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Optimization of Heat Transfer Design for High Quality 4H-SiC Ingot Growth

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Abstract. At the high growth temperatures of the PVT method, thermal radiation from the graphite crucible surface to the seed region is the dominant mode of heat transfer. In this study, we propose a newly designed crucible structure with a thinner graphite wall compared to the conventional design for SiC crystal growth. The SiC ingot grown using the conventional crucible exhibited the smallest thickness variation (flat top surface) between the center and the edge of the ingot, accompanied by polytype inclusions, which led to an increase in defect density. In contrast, SiC ingots grown using the newly designed crucibles (Design A and Design B) showed a convex top surface and a significantly lower defect density due to the improved heat transfer efficiency. Thinning the graphite crucible wall helps maintain a relatively higher temperature at the seed edge region, thereby effectively enhancing thermal radiation in the radial direction inside the crucible. These results indicate that thermal radiation in the radial direction can be achieved through appropriate optimization of the graphite wall thickness.

Introduction

Recently, commercially available SiC power devices such as MOSFETs and Schottky barrier diodes (SBDs) have been fabricated on 6-inch *n*-type 4H-SiC substrates. To further improve device performance and manufacturing yield, the development of large-diameter, high-quality SiC substrates is essential [1-3]. In high-quality epitaxial growth, such substrates must possess a low defect density, suppressed polytype inclusions, and minimal wafer bow. Achieving these characteristics requires precise control of the temperature gradient and the C/Si ratio of the vapor phase in the crystal growth region. In the physical vapor transport (PVT) method for SiC crystal growth, a non-optimized heat transfer design in the upper crucible assembly can cause instability in the crystal shape, leading to the formation of various dislocations and polytype inclusions in the grown ingot.

In this work, we aimed to optimize the heat transfer design in the growth zone by varying the lateral wall thickness of the graphite crucible in the upper crucible region, including the seed crystal area. During crystal growth, the temperature at the edge of the seed crystal is generally higher than that at the axial (center) region, primarily due to enhanced thermal radiation at high growth temperatures. This thermal radiation is the dominant heat transfer mechanism under such conditions, facilitating the transport of vapor species such as Si, Si_2C, and SiC_2 toward the center of the crucible. Consequently, this condition often leads to the formation of a slightly convex growth front in the SiC ingot [4-5]. In this study, we propose a heat transfer design that promotes polytype stability and enables precise control of defect density during crystal growth.

Experiments

Figure 1 shows schematic diagrams of two crucible designs placed inside the graphite insulation: (i) the conventional crucible and (ii) a newly designed crucibles with a relatively thinner wall. In the new design, the wall thickness was reduced to 95% (Design A) and 90% (Design B) of that of the conventional crucible (100%). SiC crystal growth experiments using these three crucible configurations were carried out at a growth temperature of approximately 2300 °C under an argon atmosphere at pressures ranging from 1 Torr to 40 Torr. A 6-inch, c-face (000-1) 4H-SiC wafer was employed as the seed crystal.

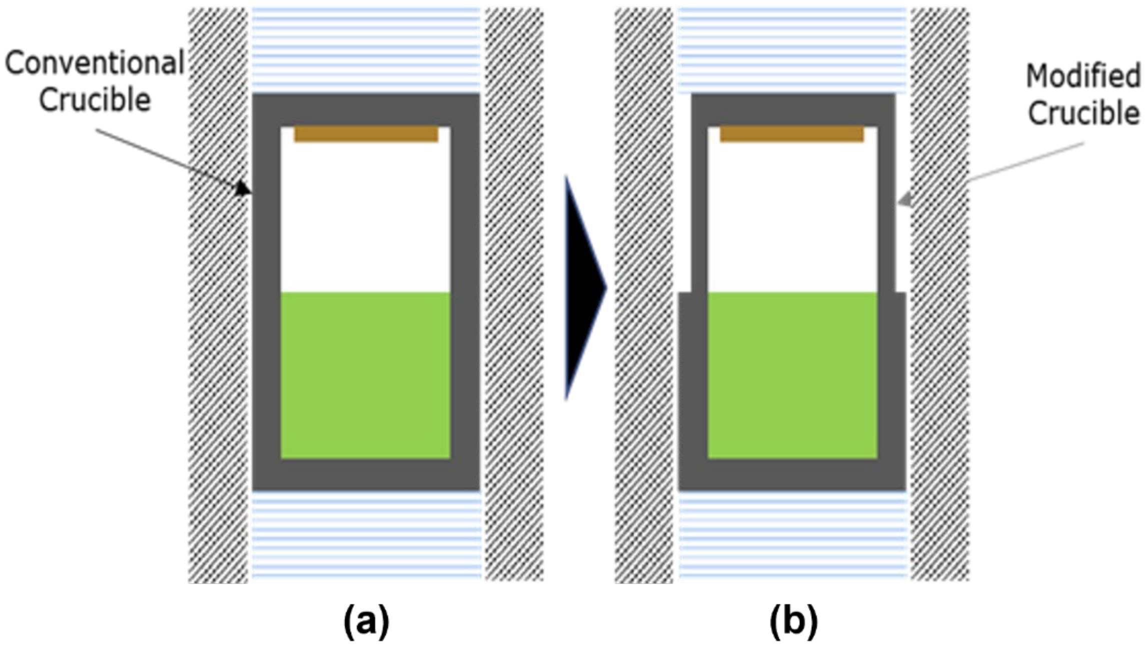


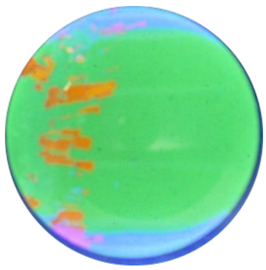
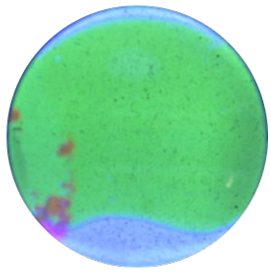
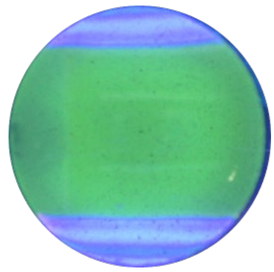
Fig. 1. Schematic diagram of two crucible designs placed inside graphite insulation: (a) the conventional design (100% wall thickness) and (b) newly designed crucibles with reduced wall thickness of 95% (Design A) and 90% (Design B) relative to the conventional one.

Result and Discussion

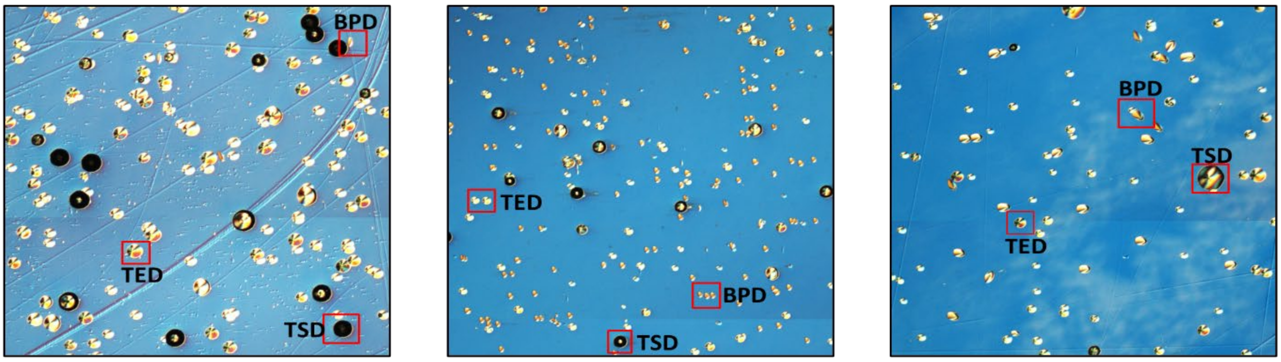
As shown in Table 1, UV fluorescence (UVF) images and photographs of SiC ingots grown using the three crucible designs are presented. The bluish regions observed at the upper and lower parts of the ingots are artifacts caused by optical interference. The UVF image of the ingot grown with the conventional crucible design reveals polytype inclusions (orange regions) on the left side. In contrast, ingots grown using both design A and design B (with relatively thinner walls) exhibited a clear suppression of polytype inclusions. The measured thickness deviation between the center and edge of the ingot grown with the conventional design was only 0.42 mm, indicating a relatively flat surface profile. In comparison, ingots grown with designs A and B displayed convex surfaces with significantly higher thickness deviations of 1.21 mm and 2.34 mm, respectively. The reduction in the graphite crucible wall thickness enhances the temperature at the seed edge region, as thermal radiation dominates heat transfer at the growth temperature (~2300 °C). Thinner crucible walls in designs A and B allow increased radial thermal radiation toward the seed crystal, which, in turn, promotes sublimation of vapor species toward the crucible center. Consequently, a more uniform temperature gradient is established, leading to the formation of convex-shaped SiC crystals and improved polytype stability.

To evaluate the defect density of the grown SiC crystals, chemical etching was carried out in molten KOH at 480 °C for 5 minutes. Figure 2 presents etched surface images (Nikon, Eclipse LV150) of selected areas near the crystal facets for ingots grown with each crucible design. As summarized in Table 2, substrates obtained from the newly designed crucibles exhibited a lower defect density compared with those from the conventional design.

Table 1. UVF images and ingot shapes of 4H-SiC crystals grown using the conventional crucible and the newly designed crucibles (Design A: 95%, Design B: 90% wall thickness).

Insulator density ratio	Conventional (100%)	Design A (95%)	Design B (90%)
UVF image			
Ingot shapes			
Thickness deviation (center-edge)	0.42 mm	1.21 mm	2.34 mm

This improvement is attributed to the optimized radial heat transfer in the thinner-walled crucibles. In particular, maintaining a relatively higher temperature at the seed edge region reduced the generation of threading screw dislocations (TSDs), likely by mitigating dislocation transformation processes at the seed-growth interface.



Conventional Design A Design B

Fig. 2. Etch pit images of 4H-SiC crystal ingots grown using the conventional crucible and modified designs (Design A: 95%, Design B: 90% wall thickness) for EPD evaluation.

Table 2. Etch pit density (EPD) for grown SiC crystal substrates for conventional and newly designed designs. (Design A: 95%, Design B: 90% wall thickness)

* TSD : Threading Screw Dislocation, TED : Threading Edge Dislocation, BPD : Basal Plane Dislocation

	Conventional	Design A	Design B
TSD [ea/cm^2]	1,680	980	500
TED [ea/cm^2]	5,200	3,000	2,000
BPD [ea/cm^2]	5,140	12	90

Summary

6-inch 4H-SiC crystals were grown at approximately 2300 °C under an argon atmosphere at 1-40 Torr. Both a conventional crucible design and newly developed crucible designs (Design A and Design B) with reduced graphite wall thickness were employed. The newly designed crucibles had relatively thinner walls, with thickness ratios of 95% (Design A) and 90% (Design B) relative to the conventional design. The SiC ingot grown using the conventional design exhibited a flat surface, the presence of polytype inclusions, and a relatively higher defect density. In contrast, ingots grown with the newly designed crucibles showed a convex surface profile, suppression of polytype inclusions, and a significant reduction in defect densities such as basal plane dislocations (BPDs) and threading screw dislocations (TSDs). These improvements are attributed to optimized control of thermal radiation within the hot zone, which is critical for achieving high-quality SiC crystal growth.

Acknowledgements

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