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Macrodefects in cubic silicon carbide crystals

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Abstract. Different sublimation growth conditions of 3C-SiC approaching a bulk process have been investigated with the focus on appearance of macrodefects. The growth rate of 3C-SiC crystals grown on 6H-SiC varied from 380 to 460 μm/h with the thickness of the crystals from 190 to 230 μm, respectively. The formation of macrodefects with void character was revealed at the early stage of 3C-SiC crystal growth. The highest concentration of macrodefects appears in the vicinity of the domain in samples grown under high temperature gradient and fastest temperature ramp up. The formation of macrodefects was related to carbon deficiency which appear due to high Si/C ratio which is used to enable formation of the 3C-SiC polytype.

Introduction
Cubic silicon carbide (3C-SiC) has several advantages over hexagonal forms in terms of higher electron mobility, higher saturated electron drift velocity and better isotropic properties which make it a preferable material for a number of device applications. Thus availability of low defect 3C-SiC substrates would be beneficial for the production of such devices. The 3C-SiC grown on foreign substrates such as silicon is highly stressed due to the 20% lattice mismatch and 8% thermal mismatch [1] and has a consequence that a high density of defects appear. Growth of 3C-SiC on 6H-SiC brings numerous advantages due to insignificant lattice mismatch and identical chemical properties. In addition, heteropolytypic structures of SiC are very promising for development of devices [2]. In order to reveal initial growth mechanisms of 3C-SiC on 6H-SiC substrates different growth methods have been investigated [3-5]. High quality 3C-SiC can be grown in very thick layers (>100 μm) by sublimation epitaxy [6]. In addition, by using this technique high quality 3C-SiC with bulk properties can be obtained by further optimizing growth conditions. However, during such growth various defects may appear due to high growth rates and in particular due to the silicon to carbon ratio which has an effect on the stability of 3C-SiC formation.

The aim of this study is to evaluate the influence of different growth conditions on the formation of macrodefects in 3C-SiC crystals grown on 6H-SiC substrates by sublimation growth.

Experimental procedure
Growth was performed using a sublimation technique where the vapor species are driven from the source to the substrate by a temperature gradient. The distance between the source and the substrate was adjusted to 1 mm for all experiments in order to facilitate direct transfer of silicon and carbon-bearing species from source to substrate. A short distance is important for the control of silicon and carbon-bearing species, since at longer distances the vapor species interact with the graphite wall and shift the vapor composition at the growth surface. Also, in this work three temperature ramp ups (slow, medium, fast) during initial nucleation stage were applied under two different temperature gradients (high and low) between the source material and the substrate. By varying initial temperature ramp-up initial supersaturation as well as silicon to carbon ratio conditions was changed. The growth was carried out at 1775 °C with a growth time of 30 min. The 3C-SiC crystals
grown on 6H-SiC substrates were analyzed by means of optical microscope with Nomarski interference contrast and electron probe micro-analysis (EPMA).

**Results and discussion**

Depending on the temperature ramp up the growth rate of 3C-SiC crystals varied from 380 to 460 μm/h with the thickness of the crystals from 190 to 230 μm, respectively. Thus the nucleation and resulting material resembles that of bulk at its initial growth stage. The crystals typically contain domains. On 6H-SiC the 3C-SiC will form as domains and there will be competition between these. The most favorable conditions are when large 3C-SiC domains are formed. The largest 3C-SiC domains were observed under the slowest initial temperature ramp up both under low and under high temperature gradient. That could be explained by an initial supersaturation set by the temperature ramp up conditions analyzed by our group previously [7]. A faster ramp up gives higher supersaturation and as a result formation of 3C-SiC as well as an increased number of 3C-SiC growth centers.

In this work we observe macrodefects appearing in the vicinity of the domains. To study the macrodefects, strips with a width of 1 mm were cut parallel to the 3C-SiC growth direction and polished. The cross sectional view was analyzed by optical microscope. As seen in Fig. 1 macrodefects having a void character are formed several micrometers above or at 3C/6H interface in different shape (oval, round, prolonged stripes and etc) and in different size ranging from 5 to 30 μm.

![Voids in 3C crystals (cross sectional view)](image)

Fig. 1 Voids in 3C crystals (cross sectional view)

They appear often as a chain of single defects propagating towards growth direction and mostly they are located at the domain boundaries (Fig. 2). The highest concentration of macrodefects were observed in the samples grown under fast temperature ramp-up which influenced smaller and higher density of 3C-SiC domains. A fast temperature ramp-up has the effect that the silicon to carbon ratio is increased. This provides conditions for formation of 3C-SiC while at the same time growth conditions a further away from stochiometry of SiC, which we believe is causing an increasing probability of void formation.
The highest concentration of macrodefect formation centers appears few micrometers above 6H steps formed at the 3C/6H interface. These defects were rarely observed above the smooth regions of 3C/6H interface. Thus, the formation of macrodefects in 3C-SiC could be related to growth disturbances due to competing growth of 3C and 6H during initial growth process.

Also, macrodefects can be preferably appearing between two 3C-SiC domains. It was clarified by additional experiments where low temperature gradient, slow temperature ramp up and very short growth time (1 min.) were used. As seen in Fig. 3 there are dominating 3C-SiC domains which are overgrowing 6H-SiC and competing with two smaller 3C-SiC domains.

Fig. 2 Voids at 3C-SiC domain boundaries (top view of polished 3C-SiC crystal)

Fig. 3 Macrodefects appearance at domain boundaries
In order to determine whether these defects are not secondary phases [8] such as can be found in hexagonal SiC bulk growth using Physical Vapor Transport technique the chemical analysis of defects containing areas in stripes was performed using EPMA. It was revealed that no higher concentration clusters of silicon or carbon exist in the samples, which confirms that these defects are mainly voids.

Summary
The growth of 3C-SiC approaching bulk properties by sublimation technique was demonstrated. We believe that void formation could be related to high Si/C ratio at the initial stage of the growth which is preferable for 3C-SiC growth. The excess of silicon creates carbon deficiency in the growing crystal and increases the probability of voids formation under conditions set for high growth rate sublimation. It was revealed that the highest concentration of voids appeared in samples grown under fast temperature ramp up which creates the highest Si/C ratio both under low and high temperature gradient.

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