

博士学位论文

单晶碳化硅基片磨削表面材料去除与损伤 机理及高效高表面质量磨削工艺研究

**Material Removal and Damage Mechanisms of Grinding
and High-Efficiency, High-Surface-Quality Grinding
Process for Single-Crystal Silicon Carbide Substrates**

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摘 要

第三代宽禁带半导体材料单晶碳化硅（SiC）具有高临界击穿电场强度、高热导率、高载流子饱和迁移速度以及耐高温等优异物理特性，是制造高压、高频、高功率器件的理想衬底材料。器件级单晶碳化硅基片在晶体生长之后，需经过切割、平整化加工、化学机械抛光等加工技术获得高面形精度超光滑表面。平整化加工是实现碳化硅基片高质高效加工的关键技术，6 英寸及以下的单晶碳化硅基片的平整化加工通常采用游离磨料研磨工艺。随着单晶碳化硅生长技术的不断进步，8 英寸及以上大尺寸单晶碳化硅基片平整化加工技术的需求愈发紧迫，利用游离磨料研磨加工大尺寸单晶碳化硅基片时，面临效率低、损伤大、成本高等问题。相比之下，基于工件旋转原理的超精密磨削技术因其加工半导体基片的效率高、面形精度与表面损伤易控制等优点，已在大尺寸硅片平整化加工中得到应用。但在单晶碳化硅基片加工中，面临磨削表面材料去除机理与损伤演化机制尚未完全揭示、表面粗糙度和亚表面损伤深度调控方法尚未建立、兼顾加工效率与表面质量的磨削工艺参数优化方法尚未提出等问题，这些问题制约了碳化硅基片平整化高质高效磨削加工的实现。为此，本文针围绕单晶碳化硅基片磨削表面材料去除机理、亚表面损伤形成与演化机理、表面粗糙度和亚表面损伤深度预测方法和高效高表面质量磨削工艺，开展了系统的研究，具体研究内容和主要结论如下：

（1）研究了单晶碳化硅磨削表面材料去除机理。通过纳米压痕、单磨粒变载荷划擦及金刚石砂轮超精密磨削试验，系统对比单晶碳化硅 C 面与 Si 面的力学特性及表面形貌特征和材料去除机理。纳米压痕结果表明，C 面硬度和弹性模量高于 Si 面，而 Si 面断裂韧性更大。划擦试验表明，尽管两者均随载荷增加由延性转向脆性去除，但 C 面弹性恢复率更低且更早进入脆性阶段。在延性去除阶段，C 面划痕两侧产生大量塑性切屑，而 Si 面未产生切屑，进入脆性阶段后，两者均产生脆性切屑和脆性坑，但 Si 面密度更高。超精密磨削结果表明，两晶面均随磨粒粒径减小由延性向脆性磨削转变，但 C 面的表面粗糙度和脆性坑密度更低、延脆转变临界切深更小。综合分析认为，两晶面去除机理差异源于本征力学性能差异，C 面较高的硬度和弹性模量导致延脆转变临界切深更小，促使材料更早发生脆性去除，而 Si 面较高的断裂韧性和弹性恢复率有助于维持延性去除状态，但在脆性断裂时释放的弹性能更强，诱发更严重的表面损伤。

（2）研究了单晶碳化硅磨削亚表面损伤形成机理与演化规律。通过单磨粒变载荷划擦试验、金刚石砂轮超精密磨削试验以及分子动力学仿真的多尺度研究方法，揭示了单晶碳化硅磨削亚表面损伤的跨尺度演化机制。划擦与磨削试验结果共同表明，C 面和 Si 面损伤分布规律一致，在延性去除阶段以非晶化、位错与滑移带等塑性变形为主，

最大损伤深度由滑移带决定，进入脆性去除阶段后，亚表面损伤在滑移带尖端处进一步扩展并形成微裂纹，此时最大损伤深度由裂纹决定。分子动力学仿真结果验证了上述损伤分布规律，并揭示了不同阶段的损伤机理。在塑性变形阶段，磨粒剪切作用导致表层原子非晶化并挤出形成切屑，同时亚表面位错运动形成滑移带。在脆性断裂阶段，滑移带尖端应力集中引发裂纹萌生，且裂纹形成后，最大主应力驱使与其方向夹角最小的 C-Si 原子键优先断裂，从而决定裂纹的扩展路径。

(3) 建立了单晶碳化硅基片磨削表面粗糙度和亚表面损伤深度预测模型。首先，通过分析砂轮磨粒和工件之间的相对运动，并基于宏观与微观材料去除面积相等原理，建立考虑磨粒轨迹、随机分布、磨粒回弹以及重叠效应影响的磨粒切深预测模型，确定了磨粒切深与工艺参数之间的解析关系。其次，结合磨削后表面形貌特征、磨粒突出高度的随机性及工件表面的弹性恢复效应，建立了表面粗糙度与磨粒切深之间的数学关系模型。然后，基于亚表面损伤的分布规律，结合“中位-径向”裂纹理论，分析了亚表面损伤深度、法向力、磨粒切深之间的关联，建立了亚表面损伤深度与磨粒切深之间的解析关系。最终以磨粒切深为中介变量，分别建立了表面粗糙度与工艺参数、亚表面损伤深度与工艺参数之间的关联模型。磨削验证试验结果表明，两个模型的预测误差都低于 5%，为后续磨削工艺的优化提供理论指导。

(4) 针对传统工艺优化主要依赖大量试验，存在周期长、成本高等问题，本章基于上述磨削表面粗糙度和亚表面损伤深度预测模型，提出一种兼顾表面质量与加工效率的磨削工艺优化方法。通过预测模型揭示了工艺参数对表面质量的影响规律，明确砂轮转速与工件转对表面质量影响显著，但对加工效率影响有限，而砂轮粒度、进给速度及粗/精磨去除厚度分配对二者均有显著影响。基于本文建立的模型，以表面粗糙度与亚表面损伤深度为质量约束条件，结合磨床参数范围及基片总去除厚度的限制，构建包含砂轮粒度与进给速度的工艺参数库，通过遍历工艺组合并计算粗磨后损伤深度，确定粗/精磨阶段的材料去除厚度分配及总加工时长，筛选出总时间最短的优化方案，并开发了配套的磨削工艺优化软件。最后，在表面粗糙度小于 1 nm、亚表面损伤深度小于 0.1 μm 、材料总去除厚度 100 μm 的约束条件下，优化方案为粗磨采用#2000 砂轮、进给速度 0.6 $\mu\text{m}/\text{s}$ 、去除厚度 95 μm ，精磨采用#10000 砂轮、进给速度 0.2 $\mu\text{m}/\text{s}$ 、去除厚度 5 μm ，砂轮与工件转速均为 3000 r/min 和 100 r/min。试验验证结果表明，该方案在保证表面质量的同时，实现了超过 30 $\mu\text{m}/\text{min}$ 的平均材料去除率，验证了所提优化方法在硬脆基片磨削中的有效性，实现了碳化硅基片的高效高表面质量磨削。

关键词：单晶碳化硅基片；材料去除机理；损伤机理；表面质量；磨削工艺优化

ABSTRACT

As a third-generation wide-bandgap semiconductor material, single-crystal silicon carbide (SiC) exhibits exceptional physical properties, including a high critical breakdown electric field, high thermal conductivity, high carrier saturation velocity, and excellent thermal stability. These characteristics make it an ideal substrate material for high-voltage, high-frequency, and high-power electronic devices. After crystal growth, device-grade single-crystal SiC substrates must undergo a series of processing steps, including slicing, planarization, and chemical mechanical polishing (CMP), to achieve high surface flatness and ultra-smooth surfaces. Among these, planarization is a key technology for achieving high-quality and high-efficiency processing of SiC substrates. For SiC substrates of 6 inches or smaller, free-abrasive lapping is commonly used for planarization. However, with the continuous advancement of SiC crystal growth technology, the demand for planarization of large-diameter (8 inches and above) SiC substrates has become increasingly urgent. The use of free-abrasive lapping for large-diameter SiC substrates face challenges such as low efficiency, severe damage, and high processing cost. In contrast, ultra-precision grinding technology based on the principle of workpiece rotation has been successfully applied in the planarization of large-diameter silicon substrates due to its advantages of high efficiency, high precision, and low damage. Nevertheless, its application in the processing of single-crystal SiC substrates remain limited due to unresolved issues, including the unclear mechanisms of material removal and damage evolution during grinding, the lack of methods for controlling surface roughness and subsurface damage depth, and the absence of grinding process parameter optimization methods that can simultaneously consider processing efficiency and surface quality. These limitations hinder the development of high-efficiency, high-surface-quality grinding techniques for SiC substrates. To address these issues, this study systematically investigates the material removal mechanisms of grinding, the formation and evolution of subsurface damage, predictive methods for surface roughness and subsurface damage depth, and high-efficiency, high-surface-quality grinding processes for single-crystal SiC substrates. The specific research contents and major findings are as follows:

(1) The surface morphology characteristics and material removal mechanism in single-crystal SiC grinding were investigated. Through nanoindentation, single-grit variable-load scratching, and ultra-precision grinding tests, a systematic comparison was made between the C-face and Si-face of single-crystal SiC in terms of mechanical properties, surface morphology, and material removal mechanisms. Nanoindentation results revealed that the C-face exhibits higher hardness and elastic modulus than the Si-face, while the Si-face possesses greater fracture toughness. Scratching tests showed that although both surfaces undergo a transition from ductile to brittle removal with increasing load, the C-face, having a lower elastic recovery

rate, enters the brittle stage earlier. In the ductile removal phase, abundant plastic chips were generated on both sides of the C-face scratch, whereas no chips appeared on the Si-face. After transitioning to brittle removal, both surfaces produced brittle chips and pits, but the Si-face exhibited a higher density. Ultra-precision grinding tests indicated that as abrasive grit size decreased, both surfaces shifted from ductile to brittle grinding. However, the C-face demonstrated lower surface roughness and pit density, as well as a smaller critical depth of cut for the ductile-to-brittle transition. Overall, the differences in removal mechanisms were attributed to intrinsic mechanical property disparities. The higher hardness and elastic modulus of the C-face resulted in a lower critical depth for the ductile-to-brittle transition, which caused the material to enter the brittle removal mode earlier. In contrast, the Si-face, with its higher fracture toughness and elastic recovery, was better able to sustain ductile removal. However, when brittle fracture occurred, the release of elastic energy was more intense, leading to more severe surface damage.

(2) The formation and evolution mechanisms of subsurface damage in single-crystal SiC grinding were investigated. Using a multiscale approach combining single-grit variable-load scratching, ultra-precision grinding, and molecular dynamics (MD) simulations, the cross-scale evolution mechanisms of subsurface damage in single-crystal SiC grinding were revealed. Results from both scratching and grinding tests showed consistent damage distribution patterns for the C-face and Si-face. In the ductile phase, subsurface damage was dominated by amorphization, dislocations, and slip bands, with maximum damage depth governed by the extent of slip bands. Upon entering the brittle phase, SSD extended from the slip band tips, where stress concentrated, leading to microcrack formation; at this stage, cracks determined the maximum damage depth. MD simulations validated this distribution pattern and further clarified the stage-specific mechanisms. In the plastic deformation stage, abrasive shearing caused surface atom amorphization and chip formation, while subsurface dislocation motion generated slip bands. In the brittle fracture stage, stress concentration at slip band tips induced crack nucleation. Once formed, cracks propagated along directions with minimal angles to the maximum principal stress, preferentially breaking C–Si bonds and determining the crack path.

(3) Prediction models for surface roughness and subsurface damage depth in grinding of single-crystal SiC substrates were established. First, by analyzing the relative motion between grinding wheel grit and the workpiece, and based on the principle of equivalent macro–micro material removal area, a model was established to predict grit depth of cut, considering grit trajectory, random distribution, elastic rebound, and overlap effects. The analytical relationship between grit depth of cut and process parameters was derived. Next, combining post-grinding surface morphology features, randomness in grit protrusion height, and elastic recovery of the workpiece surface, a mathematical model relating surface roughness to grit depth of cut was

developed. Then, based on subsurface damage distribution patterns and the median–radial crack theory, the correlations between damage depth, normal force, and grit depth of cut were analyzed, leading to an analytical model linking subsurface damage depth with grit depth of cut. Finally, using grit depth of cut as an intermediate variable, correlation models were established to link both surface roughness and subsurface damage depth with grinding parameters. Validation experiments showed that the average prediction error for both models was below 5%, providing theoretical guidance for subsequent process optimization.

(4) To address the issues associated with traditional process optimization methods, which rely heavily on extensive experimentation and often lead to long development cycles and high costs, this chapter proposes a grinding process parameter optimization method that balances surface quality and processing efficiency. The method is based on the previously established predictive models for grinding surface roughness and subsurface damage depth. Based on predictive models, the influence of grinding parameters on surface quality was clarified. Wheel speed and workpiece speed had a significant effect on surface quality while their impact on efficiency was limited. In contrast, abrasive size, feed rate, and the allocation of rough and fine grinding thickness affected both surface quality and processing efficiency. Taking surface roughness and subsurface damage depth as quality constraints, and considering practical factors such as machine limitations and total removal thickness, a parameter library was established that included abrasive size and feed rate combinations for both rough and fine grinding. Each process combination was evaluated by calculating the subsurface damage depth after rough grinding and the total machining time. The optimal combination was selected based on the shortest overall processing time, achieving a balance between quality and efficiency. A supporting software system was developed to facilitate this process. Under the constraints of surface roughness less than 1 nm, subsurface damage depth less than 0.1 μm , and a total removal thickness of 100 μm , the optimized process involved rough grinding with a #2000 wheel at a wheel speed of 3000 r/min, workpiece speed of 100 r/min, feed rate of 0.6 $\mu\text{m/s}$, and removal thickness of 95 μm . Fine grinding used a #10000 wheel at the same wheel and workpiece speeds, with a feed rate of 0.2 $\mu\text{m/s}$ and a removal thickness of 5 μm . Validation test results demonstrate that this solution not only guarantees surface quality but also achieves an average material removal rate exceeding 30 $\mu\text{m/min}$. This verifies the effectiveness of the proposed optimization method for grinding hard-brittle substrates and realizes high-efficiency, high-surface-quality grinding of silicon carbide substrates.

Key Words: Single-crystal silicon carbide substrate; Material removal mechanism; Damage mechanism; Surface quality; Grinding process optimization