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The features of the crystallization of an intermediate silicon layer during the transfer of a thin 3*C*-SiC(001) layer onto a 6*H*-SiC(0001) substrate

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The paper considers the features of crystallization of the silicon bonding layer between a (001)-oriented thin layer of cubic silicon carbide and a hexagonal (0001) 6*H*-SiC substrate. General patterns revealed in the formation of orientation relationships for the silicon layer with respect to the 3*C*-SiC layer and the 6*H*-SiC substrate are discussed.

Keywords: silicon carbide, silicon, TEM.

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Silicon carbide (SiC) is a wide-bandgap compound semiconductor. Due to its high breakdown field, good thermal conductivity, and stable electrical performance over a wide temperature range, the material is sought after by the modern electronics industry, especially in high-temperature and power electronics [1].

Silicon carbide is characterized by polytypism — a phenomenon in which the material tends to crystallize in similar structures with various subsequence of close-packed layers depending on external conditions. The most stable SiC polytypes include two hexagonal modifications: 4*H* and 6*H*. Currently, only these two polytypes can be grown as single-crystal ingots (boules) by the modified Lely method (LETI method) using seed crystals. In addition to stable hexagonal polytypes, the metastable cubic 3*C*-modification (zinc blende structure) [2] is of particular interest. Unlike stable SiC modifications, obtaining bulk crystals and hence cubic polytype substrates is a technological challenge.

The stability of cubic polytype at relatively low temperatures allows its growth by heteropolytype epitaxy on the basal facet of hexagonal 4*H*- and 6*H*-substrates [3]. Obtaining thick epitaxial layers of 3*C*-SiC with orientation (111) on such substrates involves the formation of inclusions of other polytypes [4,5] as well as double positioning boundaries (DPB) [6].

An approach aimed at creating substrates for 3*C*-SiC homopolytype epitaxy by transferring thin layers of silicon carbide of cubic modification with orientation (001) onto hexagonal polytypes substrates of SiC deserves special attention. To do this, 3*C*-SiC layers obtained by chemical vapor deposition (CVD) on silicon substrate with (001) orientation are used. This approach is promising from the point of view of further growth of thick cubic silicon carbide layers free of polytype inclusions and DPB defects [7,8]. In particular, it is shown that such substrates can be used for the epitaxy of 3*C*-SiC by sublimation growth [9]. The use of silicon as a bonding layer for 4*H*-SiC substrates was successfully shown in [10].

This paper investigates by transmission electron microscopy (TEM) the crystallization features of the silicon intermediate layer during the transfer of the 3*C*-SiC layer onto the 6*H*-SiC substrate. TEM study was performed using a Philips EM420 electron microscope operating at an accelerating voltage of 100 kV. The samples for the study were prepared by a standard technique involving mechanical thinning and ion sputtering with Ar^+ ions.

The study deals with the transfer of an 3*C*-SiC CVD film with a thickness of the order of $10\,\mu$m obtained on a silicon substrate with orientation (001) manufactured by NOVASIC. A sample of size 5×5 mm is placed face down on a 6*H*-SiC substrate of size 11×11 mm after which the resulting configuration is heated to a temperature above the melting point of silicon (1414 °C) and held for 30 min at a temperature of 1500 °C. The bonding layer is formed by penetration of molten silicon into the gap between the 3*C*-SiC layer and the 6*H*-SiC substrate. As a result of the process, a cone-shaped drop of crystallized silicon is formed on the substrate surface. An image of the drop is shown in the inset of Fig. 1, *a*. The drop is further removed by chemical etching in a mixture of hydrofluoric (HF) and nitric (HNO_3) acids.

Fig. 1, *a* shows a cross-sectional image of a TEM sample obtained using an optical microscope (the color version of the figure is presented in the online version of the paper). Unlike the substrate 6*H*-SiC layer 3*C*-SiC has a characteristic yellow hue. The silicon bonding layer is represented by a dark narrow strip in the image. The TEM image of the structure under consideration is shown in Fig. 1, *b*. Next, the orientation relationships arising from the crystallization of the intermediate silicon layer with respect to the 3*C*-SiC layer and the 6*H*-SiC substrate will be discussed.

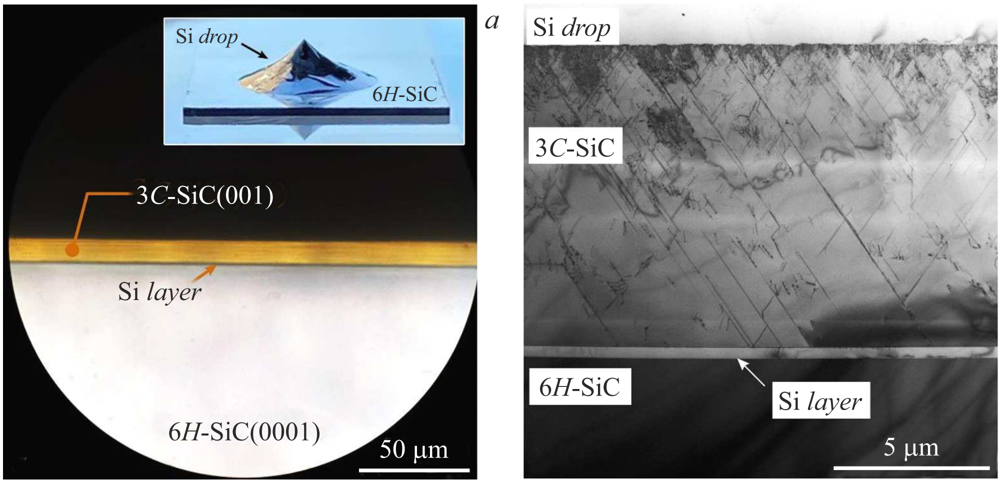

Figure 1. Cross-sectional images of the transferred 3*C*-SiC (001) layer in a silicon droplet on an 6*H*-SiC substrate. *a* — obtained using an optical microscope; *b* — obtained using a TEM. The inset shows a photograph of the droplet.

The formation of orientation relationships between silicon and cubic silicon carbide during heteroepitaxy on Si/SiC templates has been discussed in detail in a series of works [11,12]. In particular, the authors note the tendency to the formation of polycrystalline film. For the case of silicon melt crystallization in the gap between two 4*H*-SiC substrates with C and Si basal facets, the polycrystalline intermediate layer [10] is also formed.

In the considered case, crystallization of the silicon melt intermediate layer between the surface of the 3*C*-SiC (001) layer and the Si facet of the 6*H*-SiC substrate takes place during the cooling process. Analysis of the TEM study results revealed the polycrystalline nature of the structure for both the intermediate layer and the solidified silicon melt droplet. Fig. 2 shows examples of electron diffraction patterns obtained from regions near the interfaces between the silicon intermediate layer with the 3*C*-SiC layer and the 6*H*-SiC substrate.

The electron diffraction pattern for the 3*C*-SiC/Si interface in Fig. 2, *a* (top) matches the nominal epitaxial relationships with good accuracy: 3*C*-SiC$\{001\} \parallel$ Si$\{001\}$ and 3*C*-SiC$\langle 110\rangle \parallel$ Si$\langle 1\bar{1}0\rangle$. The lattice constant mismatch for this orientation is 20%. The bottom part of Fig. 2, *a* shows the diffraction pattern obtained from the same region of the intermediate silicon layer for the interface with the substrate. When obtaining electron diffraction patterns at the 6*H*-SiC/Si interface, the specimen was oriented with the 6*H*-SiC$\langle 11\bar{2}0\rangle$ zone axis parallel to the electron beam. The observed asymmetry in the intensity distribution for the reflections of the intermediate silicon layer indicates that there is no mutual orientation with the substrate. Nevertheless, the angle between the Si$\langle 1\bar{1}0\rangle$ and 6*H*-SiC$\langle 11\bar{2}0\rangle$ directions is quite small and we estimate it to be a few degrees. The tilted position of 002 reflection in the diffraction pattern relative to the 0006 reflection of substrate indicates the bending of the transferred 3*C*-SiC layer, apparently caused by the non-uniform distribution of silicon at the boundary.

Fig. 2, *b* shows the electron diffraction pattern for the 3*C*-SiC/Si interface with orientation relationship close to 3*C*-SiC$\{110\} \sim\parallel$ Si$\{11\bar{1}\}$ and 3*C*-SiC$\langle 1\bar{1}0\rangle \parallel$ Si$\langle 1\bar{1}0\rangle$. The deflection angle between the reflections 220 for 3*C*-SiC and $\overline{222}$ for silicon is of the order of 2° as demonstrated in the inset of Fig. 2, *b*. A close configuration was considered in [13], where a similar deviation was observed. This orientation differs from the previous orientation by a rotation by $\sim 35.2^\circ$ — angle between the (001) and (112) planes when observed along the $[1\bar{1}0]$ zone axis. For this orientation, the interplanar spacing mismatch for silicon carbide and silicon in the $\{001\}$ interface plane along one of the 3*C*-SiC$\langle 110\rangle$ directions is about 2% $(2d^{3C\text{-SiC}}_{\{220\}} \approx d^{\mathrm{Si}}_{\{111\}})$. Orientations of silicon crystallites for which the planes of the type $\{111\}$ are parallel to the 3*C*-SiC$\{110\}$, were frequently observed and are attributed by the authors to this circumstance. At the interface 6*H*-SiC/Si for the same region, according to the diffraction pattern in Fig. 2, *b*, in addition to the proximity of the Si$\langle 110\rangle$ and 6*H*-SiC$\langle 11\bar{2}0\rangle$ directions, no other regularities in the formation of orientation relationships are observed.

Another trend is the orientation of the close-packed direction along the similar direction of the 3*C*-SiC layer. For this configuration, two mutually perpendicular directions of the 3*C*-SiC$\langle 1\bar{1}0\rangle$ type are located in the interface plane, so two types of diffraction patterns are mainly found in the observation. The first type, when the Si$\langle 1\bar{1}0\rangle$ direction is oriented along the electron beam, corresponds to the electron diffraction patterns in Fig. 2, *a* and *b*. The second type, when the direction is oriented normal to the electron beam, is shown in Fig. 2, *c* and *d*. The fact that the Si$\langle 110\rangle$ and 3*C*-SiC$\langle 110\rangle$ directions are parallel to each other in this case is suggested by the position of the 220 reflections for silicon and silicon carbide, which are on the same straight line parallel to the interface plane.

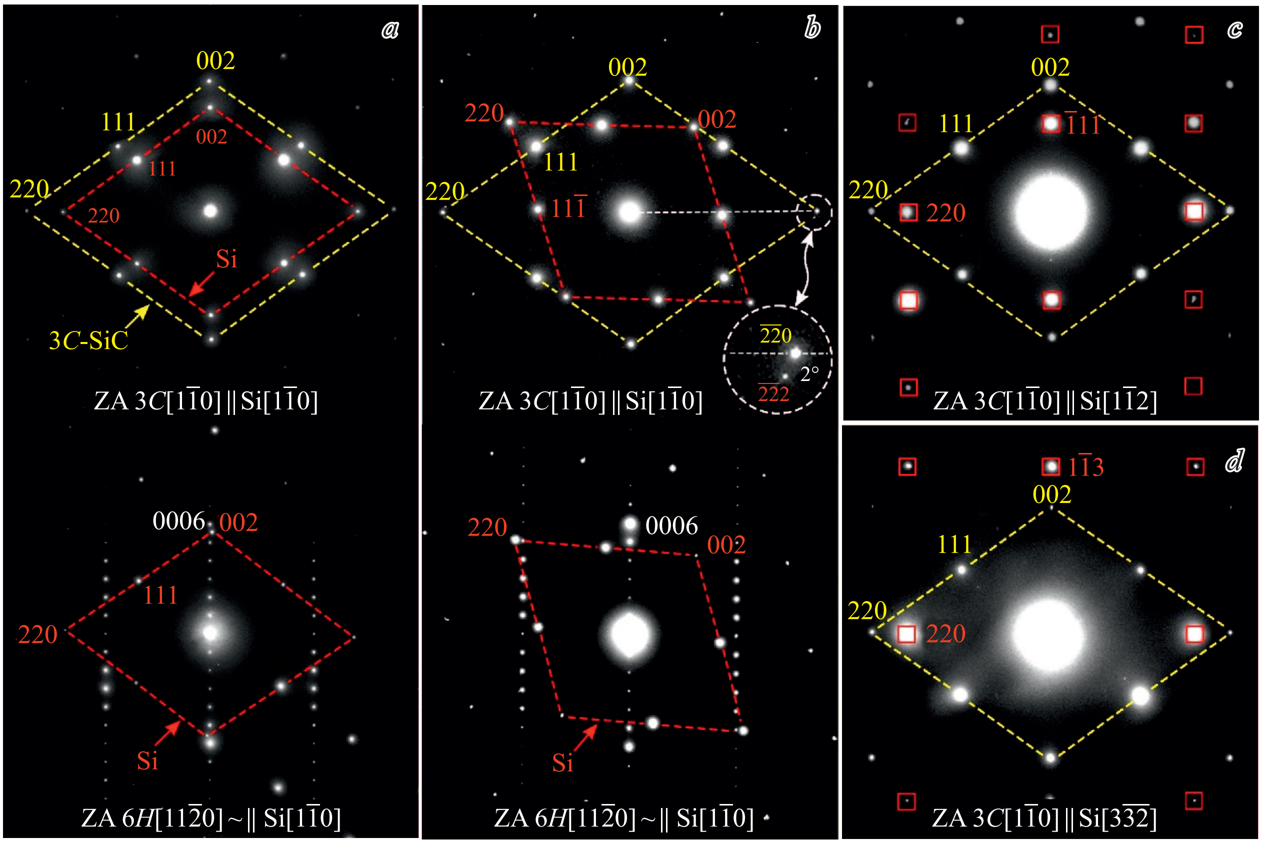

Figure 2. Examples of electron diffraction patterns obtained from the interface regions of the 3*C*-SiC layer and the 6*H*-SiC substrate with the silicon intermediate layer (*a, b*) and from the interface region between the 3*C*-SiC layer and the silicon intermediate layer (*c, d*). The yellow and red color in the notations refer to 3*C*-SiC and Si, respectively. A color version of the figure is provided in the online version of the paper.

Thus, the paper experimentally investigates the regularities of orientation relationship formation during silicon melt crystallization between the transferred 3*C*-SiC(001) layer and the hexagonal silicon carbide substrate. It is found that crystallization results in the formation of an intermediate silicon layer with a polycrystalline structure. Orientation relationships arising for such a layer correlate to a greater extent with the orientation of the cubic silicon carbide layer and to a lesser extent with the orientation of the hexagonal substrate. The following trends can be distinguished in their formation. The first trend — orientation of the Si{111} planes parallel to the 3*C*-SiC{110} planes, which is attributed to the proximity of the interplanar distances for these families of crystallographic planes. The second trend — orientation of silicon crystallites by the close-packed ⟨1$\bar{1}$0⟩ direction parallel to the transferred layer direction 3*C*-SiC⟨1$\bar{1}$0⟩.

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Conflict of interest

The authors declare that they have no conflict of interest.

References

[1] X. She, A.Q. Huang, O. Lucia, B. Ozpineci, IEEE Trans. Ind. Electron., **64** (10), 8193 (2017). DOI: 10.1109/TIE.2017.2652401
[2] F. Li, F. Roccaforte, G. Greco, P. Fiorenza, F. La Via, A. Pérez-Tomas, J.E. Evans, C.A. Fisher, F.A. Monaghan, P.A. Mawby, M. Jennings, Materials, **14** (19), 5831 (2021). DOI: 10.3390/ma14195831
[3] K. Seki, Alexander, S. Kozawa, T. Ujihara, P. Chaudouët, D. Chaussende, Y. Takeda, J. Cryst. Growth, **335** (1), 94 (2011). DOI: 10.1016/j.jcrysgro.2011.09.004
[4] R. Vasiliauskas, P. Malinovskis, A. Mekys, M. Syväjärvi, J. Storasta, R. Yakimova, Mater. Sci. Forum, **740-742**, 335 (2013). DOI: 10.4028/www.scientific.net/MSF.740-742.335

[5] R. Vasiliauskas, M. Marinova, M. Syväjärvi, E.K. Polychroniadis, R. Yakimova, J. Cryst. Growth, **395**, 109 (2014). DOI: 10.1016/j.jcrysgro.2014.03.021

[6] H.S. Kong, B.L. Jiang, J.T. Glass, G.A. Rozgonyi, K.L. More, J. Appl. Phys., **63** (8), 2645 (1988). DOI: 10.1063/1.341004

[7] F. La Via, A. Severino, R. Anzalone, C. Bongiorno, G. Litrico, M. Mauceri, M. Schoeler, P. Schuh, P. Wellmann, Mater. Sci. Semicond. Process., **78**, 57 (2018). DOI: 10.1016/j.mssp.2017.12.012

[8] P. Schuh, M. Arzig, G. Litrico, F. La Via, M. Mauceri, P.J. Wellmann, Phys. Status Solidi A, **214** (4), 1600429 (2017). DOI: 10.1002/pssa.201600429

[9] M.G. Mynbaeva, D.G. Amelchuk, A.N. Smirnov, I.P. Nikitina, S.P. Lebedev, V.Yu. Davydov, A.A. Lebedev, Semiconductors, **56** (11), 872 (2022). DOI: 10.21883/SC.2022.11.54965.9953.

[10] M. Le Cunff, F. Rieutord, D. Landru, O. Kononchuk, N. Cherkashin, J. Appl. Phys., **135** (24), 245301 (2024). DOI: 10.1063/5.0205878

[11] T. Yeghoyan, K. Alassaad, V. Souliere, G. Ferro, Mater. Sci. Forum., **897**, 87 (2017). DOI: 10.4028/www.scientific.net/MSF.897.87

[12] T. Yeghoyan, K. Alassaad, S.R.C. McMitchell, M. Gutierrez, V. Souliere, D. Araujo, G. Ferro, Mater. Sci. Forum., **924**, 128 (2018). DOI: 10.4028/www.scientific.net/MSF.924.128

[13] T. Nishiguchi, M. Nakamura, K. Nishio, T. Isshiki, S. Nishino, Appl. Phys. Lett., **84** (16), 3082 (2004). DOI: 10.1063/1.1719270

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