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Growth of 8-Inch SiC Single Crystals with Low Basal Plane Dislocation Density

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Abstract. Silicon Carbide (SiC) is a pivotal wide-bandgap semiconductor for high-power and high-frequency electronics. However, crystalline defects, particularly Basal Plane Dislocations (BPDs), severely degrade the performance and reliability of bipolar devices by nucleating stacking faults that cause fatal forward voltage drift. This work presents the successful growth of 8-inch, 4° off-axis, n-type 4H-SiC single crystals with significantly reduced BPD density via the Physical Vapor Transport (PVT) method using an improved reactor design. The key innovation involves replacing traditional graphite components with single or polycrystalline SiC for the seed holder and guide tube, subsequently coated with a thin (10 µm) tantalum carbide (TaC) film. This design ensures thermal expansion coefficient matching and reduces thermal radiation emissivity. Etch pit density analysis revealed that the improved design reduced the overall BPD density from over 1027 cm^{-2} to a remarkably low 78 cm^{-2}. Furthermore, it drastically improved the radial uniformity of BPD distribution by stabilizing the thermal gradient and suppressing parasitic polycrystalline nucleation, marking a critical advancement towards high-yield production of high-quality, large-diameter SiC substrates.

Introduction

The relentless pursuit of greater energy efficiency and miniaturization in power electronics has propelled the adoption of wide-bandgap semiconductors, among which SiC stands as a cornerstone material. Its superior properties, including a wide band gap (~3.26 eV for 4H-SiC), high thermal conductivity (~4.9 W/cm·K), exceptionally high electric breakdown field (~3 MV/cm), and large saturated electron drift velocity, enable devices to operate at higher temperatures, voltages, and switching frequencies with lower losses than traditional silicon-based devices [1,2]. These characteristics make SiC indispensable for a new generation of power converters, electric vehicle powertrains, and renewable energy systems.

However, the performance and reliability of SiC-based devices, particularly bipolar devices like PiN diodes and Insulated Gate Bipolar Transistors (IGBTs), are critically sensitive to crystalline imperfections in the substrate. Among these defects, Basal Plane Dislocations (BPDs) are notoriously detrimental. While a significant portion (>90%) of BPDs from the substrate can be converted into less harmful Threading Edge Dislocations (TEDs) in the initial epitaxial layer, the remaining BPDs pose a severe threat [3]. A perfect BPD in the hexagonal SiC crystal structure can readily dissociate into two partial dislocations, with a single Shockley-type stacking fault (SF) forming between them [4]. Under the injection of charge carriers during device operation, these stacking faults can nucleate and expand, leading to a progressive increase in the forward voltage drop (V_f drift), ultimately causing device failure [5].

The formation and distribution of BPDs during bulk crystal growth are heavily influenced by the thermo-mechanical environment within the PVT furnace. Non-uniform temperature gradients, thermal stress induced by mismatched coefficients of thermal expansion (CTE) between the crystal and crucible components, and parasitic nucleation can all promote BPD generation and clustering, especially at the crystal's periphery. Therefore, controlling the thermal field is paramount to reducing BPD density and improving its uniformity. This study addresses this challenge by introducing a novel reactor design that fundamentally alters the thermal and chemical environment, enabling the growth of 8-inch SiC crystals with record-low and highly uniform BPD densities, a vital step towards unlocking the full potential of SiC power devices.

The Critical Challenge of BPDs

To fully appreciate the significance of this work, one must understand the nature of the BPD problem. BPDs are line defects whose Burgers vector lies in the {0001} basal plane of the 4H-SiC crystal structure. Their danger lies not in their existence as perfect dislocations in the substrate, but in their behavior during device fabrication and operation. During the epitaxial or bulk growth process, the high temperatures can cause a perfect BPD (with a Burgers vector of 1/3<11-20>) to dissociate into two partial dislocations (e.g., 1/3<10-10> and 1/3<01-10>), creating a stacking fault ribbon in between [6]. This is a metastable configuration. When a bipolar device is forward-biased, electron-hole pair recombination provides the energy necessary for these partials to move, expanding the stacking fault area. This expanding fault acts as a carrier recombination center, reducing minority carrier lifetime and increasing the series resistance of the device, manifesting as the well-documented V_f drift [5]. This degradation is irreversible and fatal to the device's long-term reliability.

Consequently, the target for high-performance, high-reliability bipolar devices is a substrate with a BPD density as close to zero as possible. The industry standard, often achieved through various in-situ or ex-situ conversion techniques during epitaxy, is to reduce BPDs in the epilayer to below 0.1 cm^{-2}. However, this process is far more effective if the starting substrate has a low and uniform BPD density to begin with. Eliminating the problem at its source—the bulk crystal growth stage—is the most robust and economically viable strategy for high-yield manufacturing.

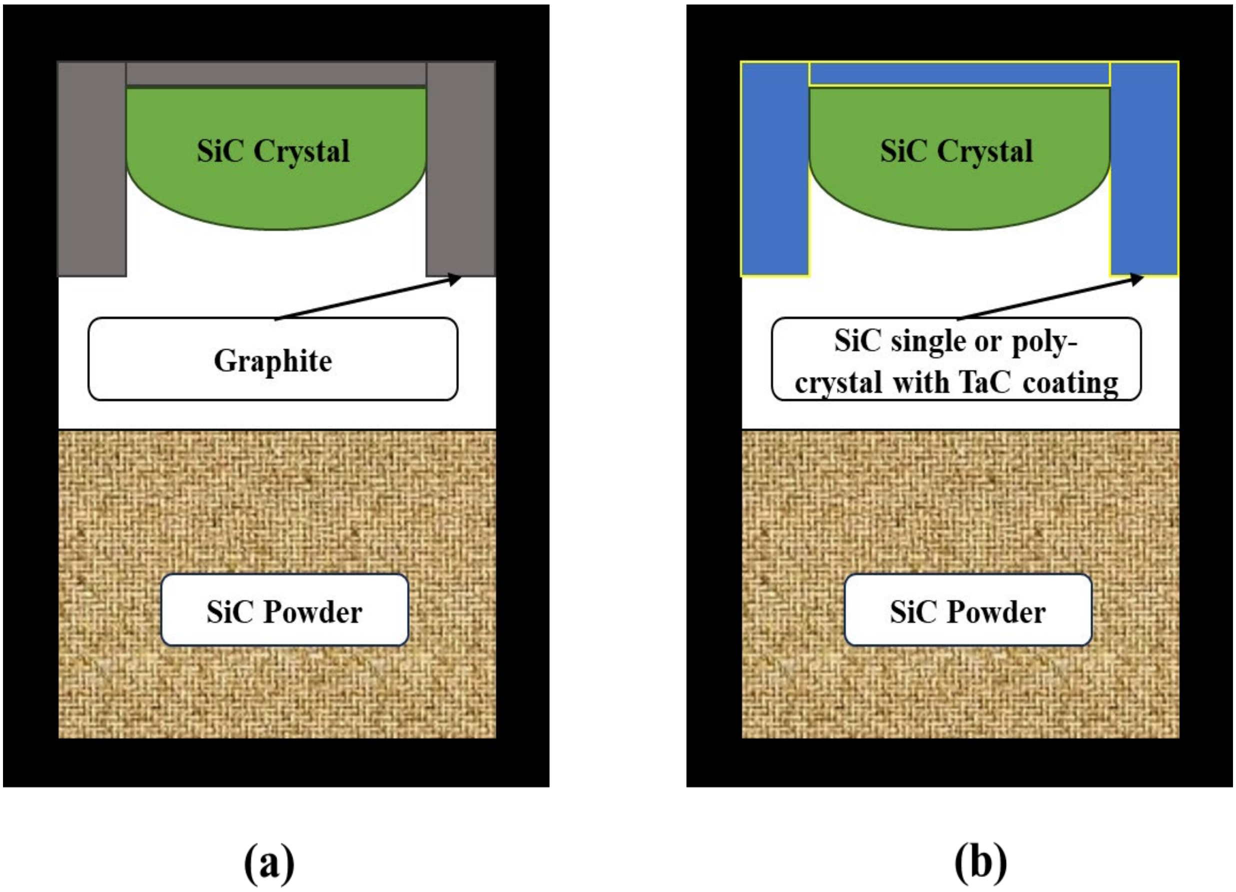


Fig. 1. The schematic diagrams of (a) traditional design and (b) improved design.

Experimental Setup: Traditional vs. Improved Design

The bulk growth of 4H-SiC single crystals is predominantly conducted using the PVT method. In a typical PVT setup, a polycrystalline SiC source is sublimated at high temperatures (>2200°C) in a sealed graphite crucible. The resulting vapor species are transported to a cooler seed crystal, where they condense and form a single-crystal boule.

The experimental work presented here involved a direct comparison between two crucible designs: Traditional Design (Fig. 1a): This configuration utilized a seed holder and a surrounding guide tube fabricated from high-purity graphite. Improved Design (Fig. 1b): This novel configuration replaced the graphite components with parts machined from solid polycrystalline SiC or high-purity single-crystal SiC (N-doping concentration:4.0-12.0E+19 atoms·cm^{-3}). Critically, these SiC-based components were then uniformly coated with a ~10 µm thick film of TaC via a CVD process. Using both designs, 8-inch, n-type, 4° off-axis 4H-SiC single crystals were grown under otherwise identical process conditions (temperature, pressure, growth rate) to ensure a fair comparison. The SiC single crystal grown through improved design are shown in Fig. 2a. After cutting, grinding and polishing, a 200mm SiC wafer was obtained (Fig. 2b).

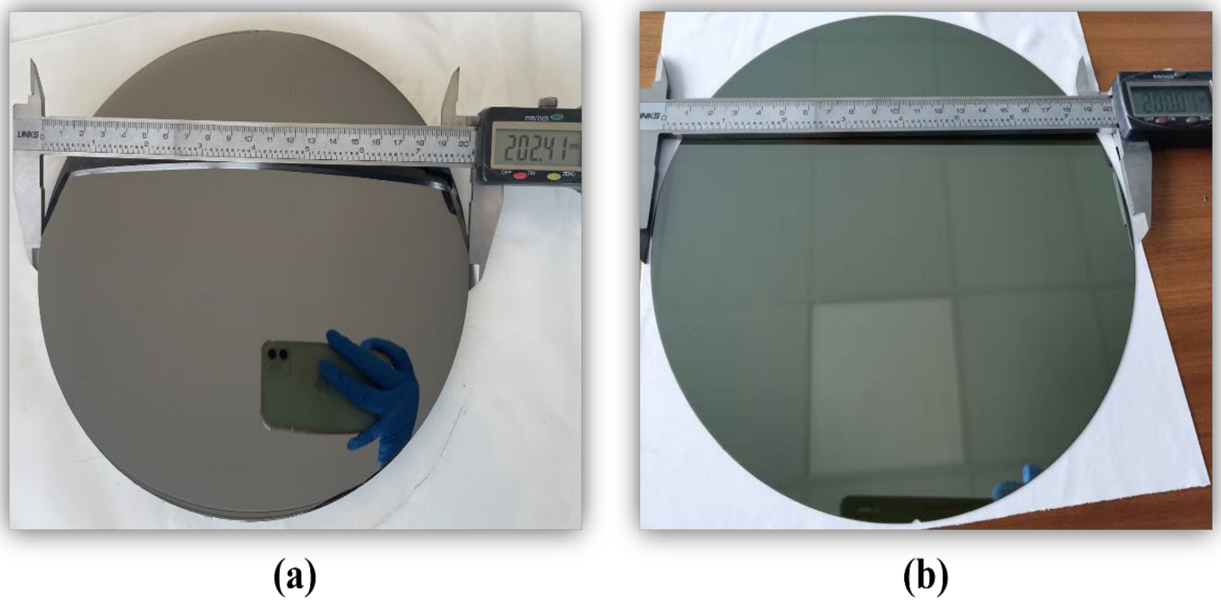
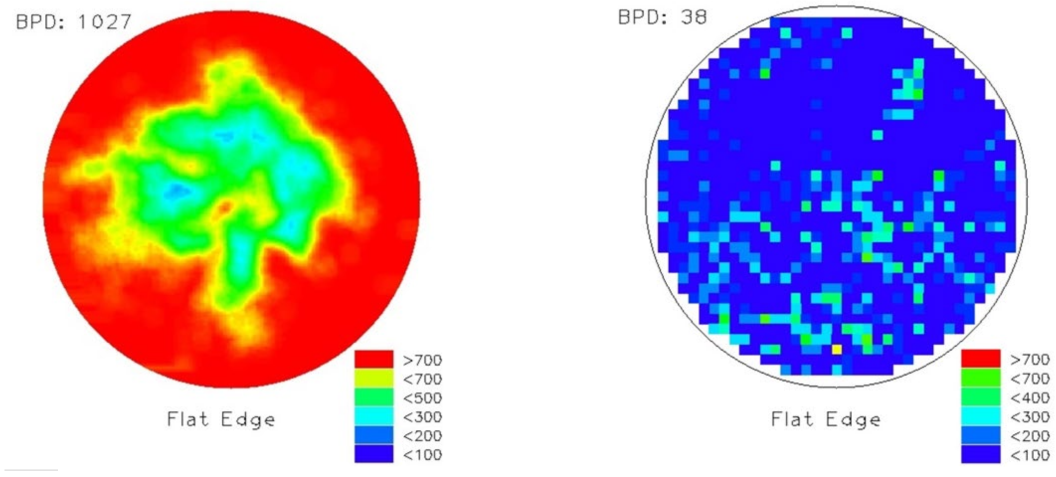


Fig. 2. The Photos of (a) SiC crystal grown through improved design and (b) processed SiC wafer.

Defect Characterization Methodology

To quantify and visualize the BPD density in the grown crystals, standard wet chemical etching was employed. Wafers sliced from the grown boules were subjected to molten Potassium Hydroxide (KOH) at a temperature of approximately 500°C for several minutes. KOH etches the SiC crystal at a much higher rate at dislocation sites than in the perfect crystal, creating characteristic hexagonal etch pits that correspond to the locations of Threading Screw Dislocations (TSDs) and oval-shaped pits that correspond to BPDs.

The etched surfaces were then analyzed using the FabXLab optical microscope equipped with automated image recognition software. This system scans the wafer surface, identifies and classifies the etch pits based on their morphology and size, and calculates their areal density (cm^{-2}), providing a precise and statistically robust map of defect distribution across the entire wafer.



(a) (b)

Fig. 3. The distribution of BPDs density in SiC crystal grown in (a) traditional design and (b) improved design.

Results: Dramatic Reduction in BPD Density

The results of the etch pit density (EPD) mapping were striking and unequivocal. Crystal from Traditional Design (Fig. 3a): The BPD density was measured to be as high as 1027 cm^{-2}. More importantly, the distribution was highly non-uniform. The edge of the wafer showed a very high density of BPDs, forming a pronounced ring-of-fire pattern. While the central region exhibited a moderately lower density. This radial gradient is a classic signature of thermo-mechanical stress-induced defect generation.
Crystal from Improved Design (Fig. 3b): Conversely, the improved design yielded crystals with a markedly lower BPD density, averaging only 78 cm^{-2}. This represents a reduction of more than an order of magnitude and a significantly more uniform radial distribution. The extreme clustering at the edge was eliminated, resulting in a wafer with consistent low defect density from center to edge.

Mechanism: The Role of Thermal Management and CTE Matching

The dramatic improvement in crystal quality can be attributed to the superior thermal and mechanical properties of the new crucible components.

Problems with the Traditional Graphite Design

Coefficient of Thermal Expansion (CTE) Mismatch: Graphite has a CTE of ~4-6 x 10^{-6} /K (in-plane), while 4H-SiC has a CTE of ~4.2 x 10^{-6} /K along the a-axis and ~4.7 x 10^{-6} /K along the c-axis. While these values seem close, any slight mismatch, combined with the extreme temperature gradients (often 5-20°C/cm) during growth and cool-down, generates significant shear stress at the interface between the crystal and the holder. This stress is a primary driver for the nucleation and propagation of dislocations, particularly at the vulnerable edge of the growing crystal.
High Thermal Emissivity and Conductivity: Graphite has a high thermal radiation emissivity (0.7-0.8) and is a good thermal conductor. This leads to two issues: Firstly, it creates a steeper and potentially unstable lateral temperature gradient ($\partial^2 T/\partial x^2$) at the crystal's periphery. Secondly, it causes excessive heat loss through the walls, cooling the inner surface of the guide tube. This cooling promotes the unwanted condensation and parasitic nucleation of SiC polycrystals on the graphite surface. These parasitic crystals disrupt the vapor flow, create local hot spots, and further distort the thermal field, exacerbating the non-uniform stress and BPD formation at the crystal edge.

Advantages of the Improved SiC/TaC Design

Perfect CTE Matching: By manufacturing the seed holder and guide tube from SiC (either poly or single crystal), their thermal expansion is perfectly synchronized with that of the growing SiC boule. This eliminates the interfacial shear stress caused by CTE mismatch during temperature changes, providing a much more stable and mechanically benign environment for crystal growth.

Low Emissivity TaC Coating: TaC is a refractory ceramic with a very low thermal radiation emissivity of approximately 0.3. This coating acts as a thermal barrier. It reduces radial heat loss from the crystal and crucible assembly, leading to a flatter, more stable, and more axially symmetric thermal profile. A smaller second derivative of temperature ($\partial^2T/\partial x^2$) means reduced thermal stress.

Suppression of Parasitic Nucleation: The combination of a stable, hotter wall temperature (due to lower heat loss) and the chemical inertness of the TaC surface makes it extremely difficult for SiC vapor species to nucleate and form polycrystalline deposits on the guide tube. This maintains a clean, predictable vapor transport path and a consistent thermal field throughout the long growth process.

In essence, the improved design transforms the growth environment from one prone to fluctuations and steep gradients (traditional) to one that is stable, uniform, and minimally stressful (improved). This directly translates to a reduction in the driving force for dislocation generation and multiplication, yielding a crystal with far fewer defects and exceptional radial uniformity.

Summary

This study achieved a significant reduction in harmful BPDs in 8-inch 4H-SiC crystals by innovating the PVT reactor design. Traditional graphite components (seed holder and guide tube) were replaced with SiC-based parts coated with a thin TaC layer. This modification eliminated thermal expansion mismatch stress and stabilized the thermal gradient due to TaC's low emissivity, thereby suppressing parasitic nucleation. Results confirmed an order-of-magnitude reduction in average BPD density, from 1027 cm^{-2} to just 78 cm^{-2}, while drastically improving radial uniformity by eliminating edge-clustering defects. This work provides a highly effective method for producing high-quality, large-diameter substrates, directly addressing the major bottleneck for reliable SiC bipolar power devices and facilitating their broader industrial application.

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