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Ultra-Pure SiC Source Material for Optical SiC Crystal Growth

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Abstract. We report on the development and systematic validation of an ultra-pure silicon carbide (SiC) source material specifically engineered for physical vapor transport (PVT) growth of optical- and electronic-grade single crystals. The material is synthesized by chemical vapor deposition (CVD) using high-purity chlorosilane and methane precursors, yielding dense, void-free polycrystalline 3C-SiC with precise 1:1 stoichiometry. Over more than two years of continuous production, bulk metallic impurities across 17 monitored elements were consistently maintained below 100 parts per billion by weight (ppbw), with most batches achieving <50 ppbw. Surface metals, assessed after proprietary crushing and cleaning processes, were similarly controlled to <100 ppbw. Nitrogen levels, determined by secondary ion mass spectrometry (SIMS), remained stable in the low 10^{15} cm^{-3} range, enabling semi-insulating or precisely doped crystal growth. Purity and reproducibility were verified by a cross-technique analytical approach including glow discharge mass spectrometry (GDMS), and inductively coupled plasma mass spectrometry (ICP-MS). Microstructural investigations confirmed dense, void-free grains and high crystallographic uniformity. With production capacity scaling toward 60 tons per month, this CVD-based SiC source material establishes a robust platform for next-generation PVT growth. Its combination of ultra-low contamination, structural integrity, and scalable manufacturing positions it as a key enabler for optical SiC applications such as transparent wafers for augmented reality (AR) systems, as well as advanced power and RF devices.

Introduction

Silicon carbide (SiC) has become one of the most critical semiconductor materials for advanced applications in power electronics, radio frequency (RF) devices, and optical systems[1-3]. Its wide bandgap, high thermal conductivity, and mechanical robustness make it the preferred substrate for high-performance devices that must operate under extreme thermal and electrical conditions. Beyond traditional electronic applications, recent interest in transparent and semi-insulating SiC has opened new opportunities in optoelectronics and augmented reality (AR) systems, where crystal transparency and ultra-low contamination are essential requirements[4,5].

A fundamental prerequisite for high-quality SiC crystal growth is the availability of ultra-pure feedstock material[6-8]. Physical vapor transport (PVT) growth, the dominant industrial method for producing single-crystalline 4H- and 3C-SiC, is highly sensitive to the purity and stoichiometry of the source. Even trace amounts of metallic impurities, uncontrolled nitrogen incorporation, or residual free silicon and carbon can destabilize sublimation chemistry, increase defect density, and compromise device performance. Consequently, developing reliable and scalable SiC source materials with exceptionally low impurity levels has become a critical challenge for the industry.

Conventional polycrystalline SiC powders, often produced via carbothermal reduction, suffer from limitations in chemical purity, batch-to-batch reproducibility, and structural homogeneity. Alternative approaches, such as advanced chemical vapor deposition (CVD), have emerged as promising routes to engineer feedstock with controlled stoichiometry, dense microstructure, and minimal defect density. CVD-based processes further offer the potential for scalability and independence of supply-

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factors that are increasingly relevant as demand for SiC substrates accelerates across multiple industries.

In this work, we present the development and validation of a new CVD-derived SiC source material tailored for PVT growth of high-quality crystals. Using ultra-high-purity chlorosilane and methane precursors, we deposit dense, void-free polycrystalline 3C-SiC with precise atomic stoichiometry. Over a multi-year production period, we demonstrate outstanding reproducibility and impurity control, with bulk metallic concentrations consistently below 100 parts per billion by weight (ppbw) and nitrogen incorporation stabilized in the low 10^{15} cm^{-3} range. A multi-technique analytical strategy—including glow discharge mass spectrometry (GDMS), secondary ion mass spectrometry (SIMS), and inductively coupled plasma mass spectrometry (ICP-MS)—was employed to establish the reliability of impurity quantification and to validate surface cleaning processes.

The results confirm that this material platform provides one of the purest and most structurally uniform polycrystalline SiC feedstocks available today. Its reproducibility, combined with ongoing capacity expansion toward industrial-scale volumes, positions it as a robust and cost-effective enabler for next-generation optical SiC applications, as well as for advanced power and RF devices.

Materials and Methods

The production of the ultra-pure SiC source material was carried out in a former CVD silicon facility located within the chemical infrastructure of Chemiepark Bitterfeld, Germany. The complete process flow, comprising CVD synthesis, comminution, surface treatment, and packaging, is illustrated in Figure 1.

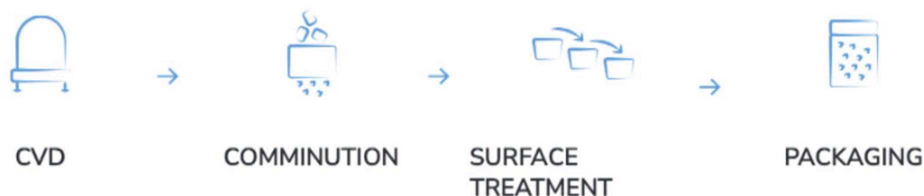

Fig. 1. Process steps for the production of ultra-pur SiC source material.

CVD Synthesis

The SiC source material was produced by chemical vapor deposition (CVD) using ultra-high purity chlorosilane and methane as precursors. The process yields dense, void-free polycrystalline 3C-SiC layers with precise 1:1 Si to C stoichiometry, free of elemental silicon or carbon inclusions. The deposition was carried out under tightly controlled conditions in a dedicated CVD facility in Germany, ensuring reproducibility and scalability across extended production campaigns[6-8].

Comminution

Following deposition, the bulk polycrystalline SiC blocks were subjected to a comminution step. Mechanical crushing and milling were optimized to preserve microstructural integrity while achieving controlled particle size distributions. Tailored particle sizes ranging from 0.5 to 15 mm were produced, with bulk densities up to 1.9 g/cm^3. This flexibility allows the feedstock to be adapted to diverse PVT loading strategies and crystal growth systems.

Surface Treatment

To remove any residual surface contamination introduced during comminution, a proprietary surface treatment protocol was applied. This included multi-stage acid leaching designed to dissolve trace metallic residues without altering the SiC bulk. Surface analysis confirmed that metallic contamination after treatment remained consistently below 100 ppbw.

Packaging

Finally, the purified SiC granules were packaged in contamination-controlled environments to ensure preservation of purity during storage and shipping. The packaging design minimizes environmental exposure and enables reliable long-distance transport for both industrial and research use.

Analytics and Characterization

To rigorously validate the purity and structural quality of the SiC source material, a multi-technique analytical strategy was implemented. This cross-validation approach ensured high confidence in both bulk and surface measurements and minimized the risk of systematic error from any single method.

Bulk Impurity Analysis

Used to quantify metallic impurities within the bulk polycrystalline SiC Glow Discharge Mass Spectrometry (GDMS) offered high sensitivity, with detection limits in the low parts-per-billion by weight (ppbw) range[9]. Here we were able to optimize the characterization process and sample preparation to achieve detection limits in the single digit ppbw (parts per billion weight) region. Across more than two years of production, all 17 monitored elements were consistently maintained below 100 ppbw, with most batches showing <50 ppbw (see figure 2).

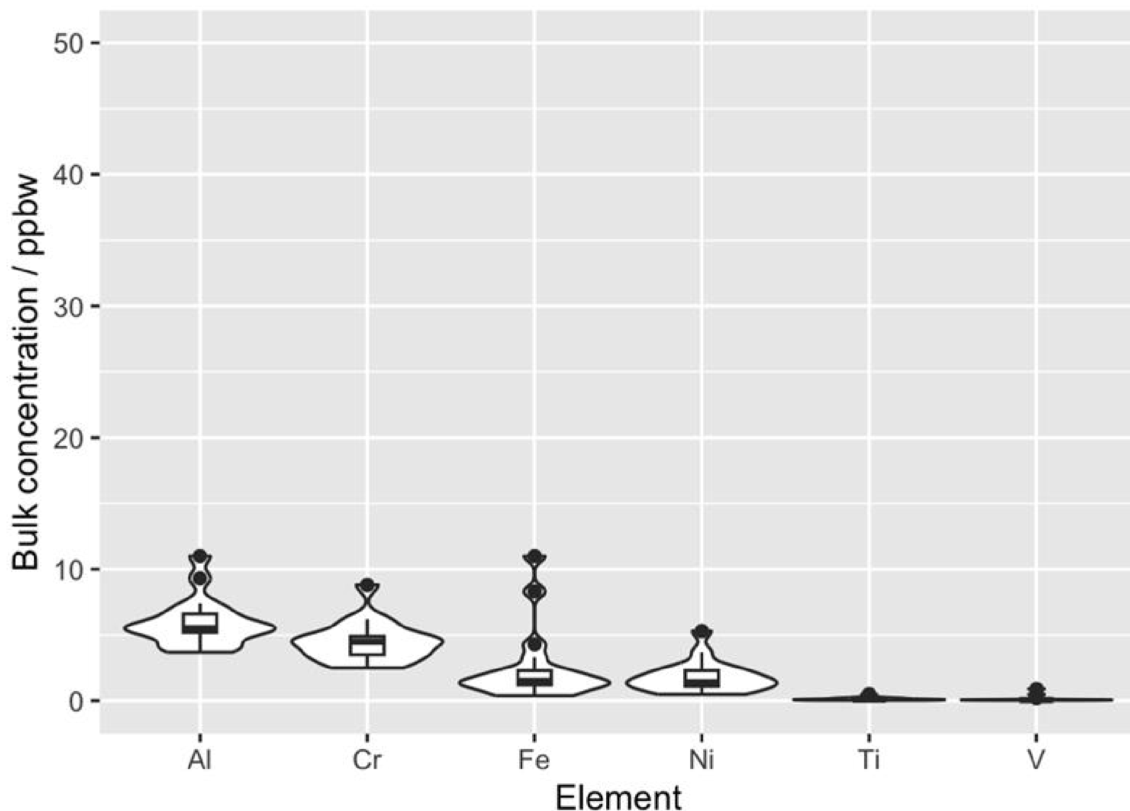

Fig. 2. Bulk concentration for selected elements of concern in ppbw (parts per billion weight) shown in boxplots over the last 12 months.

Nitrogen Incorporation

High-sensitivity Secondary Ion Mass Spectrometry (SIMS) was used to quantify nitrogen concentrations[10], which remained in the low 10^{15} cm^{-3} range. In figure 3 a production chart is given to show the consistency of the incorporation level over time (please note that 30 ppba correspond to $2.9*10^{15}$ atoms/cm^3). This enables both semi-insulating material growth and controlled doping strategies for device applications.

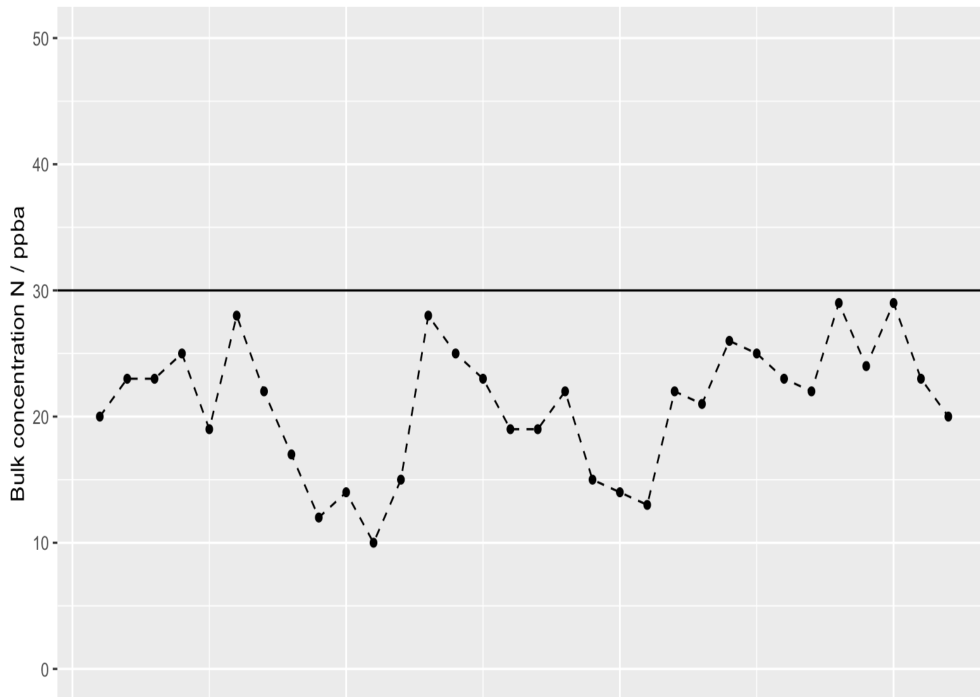

Fig. 3. Nitrogen concentration in ppba (parts per billion atoms) < 30 ppba corresponding to $2.9*10^{15}$ atoms/cm^3.

Surface Purity Determination

We applied inductively coupled plasma mass spectrometry (ICP-MS) to quantify residual surface contamination following the proprietary cleaning process[11-13]. Prior to analysis, hot acid leaching was employed to dissolve trace residues from the SiC surface. The completeness of this procedure was verified through successive leaching steps, which showed no detectable contamination (i.e., below the instrument detection limit), confirming the effectiveness of the initial treatment. Across all batches, the combined concentration of surface metals remained consistently below 100 ppbw (see Figure 4). Through a combination of optimized sample preparation and refined analytical methodology, absolute detection limits below 1 ppbw were achieved for all elements of concern.

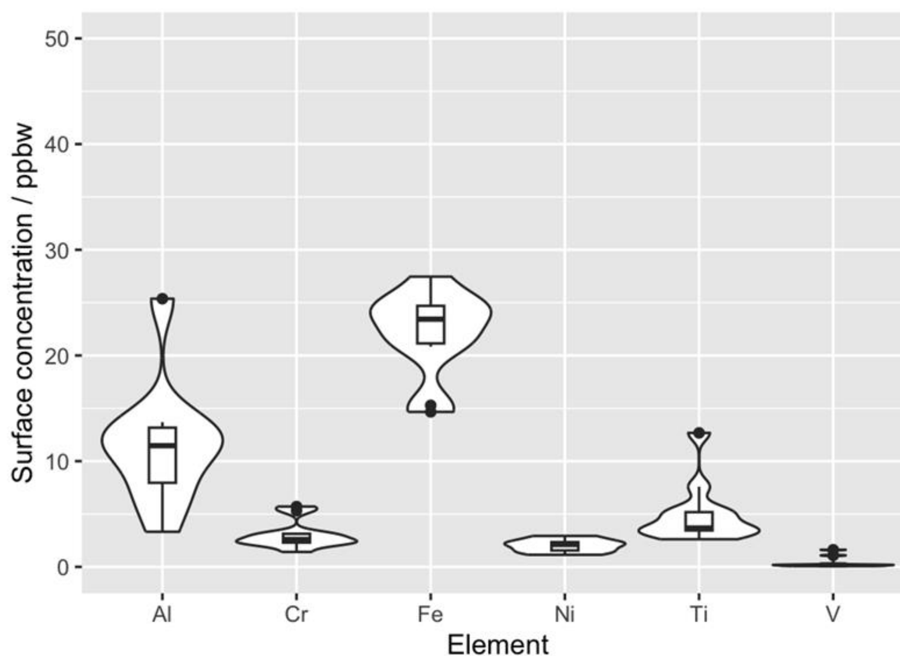

Fig. 4. Surface concentration for selected elements of concern in ppbw (parts per billion weight) shown in boxplots over the last 12 months.

Structural and Stoichiometric Analysis

The High-Resolution Scanning Electron Microscopy (HRSEM) revealed dense, void-free microstructures with average grain sizes of ~50 µm (see figure 5). The analysis was provided by the Fraunhofer IKTS in Dresden, Germany.

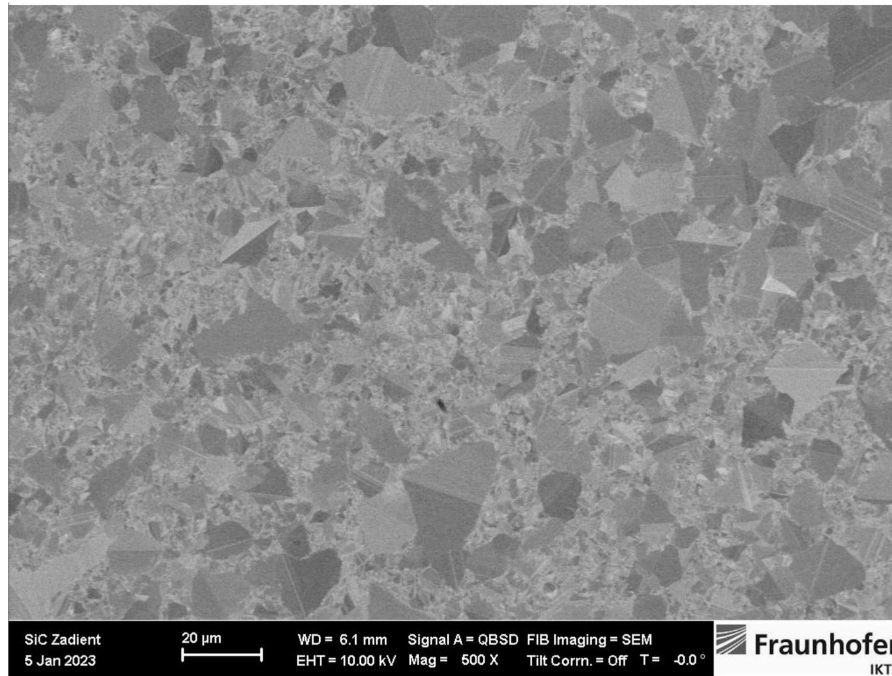

Fig. 5. High resolution TEM image of the polycrystalline SiC structure.

The crystalline structure of the material was analyzed by X-ray diffraction (XRD). The resulting diffraction pattern confirmed the presence of a single polycrystalline 3C-SiC phase, with no detectable secondary phases. The slight broadening of the dominant diffraction peak at 35.4° is attributed to the limited grain size and the associated grain boundary effects. Notably, the typical side peaks characteristic of 4H- and 6H-SiC polytypes—appearing around 38° and below 35°—were completely absent. Furthermore, the peak observed at 41.3° is uniquely consistent with the 3C polytype and does not occur in 4H or 6H samples, reinforcing the phase purity of the deposited material[14-17].

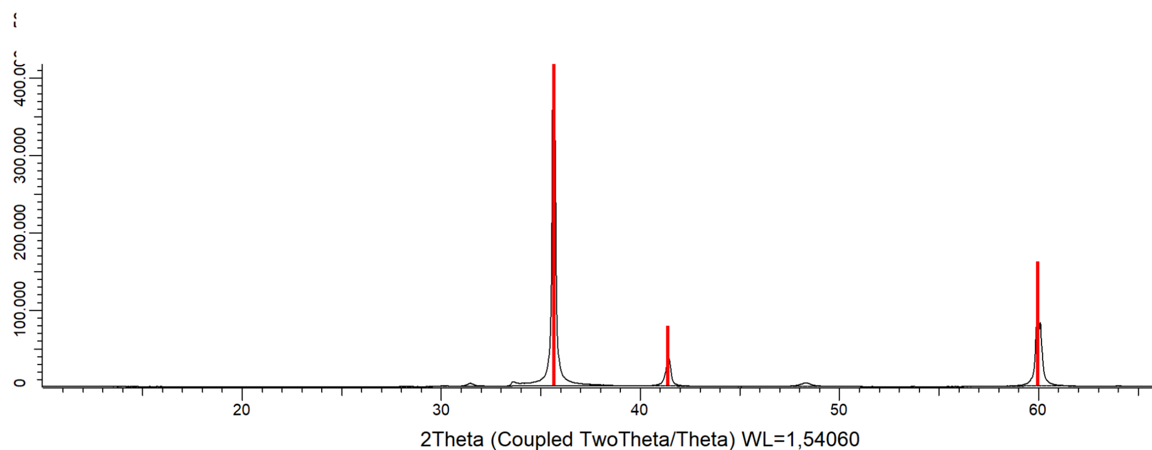

Fig. 6. XRD scan confirming the 3C structure of the polycrystalline SiC.

The precise 1:1 Si:C atomic ratio was confirmed by the exclusion of excess silicon and carbon within the material. Excess silicon was investigated using XRD on finely powdered samples, which would reveal any residual elemental silicon on the surface. However, it should be noted that the detection limit of this method remains relatively high, in the range of 100–500 ppmw, leaving room

for further sensitivity improvements. Excess carbon was assessed by combustion analysis, which did not indicate any detectable carbon inclusions above the method's detection threshold. Similar to silicon, the current detection limit for free carbon lies in the ~500 ppmw range, highlighting the need for enhanced analytical resolution in future studies.

Summary

This work demonstrates that chemical vapor deposition (CVD) is the most effective route to produce ultra-pure silicon carbide (SiC) source material for physical vapor transport (PVT) growth. Unlike conventional synthesis methods, CVD enables precise control over stoichiometry, microstructure, and impurity levels, resulting in dense, void-free 3C-SiC with reproducible properties across multiple production batches.

Extensive characterization is essential to optimize the production process and to ensure reproducibility. A multi-technique analytical framework, combining GDMS, SIMS, ICP-MS, SEM, and XRD, provides the resolution and confidence required to confirm trace-level purity and structural integrity. This systematic validation not only guarantees the material's suitability for advanced optical and electronic applications but also builds a robust foundation for further process optimization.

Finally, CVD offers a straightforward and scalable path to mass production. With demonstrated long-term reproducibility and ongoing capacity expansion, the technology is positioned to support industrial-scale volumes while maintaining the highest levels of purity. This makes CVD-derived SiC source material a reliable and future-proof enabler for next-generation applications ranging from augmented reality optics to high-performance power and RF devices.

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