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Growth Mechanism of (111)-Textured 3C-SiC Films on Si(100) Substrates

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Heteroepitaxial growth of 3C-SiC films on a Si(100) substrate can be achieved by chemical vapor deposition [1,2]. Under certain processing conditions, there is a transition from 3-D epitaxial islands to columnar grains, modifying the film texture from (100) to (111). This transition is more pronounced with increasing thickness and decreasing deposition temperature. The current work uses transmission electron microscopy to characterize the microstructure and investigate the mechanism of 3C-SiC film growth on Si(100) substrates.

SiC films are deposited on Si(100) substrates by CVD using a single precursor DSB (1,3-disilabutane, molecular structure CH_3-SiH_2-CH_2-SiH_3). The deposition begins by pressurizing the CVD reactor with DSB to approximately 5×10^{-5} torr at a reactor temperature of 100°C. The temperature is then increased to the ultimate growth temperature of 850°C at a rate of 50°C/min at constant DSB pressure. The film growth rate under these conditions is about 150nm/min. Conventional transmission electron microscopy was carried out in a JEOL 200CX microscope, operating at 200kV, and high resolution microscopy in a CM300 FEG microscope operating at 300kV.

We have found that the columnar grains (Fig. 1a) do not originate at the substrate surface but on a buffer layer (Fig. 2a) about 3 to 5 nm thick, consisting of interconnected 3D-islands (Fig. 2b), as proposed by Ernst and Pirouz [3]. The growth of epitaxial 3-D islands in a one-step deposition process using a single precursor has not been shown before. Initial nucleation of SiC grains occurs in parallel-cube orientation relationship at the interface with the substrate, and twinning is abundant even at the earliest stages of growth. It is apparent that growth is limited by the slow growth rate of the {111} planes. From these observations, it is possible to understand the growth mechanism as follows. Initially, 3C-SiC grains nucleate epitaxially on the Si(100) substrate in a parallel-cube orientation relationship. The anisotropy in growth rate along {100} and {111} planes differs by at least a factor of $\sqrt{3}$, making {111} faces the growth limiting form. However, twinning occurs frequently and appears to be associated with enhanced growth. Higher order twinning leads to new crystal orientations. During the growth competition following nucleation, the slower-growing grains are overgrown by faster-growing grains [4]. Growth will be most rapid in the directions that make the largest angle with the growth facets. This means that the grains that are aligned with their fastest growth direction normal to the substrate survive and become the {111} oriented columnar grains we observe (Figs. 1 b and c). Our observations show that nucleation occurs in <100> orientation (Fig. 2b). Growth in this orientation will be limited until subsequent twinning generates new orientations that are closer to the <111> growth direction favored by twinning. For example, first order twins will be oriented with their <122> direction normal to the substrate, bringing a <111> direction within 16° of the substrate normal. Higher order twins can generate even more favorable orientations, until a <111> direction is close enough to the substrate normal, within $\pm 9^{o}$, to allow uninhibited growth. Thus, as observed, the largest columnar grains are those that are closest to a <111> orientation. This leads to the observed <111> fiber texture.

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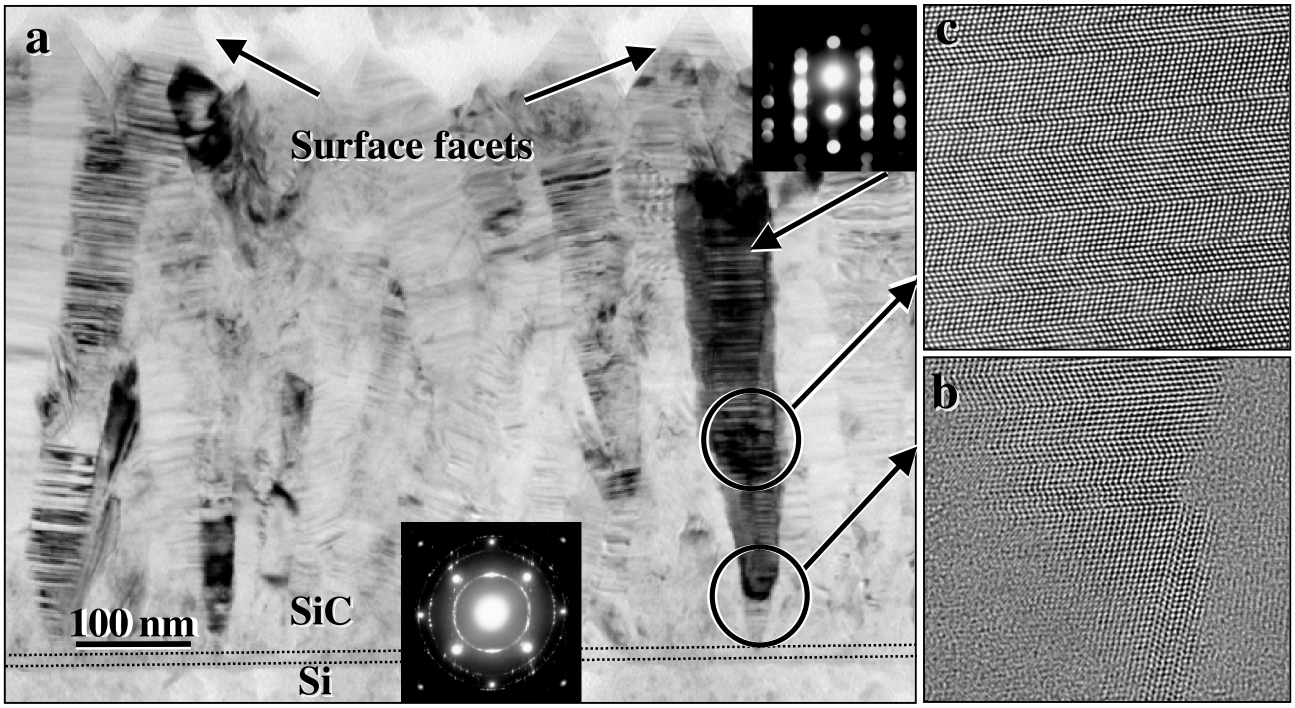

Fig. 1. a) TEM micrographs of SiC film in cross section demonstrating columnar growth morphology; upper right inset: nanodiffraction from arrowed grain; middle bottom inset: selected area diffraction pattern from Si substrate and SiC film; b) and c) HREM images of the encircled regions in (a); showing extensive twinning on a single set of 111 planes. From this and similar observations, an average fault density of one fault every twelve {111} planes was measured.

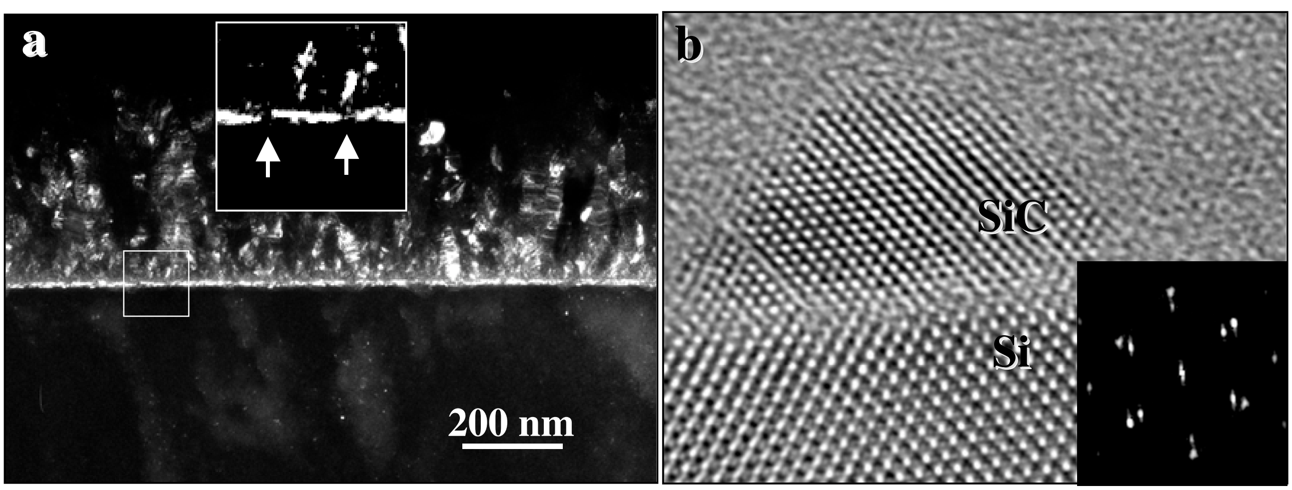

Fig. 2. a) Dark field image taken using 111 3C-SiC reflection; b) HREM micrograph showing nucleus of SiC on Si substrate in parallel-cube epitaxial orientation. The inset Fourier diffractogram indicates the orientation relationship and relative lattice parameters of Si and SiC.

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