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Transfer of 3C-SiC heteroepitaxial layers grown on silicon to a 6H-SiC substrate by direct bonding technique

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Abstract. This paper reports on the development of direct bonding of 3C-SiC epitaxial layers grown by chemical vapor deposition on silicon substrates and 6H-SiC single crystal wafers. It has been found that the bonding temperature is a critical parameter to obtain mechanical contact between the transferred 3C-SiC layers and the 6H-SiC carrier plates. The results of structural characterization showed that the structure of epitaxial layers grown by sublimation on bonded substrates corresponds to a pure cubic phase of high quality.

Keywords: Silicon carbide, polytypes, direct splicing, templates, sublimation epitaxy

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Материалы конференции
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Перенос гетероэпитаксиальных слоёв 3C-SiC, выращенных на кремнии, на подложку 6H-SiC методом прямого сращивания

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Аннотация. В представленной работе сообщается о разработке метода прямого сращивания гетероэпитаксиальных слоев 3C-SiC, выращенных на Si подложках, и монокристаллических пластин 6H-SiC. Обнаружено, что температура сращивания является критическим параметром для получения механического контакта между переносимыми слоями и несущими пластинами. Результаты характеризации показали, что кристаллическая структура гомоэпитаксиальных слоёв 3C-SiC, выращенных на подложках, полученных методом сращивания, соответствует чистой кубической фазе высокого качества.

Ключевые слова: Карбид кремния, политипы, прямое сращивание, темплейты, сублимационная эпитаксия

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Introduction

Silicon carbide (SiC) is considered as a prime candidate to replace silicon in today's electronics due to inherent physical properties such as wide band gap, thermal and corrosion stability, as well as higher blocking voltage, lower losses, and faster switching speed [1]. Compared to the other two most known polytypes, hexagonal 4H- and 6H-SiC used in power microelectronics, the cubic 3C-SiC polytype is the promising material for high-frequency electronic devices [2]. A topic problem of 3C-SiC technology is the lack of methods for the 'bulk' growth of a single-crystal material necessary for the manufacture of substrates for 3C-SiC homoepitaxy. It could seem that in this case, a natural solution would be to use existing SiC wafers of hexagonal polytypes as substrates. However, achieving high-quality homoepitaxy of 3C-SiC on 4H- and 6H-SiC is problematic due to the difference in the types of crystal lattices. At the same time, cubic SiC can be grown on widely available silicon wafers with a similar syngony. At present, however, such heteroepitaxial technologies have not yet reached the crystalline quality acceptable for the production of electronic devices. There are two main problems to be resolved here. First, it is the level of internal stresses caused by the mismatch between the lattice parameters of 3C-SiC (4.36 Å) and Si (5.43 Å). The mismatch is the reason for the formation of a highly defective nucleation layer resulting in the formation of wide set of extended defects. The electrical activity of these defects is the dominant problem that adversely affects the efficiency of electronic devices based on 3C-SiC. The second problem is related to the presence of thermoelastic stresses arising from the difference in the thermal expansion coefficients of Si and 3C-SiC, which is 8%. As a result, cracking of epitaxial layers is often observed when they are cooled from the growth temperature to the room temperature. Cracking determines a significant deterioration in the quality of the epitaxial layers. A comprehensive solution of the problems mentioned above can be the development of an alternative substrate (template) using the approach of transferring the already grown 3C-SiC seeding layer onto a carrier wafer which would be close to the layer in terms of lattice parameters and thermal expansion coefficients. Notice that such transfer technologies (called *wafer bonding*) are widely used in epitaxial and device technologies of materials for which there is no matched substrate [3–6]. This paper reports on the development of a template by direct bonding of 3C-SiC epitaxial layers grown by chemical vapor deposition (CVD) on silicon substrates and single-crystal 6H-SiC wafers, for which the lattice mismatch with 3C-SiC does not exceed 0.3%; these two polytypes also have close thermal expansion coefficients. The effectiveness of the proposed transfer approach is confirmed by the results of sublimation homoepitaxy on the 3C-SiC/6H-SiC templates obtained.

Materials and Methods

CVD-grown (001)3C-SiC/Si structures with 40 μm-thick epitaxial layer and single-crystal (0001)6H-SiC wafers (manufactured by Nitride Crystals, LLC) were used for bonding experiments. The bonding was carried out at temperature T = 1300–1550 °C in vacuum without any adhesive layers and without applying external mechanical pressure. The next step after the bonding was the removal of silicon with a liquid etchant. Homoepitaxial 3C-SiC layers were grown on the resulting templates by the sublimation method at T = 1700–1800 °C in vacuum of (4–5) × 10^{-6} Torr. The layer thickness was 10–15 micrometers. Structural characterization was carried out with X-ray double-crystal diffractometry (XRD) and Raman spectroscopy. Room temperature Raman spectra were recorded in the backscattering geometry using a LabRAM HR Evo UV-VIS-NIR-Open spectrometer (Horiba, France). Nd:YAG laser with a wavelength of 532 nm was used as the excitation source. The laser beam was focused into a spot up to 1 μm in diameter using Olympus confocal microscope.

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Results and Discussion

Fig. 1, *a*, *b* shows the technological scheme of the bonding process and photographs of the processed experimental samples.

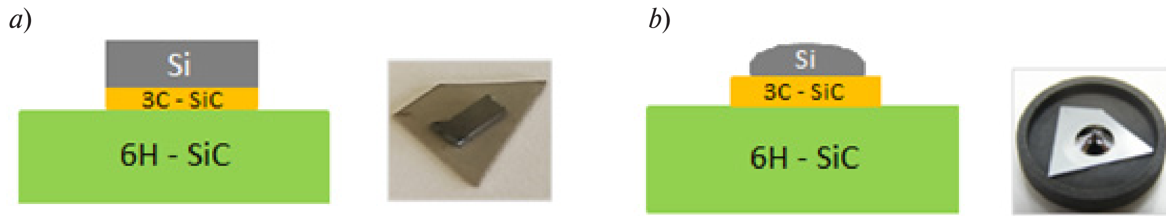

Fig. 1. Scheme of bonding process (left) and the corresponding photographs (right) of experimental samples: before annealing (*a*), after unloading from the annealing chamber (*b*)

It was found that the transferred CVD-layers had strong mechanical contact with SiC wafers when the annealing temperature exceeded the melting temperature of Si (1400 °C). Annealing under these conditions results in conversion of silicon substrate into a droplet of Si melt as shows the photograph in Fig. 1, *b*. Before using the bonded 3C-SiC/6H-SiC structures as a substrate for subsequent sublimation homoepitaxy, the solidified Si melt was removed by wet etching in a 1 : 3 mixture of hydrofluoric (HF) and nitric (HNO_3) acids, which has no etching effect on the underlying silicon carbide.

Structural characterization showed that the best quality was achieved for sublimation epitaxial layers grown on a bonded substrate fabricated at $T = 1500$ °C. XRD rocking curves (RC) obtained on homoepitaxial layers grown by sublimation on a substrate with a transferred CVD adlayer had a full width at half maximum (FWHM) in the range of 120–170 arc seconds whereas RC with FWHM of 300 arc seconds were recorded on starting heteroepitaxial 3C-SiC grown by CVD on a Si substrate. Based on the XRD data, two main conclusions can be drawn: (I) the quality of sublimation epitaxy of 3C-SiC on the combined substrates is at the level of epitaxy of cubic silicon carbide by chemical vapor deposition; (II) despite the fact that the transferred layer had the (001) orientation, its overgrowth proceeded in the [111] direction. To clarify the latter discrepancy, we can consider the data obtained by optical microscopy (Fig. 2, *a*, *b*). A micrograph of the back side of the 3C-SiC CVD layer transferred onto a SiC wafer is shown in Fig. 2, *a*.

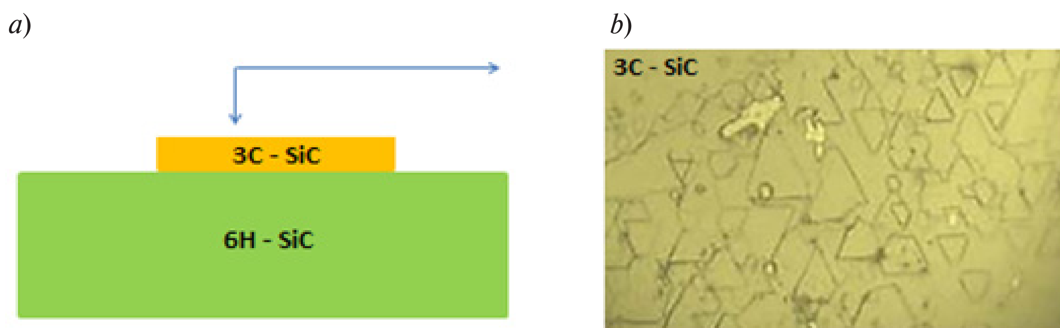

Fig. 2. Results obtained by optical microscopy: explanatory diagram of the studied sample (*a*); back side surface view of 3C-SiC layer transferred on 6H-SiC wafer (×500) (*b*)

An island-like character can be detected in the structure formed at the initial stage of 3C-SiC growth on the Si substrate. The structure is formed by small randomly distributed triangular islands, which are crystallographic twins lying in the (001) plane. Based on this observation and the results of XRD analysis, we can assume that the initial island-like microstructure develops into a microstructure with different island orientation in accordance with van der Drift model of self-regulation of crystal growth from the vapor phase on a substrate with randomly oriented nucleation islands. The evolutionary selection rules proposed in the model determine the termination of the growth in the direction of slowly growing orientations and the development of preferred orientations with a maximum growth rate. In case of cubic crystals, these regularities determine the growth transition from the [100] direction to the [111] direction [7].

Results obtained by XRD analysis were fully confirmed by the results of Raman spectroscopy studies of initial 3C-SiC CVD-grown layers and grown on combined substrates. Raman studies are used in SiC technologies as the main diagnostic method for determining the polytype of experimental samples, the presence of polytype inclusions in them, and evidence of polytype transformations. It is known that in the Raman spectra of 3C-SiC there are two characteristic lines corresponding to the transverse optical mode (TO) at a frequency of 796.2 cm^{-1} and the longitudinal optical mode (LO) at a frequency of 972.7 cm^{-1} [8, 9]. Fig. 3 shows the Raman spectra of CVD-grown 3C-SiC layer on Si and of the layer grown by sublimation layer on the bonded substrate.

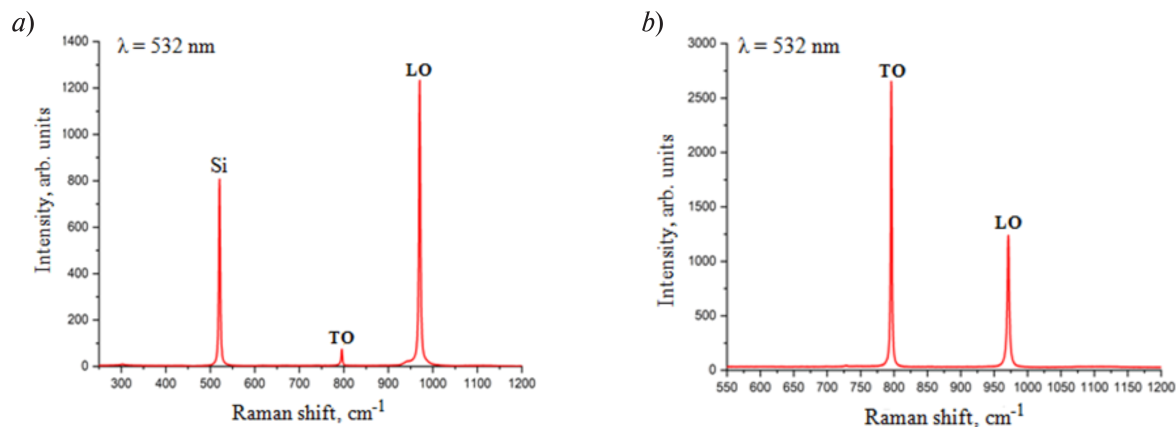

Fig. 3. Raman spectra measured in the starting 3C-SiC/Si sample (*a*) and in the layer grown by sublimation on the transferred 3C-SiC seed adlayer (*b*)

Both spectra contain narrow peaks of TO and LO phonon modes at frequencies ~794 cm^{-1} and ~968 cm^{-1}, respectively. This confirms that the layers correspond to the pure cubic phase of high quality. The spectrum of the CVD-grown layer additionally contains a peak at 520 cm^{-1} corresponding to the silicon substrate. Observed change in the ratio of intensity of the LO and TO phonon lines confirms the phenomenon of changing of orientation from [001] to [111] for the CVD layer and the layer grown by sublimation epitaxy, respectively.

Conclusion

We established that the transfer of 3C-SiC heteroepitaxial CVD-grown layers onto a 6H-SiC wafer makes it possible to develop combined 3C-SiC/6H-SiC structures suitable for use as substrates for high-quality homoepitaxy of cubic polytype silicon carbide. We found that a bonding temperature above the melting temperature of Si is a critical parameter for obtaining good mechanical contact between the transferred 3C-SiC layers and carrier 6H-SiC wafers. Interpretation of the observed phenomenon of the change in the crystallographic orientation of the grown layers relative to the transferred ones requires additional investigation.

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