Application of $6H$-SiC/$3C$-SiC(001) composite substrates for growth of cubic silicon carbide by sublimation method

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The paper presents the results of a study of thick layers of cubic silicon carbide polytype grown using $6H$-SiC/$3C$-SiC(001) composite substrates of our own manufacture. The layers were grown by the sublimation method in a vacuum chamber in the temperature range of 1600–1800 °C. The study was carried out using optical and transmission electron microscopy and was aimed to characterize the stability of growing a layer of cubic silicon carbide with the orientation (001). An analysis of the defect structure of the layer is presented in comparison with a layer of silicon carbide with the orientation (111), obtained on a wafer of a hexagonal polytype.

Keywords: silicon carbide, cubic polytype, sublimation epitaxy.

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Silicon carbide (SiC) is distinguished by an array of useful electrical and mechanical properties, such as high breakdown field, high thermal conductivity, and stability of characteristics within a wide temperature range. These make the material highly sought after in the modern semiconductor industry, especially in high-temperature and power electronics [1]. The modified Lely method is used at present to grow bulk SiC. This method allows one to obtain substrates of just the two most stable hexagonal polytypes: $4H$ and $6H$. At the same time, metastable cubic polytype $3C$ has a number of advantages (specifically, higher carrier mobility [2,3]), which stimulates the research aimed at its synthesis [4].

The process of heteropolytypic epitaxy of cubic polytype crystals with readily available hexagonal single-crystal silicon carbide substrates faces two major challenges that limit its applicability. The first (and most significant) is the inclusion of other polytypes, which may exert a negative influence on the electrical characteristics of the resulting structures. The second problem is related to the existence of two possible sequences of crystallite nucleation (ABC and ACB), which leads to the formation of defect boundaries between the corresponding regions (the so-called double position boundaries (DPB) defects) [5].

Chemical vapor deposition (CVD) with single-crystal silicon substrates of the (001) orientation is currently used widely to obtain $3C$-SiC structures. Heteroepitaxy provides films of the cubic polytype of silicon carbide free from inclusions of other polytypes and helps avoid the formation of DPB defects. However, this approach has limitations associated with the melting point of silicon (1414 °C) and with a significant mismatch of lattice parameters, which leads to high defect densities in the films. In addition, the difference in thermal expansion coefficients imposes restrictions on the maximum film thickness. This is an important point to consider in the design of devices based on them.

The method of bonding of wafers of different semiconductor materials is worthy of special notice; it is widely used to fabricate composite substrates with the required characteristics [6]. This approach is also relevant for silicon carbide [7,8]. Specifically, the transfer of thin layers of silicon carbide of the cubic modification with the (001) orientation onto a substrate of hexagonal polytypes is considered [9,10] as a means of growth of thick $3C$-SiC layers by sublimation. CVD-grown $3C$-SiC layers on a silicon substrate are used for this purpose. When the (001) face of $3C$-SiC is used for homopolytypic epitaxy, the direction of stacking of close-packed planes differs from the direction of layer growth, which should suppress the emergence of polytypic inclusions. A dissimilar stacking of layers along the 4th-order symmetry axis of such a substrate should also exclude DPB defects. As for anti-phase domain boundaries (ADBs) inherent in heteroepitaxy on a monoatomic silicon substrate, homopolytypic epitaxy should not alter their density in the layer in any significant way relative to the density in the initial CVD layer. It was noted in [11] that ADBs may close within the bulk of a crystal as the layer thickness increases. Thus, the aim of the present study is to characterize polytypic inclusions and structural defects in a silicon carbide layer, which was grown by sublimation on a $6H$-SiC/$3C$-SiC(001) composite substrate, by optical and transmission electron microscopy (TEM). TEM studies was carried out using a Philips EM420 microscope operating at an accelerating voltage of 100 kV. An Olympus CX41 microscope was used for optical imaging. Cross sections of

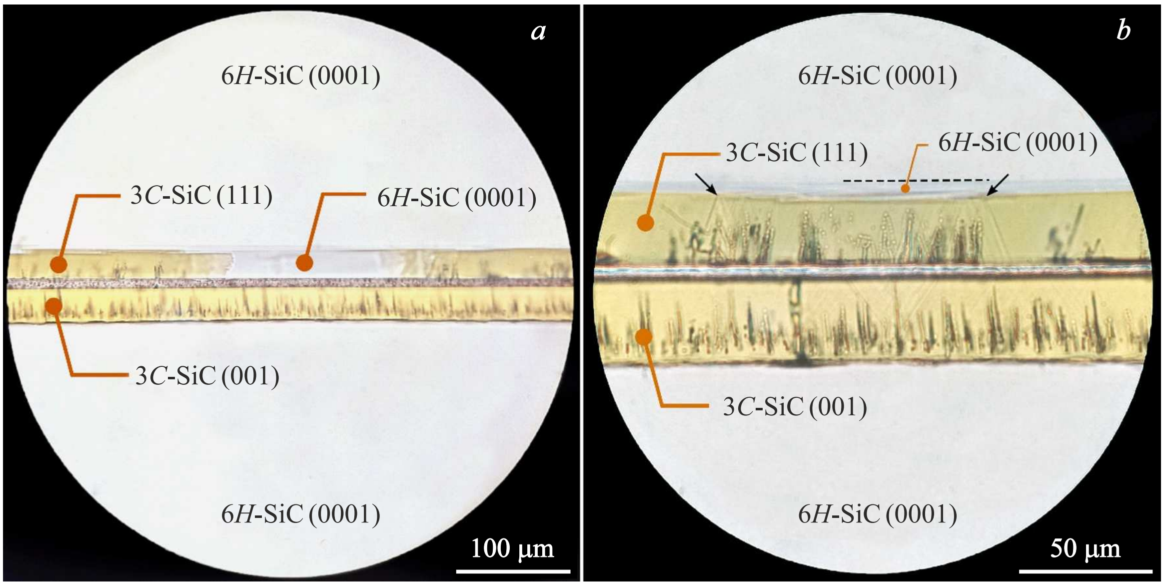

Figure 1. Cross-sectional images of bonded silicon carbide layers grown directly on the 6*H*-SiC substrate (top half of images) and with the use of a CVD 3*C*-SiC seed layer (bottom half of images). The presence of hexagonal polytypic inclusions in the 3*C*-SiC(111) layer (panel *a*) and DPB defects indicated by black arrows (panel *b*) is demonstrated. The dotted line represents the layer–substrate interface.

the structures for study were prepared in accordance with the standard TEM procedure, which included mechanical thinning and ion polishing (Ar^+).

Composite 6*H*-SiC/3*C*-SiC(001) substrates of our own production were used in experiments on growth of epitaxial layers of the cubic polytype. Commercially available single-crystal 6*H*-SiC(0001) wafers (CREE, Inc.) served as a carrier substrate. CVD 3*C*-SiC(001) layers with a thickness of 10 μm (NOVASIC) were used as a seed layer of the cubic polytype with the (001) orientation. The process of layer transfer onto the 6*H*-SiC wafer was detailed in [12]. Silicon carbide layers were grown by sublimation using a laboratory setup with induction heating. The maximum temperature in this process was $\sim 1800\,^\circ$C, and the pressure in the growth chamber was maintained at $5 \cdot 10^{-6}$–$6 \cdot 10^{-6}$ Torr. The growth time was 1–2 h.

The total area of the composite substrate was $\sim 11\times 11\,\mathrm{mm}^2$, of which the seed CVD 3*C*-SiC layer accounted for $\sim 7\times 7\,\mathrm{mm}^2$. The remaining surface corresponded to the Si face of the 6*H*-SiC(0001) wafer. For structural TEM characterization, regions with and without the seed layer were bonded. The cross-sectional images of the prepared TEM sample obtained with an optical microscope are shown in Figure 1. Cubic silicon carbide with a band gap of 2.4 eV has a transparent yellow tint, while hexagonal polytypes may come in different shades depending on the type of dopant. This effect allows one to differentiate silicon carbide polytypes by their shades using optical microscopy [13].

In Figure 1, the yellow tint of 3*C*-SiC layers makes them easily distinguishable on the transparent substrate. The layers are continuous with a uniform thickness of $\sim 30\,\mu$m in both regions. In the region without the seed layer (top half of the image in Figure 1, *a*), the 3*C*-SiC layer has orientation (111). A significant polytypic inclusion of 6*H*-SiC is seen. It is also evident that polytypic instability is typical of the entire interface with the substrate. As for the region with the seed layer shown in the lower half of the image, no similar hexagonal inclusions are found in the 3*C*-SiC layer with the (001) orientation. The formation of vertical defects at a distance of $\sim 6\,\mu$m from the interface is apparently attributable to the features of surface morphology of the seed layer that form as a result of interaction of the silicon melt and the CVD silicon carbide layer during its transfer to the 6*H*-SiC wafer [4]. The process is accompanied by dissolution of a part of the original CVD layer with the highest defect density, which explains the fact that its thickness decreases from 10 to 6 μm. It can be seen from the figure that the density of these defects decreases rapidly as the sublimation layer thickness increases.

V-shaped outlines of DPB defects, which are marked for clarity with black arrows, are visible in the 3*C*-SiC(111) layer in Figure 1, *b*. Similar inclined lines are seen in the 3*C*-SiC(001) layer. As was found in subsequent TEM studies, these are caused by twinning along the {111}-type planes. The emergence of such twins in the 3*C*-SiC film with the (001) orientation was associated in [14] with waviness of the substrate surface. Twins may be suppressed at a sufficient film thickness.

TEM images of the cross section of the SiC layer are shown in Figure 2. The region without the seed layer imaged in Figure 2, *a* demonstrates two main types of

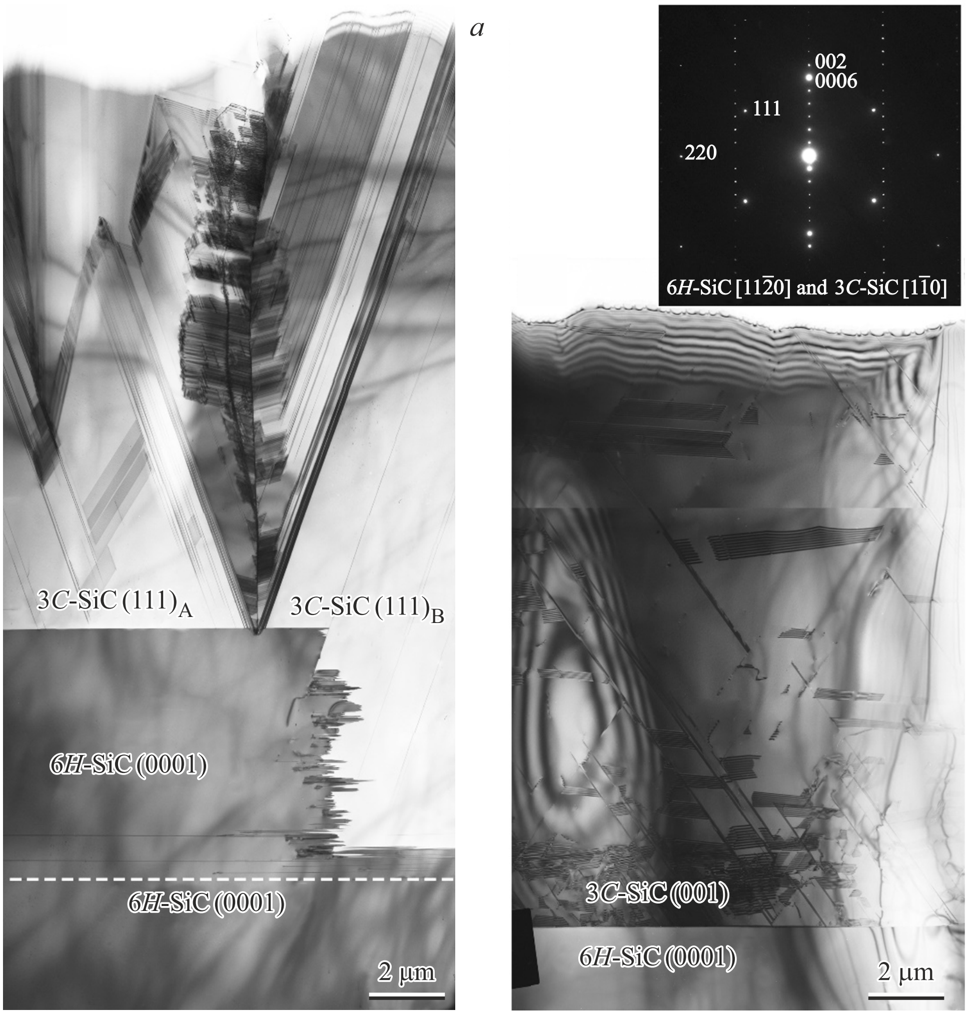

Figure 2. Bright-field TEM images of the cross section of the SiC layer: *a* — the substrate region without the seed layer; *b* — the region with the CVD seed layer. The electron diffraction pattern corresponding to the interface region is shown in the inset.

defects inherent in homopolytypic epitaxy of 3*C*-SiC on hexagonal substrates. These are hexagonal inclusions with needle-like interphase boundaries and DPB defects between regions 3*C*-SiC$(111)_A$ and 3*C*-SiC$(111)_B$ with differing stacking sequences (ABC and CBA, respectively).

The orientation of grown layers was determined via electron diffraction. The electron diffraction pattern recorded in the region of the interface with the hexagonal substrate is shown in the inset in Figure 2, *b*. It confirms that the layer has orientation (001) with the 3*C*-SiC(001) plane parallel to plane 6*H*-SiC(0001) of the substrate. The boundary between the CVD and sublimation layers is not visible in TEM images. A high density of stacking faults is seen in the obtained structure near the interface with the substrate, but this density decreases with increasing layer thickness. ADBs were not detected, which is apparently attributable to high locality of the TEM method.

As was noted above in the description of optical images, twins with the $\{111\}$-type twinning plane were detected in the layer. Twins are present in the layer in the form of flat inserts parallel to the basal planes. Their images are not provided here.

TEM and optical microscopy methods were used to demonstrate that the use of a composite 6*H*-SiC/3*C*-SiC(001) substrate ensures the production of cubic silicon carbide free of polytypic inclusions. The grown layer inherits the (001) orientation of the seed layer. This crystallographic orientation of the layer excludes DPB defects; however, it was found that it does not prevent the emergence of twins with the $\{111\}$-type twinning plane. It was also demonstrated that the proposed approach of homoepitaxial growth on composite substrates provides an opportunity to form thick ($> 30\,\mu$m) layers of cubic SiC at higher temperatures than the CVD method applied to epitaxy on silicon.

Conflict of interest

The authors declare that they have no conflict of interest.

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