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Development of High Quality 8 inch 4H-SiC Substrates

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Abstract. 8 inch 4H-silicon carbide (SiC) development faces challenges first from obtaining high-quality 8 inch SiC seed substrate, then reducing grown-in crystal residual stress and defects in the following crystal growth process. Here we report the diameter expansion process from 6 inch 4H-SiC seed substrate to 8 inch 4H-SiC crystal. Based on simulation and experimental results, it is deduced that an optimized radial temperature gradient (RTG) zone in the range of 0.10-0.12 °C/mm is essential for high-quality and efficient SiC crystal diameter expansion. According to the RTG calculation, diameter expansion process is designed and 8 inch 4H-SiC crystal as well as seed substrate is achieved. With the obtained seed substrate, high-quality 8 inch 4H-SiC crystal is developed and the following polished 4H-SiC substrate quality is characterized.

Introduction

4H-SiC is recognized as one of the most suitable semiconductor material for high-power and high-frequency devices due to its superior physical properties. Nowadays, 6 inch 4H-SiC substrates are in mass production for power device fabrication while 8 inch 4H-SiC substrates are still in rapid development. To develop 8 inch SiC crystal and substrate, the first obstacle is how to expand the crystal diameter to 8 inch from smaller-sized seed substrates. Considering the driving force of SiC lateral growth is mainly provided by radial temperature gradient (RTG), the difficulty in SiC crystal diameter expansion is how to balance the lateral growth of SiC crystal while keeping a minimum grown-in residual thermal stress in the lattice to guarantee the crystal quality [1-3]. Besides, residual thermal stress in as-grown 4H-SiC crystal increases with the diameter expansion due to the non-uniform temperature distribution inside the growth chamber. Since the key defects such as basal plane dislocations (BPDs) are closely related to the thermal stress [4-6], it is important to design homogenously temperature distributed growth chamber for 8 inch SiC crystal, which is essential to reduce stress introduced defects and keep the following sliced substrates in small bow/warp values.
Here we demonstrate the diameter expansion process of SiC crystal from 6 inch to 8 inch and the following obtained 8 inch SiC crystal and substrates. The temperature gradient suitable for diameter expansion is calculated and demonstrated, the grown-in thermal stress and resulted defects in the 8 inch 4H-SiC crystals are discussed.

Experiments

4H-SiC crystals were grown on 4° off-cut C-face 4H-SiC seed substrates with physical vapor transportation (PVT) method in graphite-made growth chambers. The growth temperature is set at 2000-2300 °C under pressure 10-30 mbar in argon and nitrogen atmosphere. Nitrogen was doped for both resistivity optimization and 4H polytype stabilization during diameter expansion process [7]. It is noted that the nitrogen doping concentrations during different diameter-expansion processes are not necessarily the same. An initial self-produced 6 inch 4H-SiC seed substrate was used for crystal diameter expansion process. With each run of crystal diameter expansion growth, SiC crystals with

increased diameter were acquired. The enlarged crystals were then sent to wafer fabrication process for new seed preparation and next run of crystal diameter expansion growth process. It should be stressed that the temperature gradient and corresponding diameter expansion structure for each run of crystal diameter expansion differs a lot. In order to have a better understanding and design of each diameter expansion process, Virtual Reactor simulation was carried out before crystal growth. The temperature distribution and the RTG required for diameter expansion is calculated in combination with the experimental results. After the SiC seed substrate reached 8 inch in diameter, the seed substrate was then used for 8 inch SiC crystal growth. A crystal growth thermal field differs from diameter expansion process was designed in order to minimize the residual crystal stress. The finally obtained 8 inch SiC crystal was then sliced into 8 inch SiC substrates.
To characterize the quality of the 8 inch SiC substrate, micro-Raman spectroscopy was carried out for polytype inspection. Besides, the typical peak shift is taken to characterize the grown-in thermal stress [8,9]. To further characterize the crystallization quality, high-resolution X-ray diffraction (HRXRD) measurement of 121 points with a step size of 15 mm across the 8 inch substrate was carried out, the full width at half maximum (FWHM) mapping of (004) diffraction rocking curve was exhibited.

Results and Discussion

To understand the correlation between the grown-in thermal stress and RTG during continuous diameter expansion processes, simulations are carried out in SiC crystal growth models with different SiC crystal diameters. Identical thermal field and crystal growth chamber structures for SiC diameter-expansion are used in the simulation processes in order to fix the crystal diameter as the single variable. As the calculated data shown in Fig. 1, the obtained RTG keeps decreasing from 0.24°C/mm to 0.05 °C/mm as the diameter increases from 75 mm to 200 mm, which indicates the lateral growth driving force diminishes when the crystal diameter grows larger. Meanwhile, the grown-in thermal stress in the crystal keeps increasing with the enlarged SiC crystal diameter. The results in Fig. 1 clearly shows that the crystal diameter expansion will become more and more difficult as the SiC crystal diameter increases, which is caused by the decreased RTG and increased grown-in thermal stress in crystal. Therefore, it is necessary to design different growth chamber structures and RTG when crystal diameter expands to certain size in order to balance the thermal stress and lateral growth driving force.

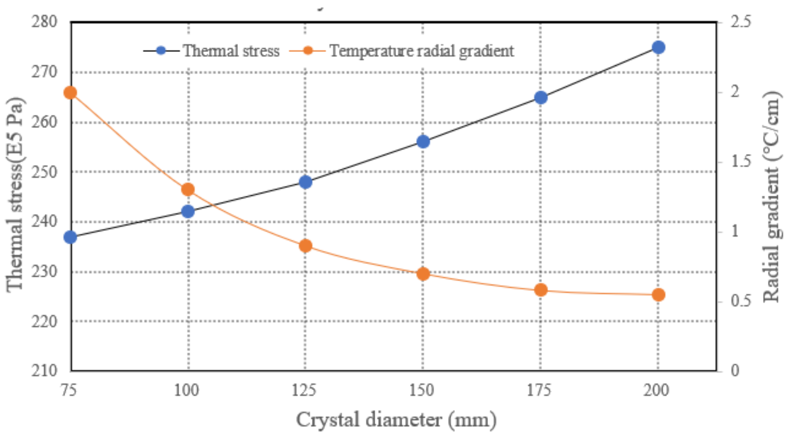

Fig. 1 Calculated correlation of the radial temperature gradient and residual thermal stress in SiC crystals with varied diameter.

In Fig. 2(a), a deduced RTG value of 0.10-0.12 °C/mm is demonstrated based on simulation and experimental results, which is considered to be the most optimized zone for high-quality crystal diameter expansion. As shown in Fig. 2(b), a smaller RTG value below 0.10 °C/mm cannot provide enough lateral growth driving force, which results in polycrystal deposition around the periphery of the crystal. When a RTG value larger than 0.12 °C/mm is applied, single crystal lateral growth can be achieved. However, the grown-in thermal stress in the crystal is also increased due to the larger RTG value, resulting in macro defect formation or even crystal cracking. To balance the crystal lateral driving force and grown-in thermal stress, the radial temperature distribution should be carefully designed. It is proposed that, larger local temperature gradient should be exerted on the crystal periphery to support the lateral growth, while smaller radial gradient should be kept in the central region of the crystal to reduce thermal stress. Moreover, the SiC crystal diameter expansion process is a combination of temperature gradient and growth chamber structure, such as the tilt (expansion angle) of the graphite ring in which crystal grows. The expansion angle is usually set at 10° to 45°, even bigger angle requires larger temperature gradient, which may lead to polycrystal deposition or crystal cracking problem.

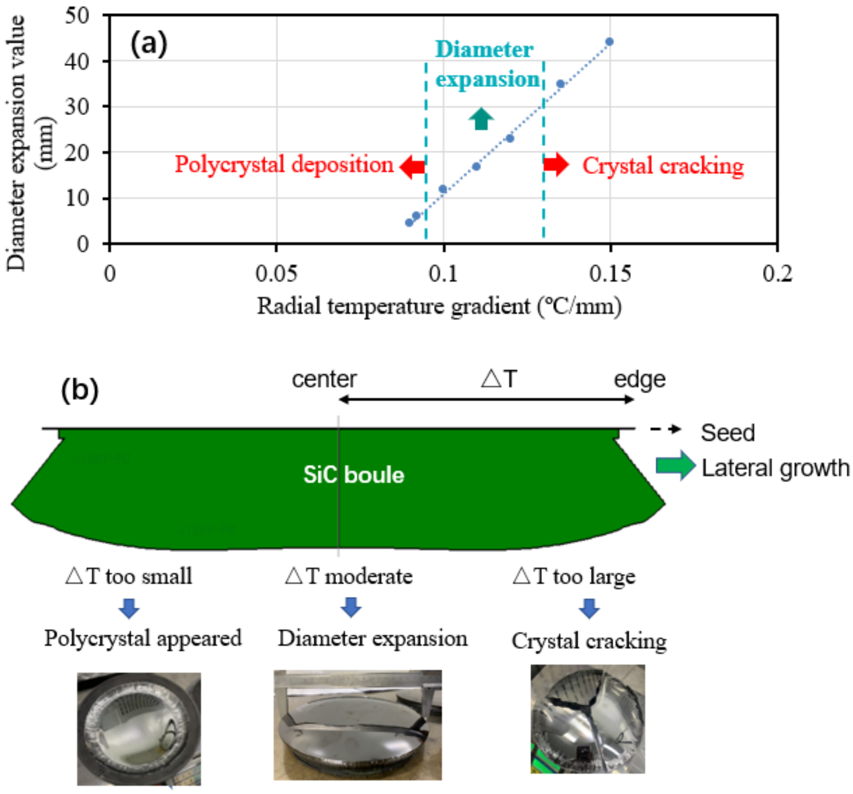

Fig. 2 (a) Calculated radial temperature gradient for 8 inch SiC crystal diameter expansion; (b) Schematic diagram of crystal diameter expansion and corresponding crystal results with different RTG.

On the basis of the above discussion, RTG value is set among 0.10-0.12 °C/mm for different-sized SiC crystal growth processes. The diameter expansion angle and related growth structure is optimized accordingly. After several runs of crystal diameter expansion processes, 8 inch SiC crystal is achieved starting from 6 inch seed substrates, as shown in Fig. 3(a). The quality optimization process of the obtained SiC substrates is also shown in Fig. 3(b). The typical polarizer images of the 8 inch SiC substrates indicate that local stress mainly aggregates around the periphery of the substrate. This is usually caused by macro defects in the peripheral zone where RTG is mostly exerted. With the optimized temperature distribution and growth process, the crystal quality can be much improved and local stress can be eliminated.

Considering the crystal diameter increase during an equivalent-diameter crystal growth process is much smaller than that in diameter expansion process, the RTG can be set at a relatively small value across the whole growth surface in order to minimize the thermal stress in the crystal. Furthermore, the expansion angle for crystal growth can also be designed according to the expected crystal diameter to minimize the space of polycrystal deposition.

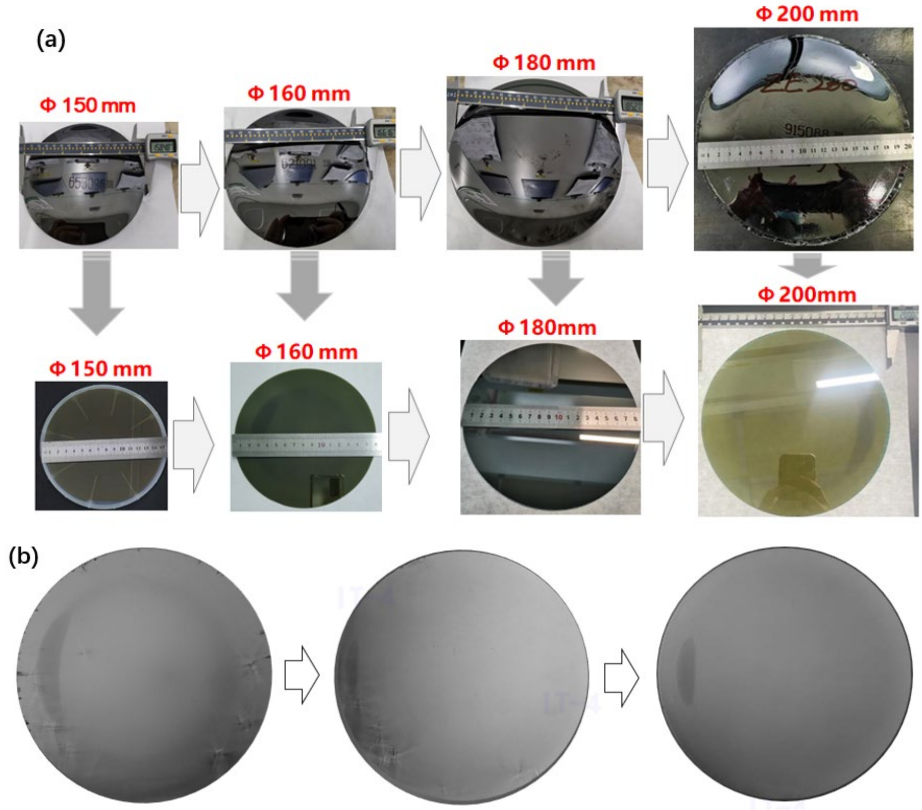

Fig. 3 (a) Diameter expansion process from 6 inch SiC seed substrate to 8 inch SiC substrate; (b) Polarizer images of 8 inch seed substrates quality improvement process.

Fig. 4 shows the 8 inch 4H-SiC ingot and substrates obtained from 8 inch SiC seed substrates. It can be seen that the thickness of the ingot is over 30 mm. The substrates are well polished to 500 μm thickness according to SEMI standard. The bow values of the substrates are around 5 μm which indicates no huge residual thermal stress exists in the as-grown 8 inch SiC crystal. Fig.5(a) demonstrates the Raman mapping characterization results. The red color in the left figure represents that the whole substrate is 100% 4H polytype without 6H or 15R inclusions. Raman spectra of nine points (A to I as labeled in the left figure) are selected to show the peak shift. It's known that the FTO(2/4)E2 peak shift of planar mode phonon in (0001) surface is among 776 cm^{-1} to 777 cm^{-1}, local stress introduced by non-uniform temperature distribution or macro defects in the lattice will lead to peak shift to low or high frequency side in accordance to the tensile or compressive strain [9]. The data plotted in Fig. 5 shows clearly that the FTO(2/4) peak is 776.5 cm^{-1}, indicating the lattice strain of the as-grown crystal is quite small. Fig. 5(b) further shows the XRD measurement result of the substrate. It's known that FWHM value of the (004) diffraction rocking curve is not only influenced by the strain in SiC crystal, but also the lattice defects such as dislocations. Local high density of dislocations will result in diffraction peak broadening or even multi peaks in the XRD spectra. We selected 121 points with a step size of 15 mm across the substrates and measured the FWHM values of the (004) diffraction peaks. Results show that almost all tested points have FWHM values smaller than 30 arcsec except for certain points in the periphery of the substrate, demonstrating good crystallization quality of the 8 inch 4H-SiC substrates. The slight difference between the periphery area and central area is attributed to the dislocation distribution. It's well understood that crystal edge is inclined to have more defects due to stress and defect aggregation, which is caused by larger temperature gradient and misfit with the graphite parts.

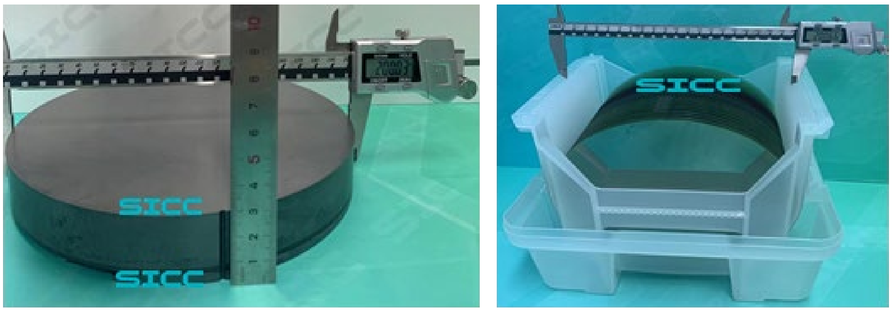

Fig. 4 8 inch 4H-SiC ingot and polished substrates obtained from self-enlarged 8 inch 4H-SiC seeds.

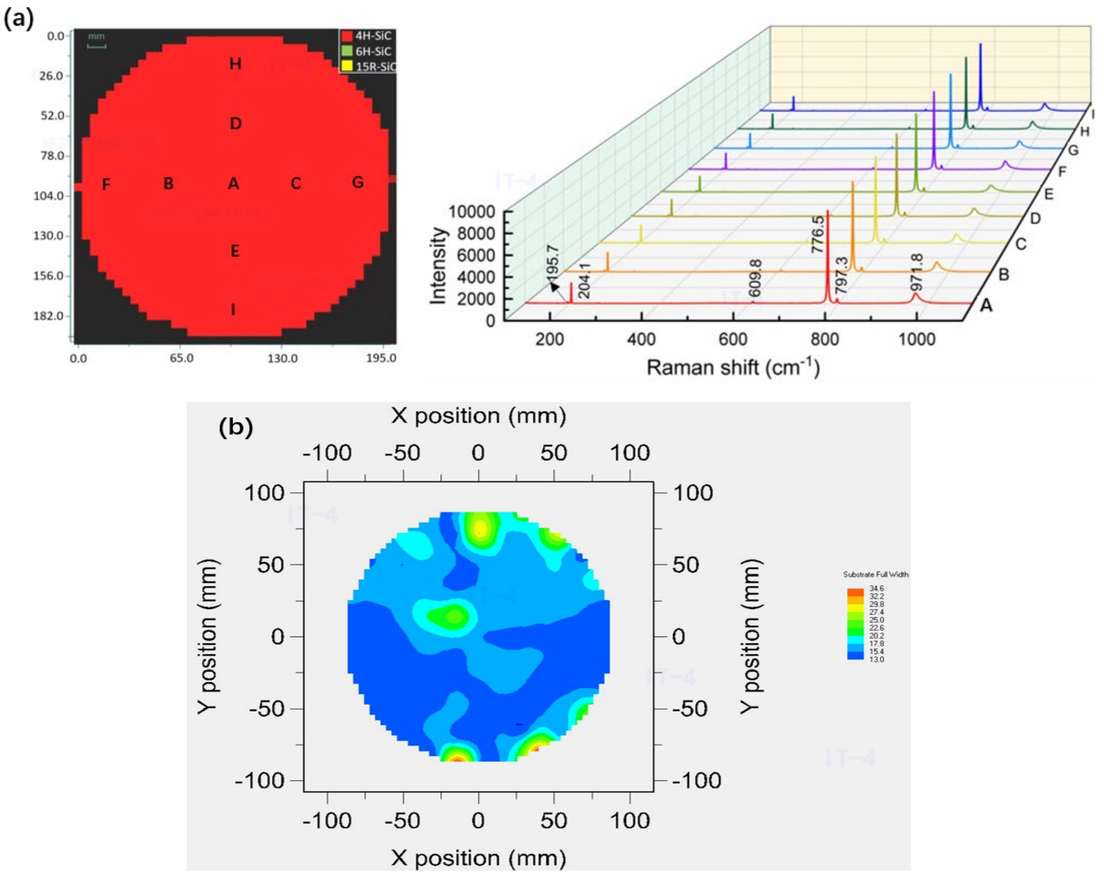

Fig.5 (a) Raman characterization of the 8 inch SiC substrates, the left figure shows the mapping data and the right figure shows the spetrca of typical points in the substrate; (b) FWHM maps of the (004) diffraction peak across an 8 inch SiC substrate measured by HRXRD equipment.

Summary

The diameter expansion process from 6 inch to 8 inch SiC crystal is demonstrated and the following obtained 8 inch 4H-SiC substrate quality is characterized. It's demonstrated that a key factor in achieving high quality diameter-expanded SiC crystal is the design of RTG which is deduced to be reasonable in the range of 0.10-0.12 °C/mm. With the 8 inch SiC seed substrate and optimized temperature gradient, residual thermal stress in the 8 inch 4H-SiC crystal is minimized and high quality 8 inch 4H-SiC substrates are achieved.

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