large grains emerge above the near-interface region and grain boundaries become the main defects in the upper part of the BP film.

1. Introduction

Boron phosphide (BP) is an indirect bandgap semiconductor with potential for use as a solid state thermal neutron detector. ^{10}B (20% of natural abundance boron) has a large neutron absorption cross section (3840 barns) and generates 2.3 MeV of energy by the reaction [1], $^{10}B + n \rightarrow {}^{7}Li + \alpha + 2.3\ MeV$.

To optimize the detection efficiency of a BP based neutron detector, it is important that BP be of high crystal quality and detrimental defects in the material be limited and not serve as charge traps or electron-hole recombination sites.

Most of previous work on chemical vapor deposition of BP was done on silicon (Si) [2–6] and sapphire substrates [7,8]. Unfortunately, the poor lattice mismatches between Si/BP (16.5%) and sapphire/BP (4.6% and 11.5% depending on direction), are known to produce discontinuities across the interface and large amount of dislocations in the hetero-epilayer [8]. As an alternative, SiC has a {0 0 0 1} basal plane which offers only 4.5% mismatch with a BP {1 1 1} plane and therefore should be a better substrate for BP epitaxy. In 1971, Chu et al. performed the first BP growth on SiC, but characterized only the surface crystallinity using reflection electron diffraction [9]. In 2005, Udagawa et al. characterized a thin <1 1 1> BP layer (200–440 nm) grown on (0 0 0 1) 6H-SiC using high-resolution transmission electron microscopy (HRTEM) [10]. They observed coherent twin boundaries and random atomic configurations at the BP/SiC interface, but yet were unable to study the microstructure evolution in a larger scale due to the limited film thickness. In this paper, we present a detailed analysis of the defect generation, structural evolution and strain management in a thick BP film (~3 μm) grown on 4° offcut (0 0 0 1) 4H-SiC.

2. Experimental

Heteroepitaxial BP films were grown by CVD on the (0 0 0 1) surface of 4H-SiC substrates with a 4° offcut in a <11-20> direction using diborane (B_2H_6) and phosphine (PH_3) precursors. The reactor pressure was maintained at 630 Torr and the flow rates used were 20 sccm B_2H_6 (1% in H_2), 100 sccm PH_3 (5% in H_2) and 2500 sccm of H_2. Crystalline BP films have been grown at temperatures ranging from 800 to 950 °C. The detailed structural and strain analysis presented here was on a film grown at 850 °C. Details of the reactor design will be reported elsewhere. Angular offcut wafers were used to promote step-flow growth.

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TEM samples were prepared with a Zeiss Auriga dual beam SEM/FIB. High resolution phase contrast and Z-contrast imaging was performed using a Zeiss Libra 200 MC transmission electron microscope and a VG HB 603 UX scanning transmission electron microscope. Both of the microscopes can reach Angstrom level resolution and reveal easily the {1 1 2} and {1 1 1} atomic planes in BP, which enables us to determine the microstructure. Strain and defects were analyzed utilizing electron micrographs, diffractograms and X-ray diffraction.

3. Results and discussions

3.1. Structure overview of the BP film

Fig. 1 is an overview bright-field image of the BP/SiC cross-section taken under a SiC <11-20> zone-axis. The bright-field detector in TEM collects mostly the transmitted electrons, therefore, the more severe the electron diffraction the darker the image will be. Electron diffraction is particularly strong when a crystal is illuminated in zone-axis. As we can see in the image, the near-interface region has more dark contrast, while the upper part of the film has more bright contrast. This means BP grew epitaxially from the interface but deviated from epitaxial growth and became non-epitaxial as the film develops.

To determine the structural evolution of the BP film, selected area diffraction (SAD) experiments were performed under a <11-20> zone-axis of SiC throughout the entire film. The SAD aperture diameter was approximately 850 nm. The results are shown in Fig. 2 where the approximate regions that contributed to the diffractions are indicated by a circle in the bright-field TEM image. While details of the diffraction pattern analysis will be discussed in the following text, the following sequence will serve as an overview:

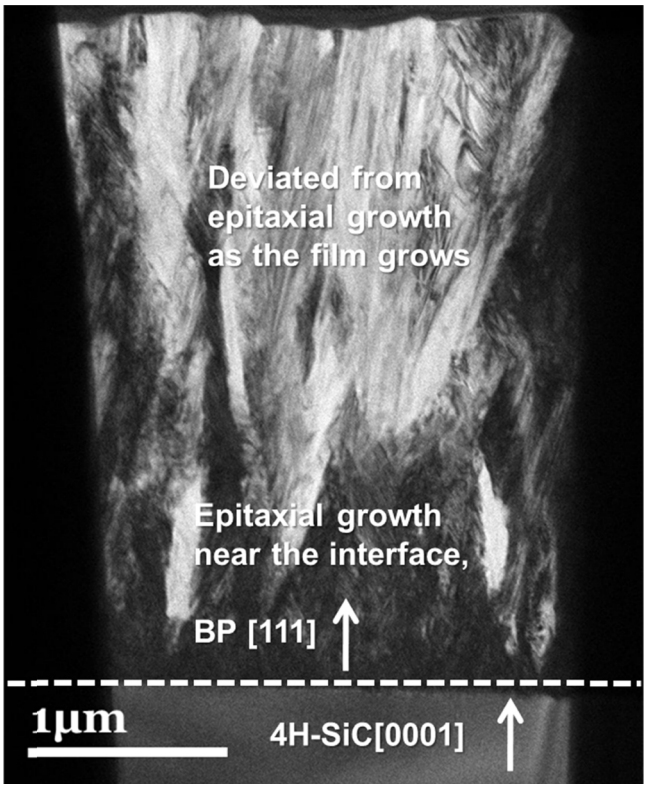

Fig. 1. An overview bright-field TEM image of the BP/SiC cross-section taken under a SiC <11-20> zone-axis. The dark contrast near the interface indicate epitaxial growth, the bright contrast in the upper part indicates the epitaxial growth is not retained as the film develops.

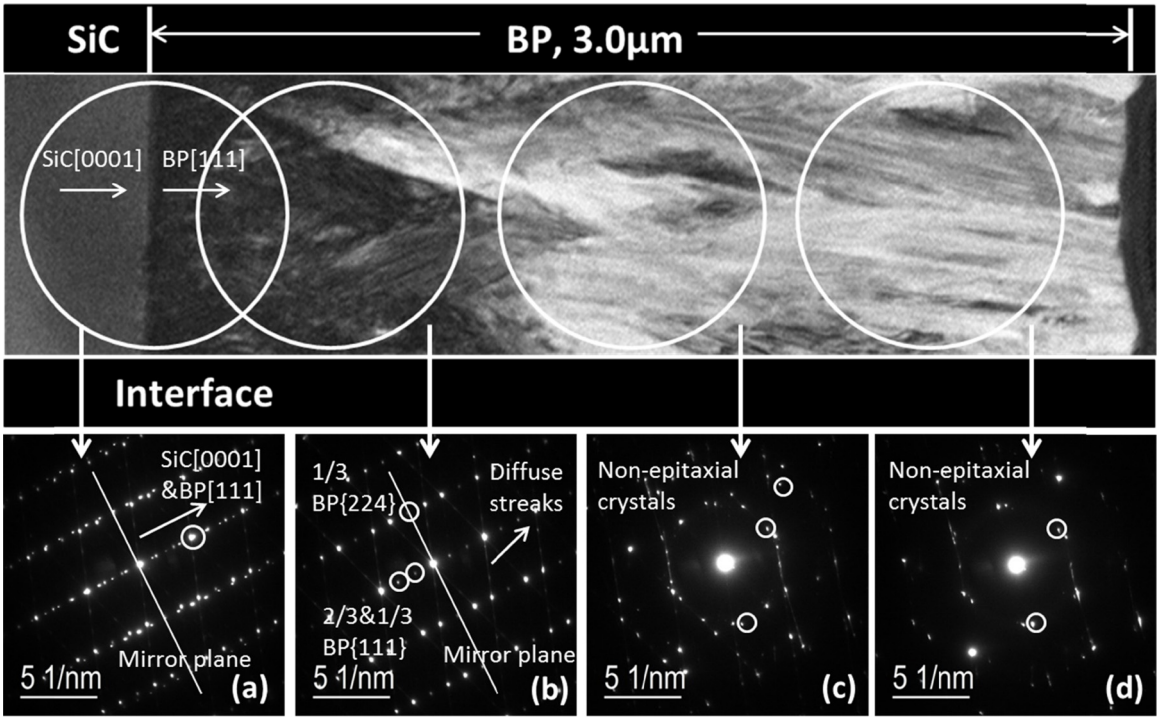

Fig. 2. Sequential SAD patterns taken under a SiC <11-20> zone-axis. (a) is the SAD pattern of the 4H-SiC/BP interface. The epitaxial relationship of BP with SiC is SiC (0 0 0 1), <11-20>//FCC BP (1 1 1), <1 1 0>. (b) represents the-near interface region. The mirrored pattern and diffuse streaks imply twin boundaries and planar defects, respectively. (c) shows the mid-film region. Less twins and planar defects are observed, instead, grain boundaries between epitaxial and non-epitaxial BP crystals (circled diffraction spots) become the main defects. (d) is the surface region. Grain boundaries are the dominating defects.