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Suppression of In-Grown SF Formation and BPD Propagation in 4H-SiC Epitaxial Layer by Sublimating Sub-Surface Damage before the Growth

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Abstract. It is known that basal plane dislocations (BPDs) and in-grown stacking faults (IGSFs) in the 4H-SiC epitaxial layer cause severe electrical degradation in SiC devices. The impact that sub-surface damage (SSD) on a production-grade 4H-SiC substrate with CMP-finished surface causes on both the BPD propagation and IGSF formation during epitaxial growth was investigated by Dynamic AGE-ing® (DA). The substrates etched by DA sublimation etching to adjust the residual amount of SSD maintaining a smooth surface without macro step bunching were grown to observe BPD and IGSF density. The obtained results showed that these defect densities decreased exponentially with increasing etching depth. We demonstrated SSD introduced by mechanical processing led BPDs and IGSFs to extend or introduce to the epitaxial layer.

Introduction

The degradation of electrical characteristics of 4H-SiC power devices caused by basal plane dislocations (BPDs) and in-grown stacking faults (IGSFs) in the epitaxial layer has been a critical issue [1]. It is known that the BPD is propagated from the 4H-SiC substrate and the IGSF is formed near the epi/sub-interface during CVD epitaxial growth [1,2]. The BPDs can be reduced by converting to threading edge dislocations (TEDs) through optimization of H_2 etching conditions prior to CVD epitaxial growth [3,4]. On the other hand, the IGSFs can be decreased by removing high-density defects of scratches introduced during mechanical contacts such as grinding and mechanical polishing (MP) [5-7]. However, the densities of both BPD and IGSF have not been suppressed simultaneously to less than 0.1 cm^{-2}.

Therefore, we assumed that the sub-surface damage (SSD) caused by the mechanical contact still remains at the CMP-finished substrate even after the H_2 etching and it affects both the BPD propagation and the IGSF formation. Considering the difficulty in the H_2 etching to avoid the arising of thermally stable macro step bunching, the controllable depth is limited to about 100 nm. In order to verify the assumption beyond that limitation, an alternative etching method is required. For this purpose, we have developed a sublimation-controlled non-contacting type process as "Dynamic AGE-ing®" (DA), which enables etching, epitaxial growth, and annealing in the wide temperature range of 1200-2100°C [8].

The DA is conducted under a near-equilibrium condition inside a quasi-closed container made of polycrystalline SiC as shown in Fig. 1. Controlling the temperature gradient between the substrate and the container, the three different thermal processes can be performed. In addition, This process creates Si-rich or C-rich conditions around the SiC substrate by the simple arrangement of components capable of supplying Si vapor. Fig. 2 (a) shows the Si/C ratio during the DA process at 1500-2000°C obtained by thermodynamic calculation using JANAF Thermochemical Tables. This result indicates the Si/C ratio remains stable over a wide temperature range, so the surface morphology of SiC substrates can be easily controlled as observed by the SEM images in Figs. 2 (b)-(e). For the removal of the SSD from SiC sub-surface using the DA sublimation etching at the Si-rich condition, a smooth surface as shown in Figs. 2 (b), (c) can be maintained without the macro step bunching independent of the etching depth. In this study, epitaxial layers were grown directly after removing SSD from the substrates using DA sublimation etching to observe BPD and IGSF density.

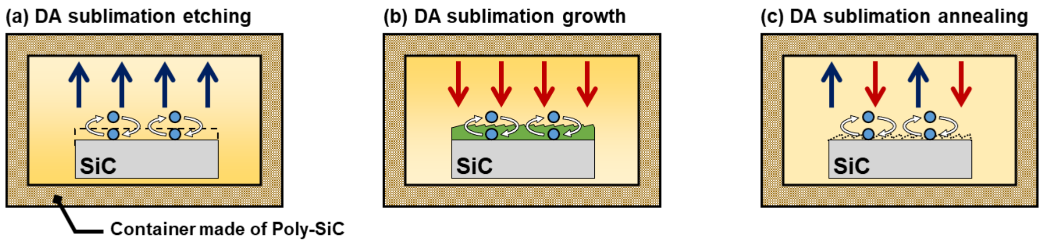

Fig. 1. The functions of DA process controlled by the change in temperature gradient between the SiC substrate and the container. (a) DA sublimation etching, (b) DA sublimation growth, and (c) DA sublimation annealing.

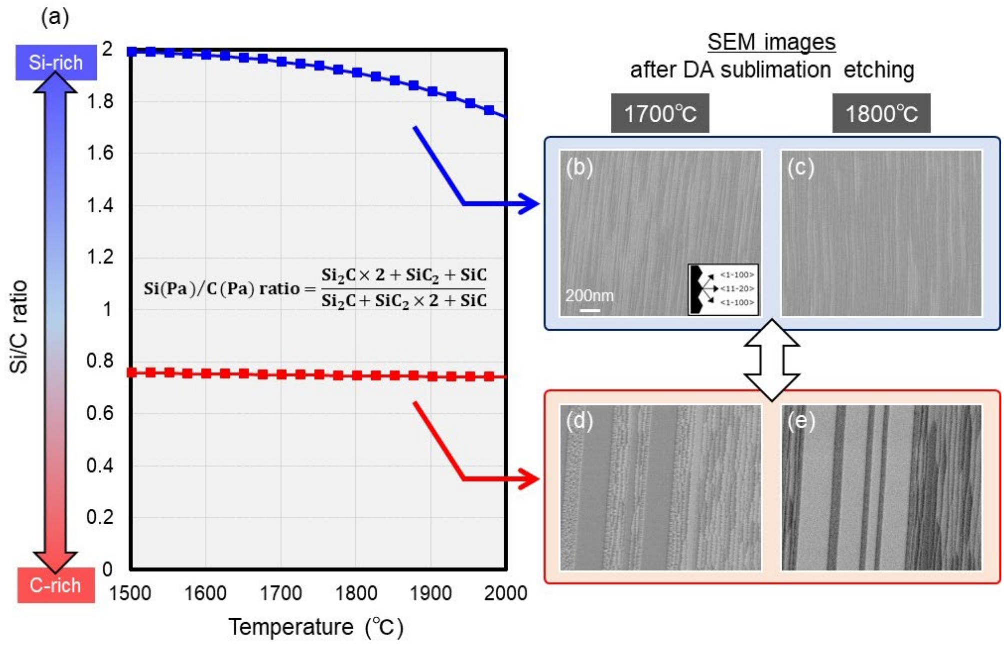

Fig. 2. (a) Si/C ratio during the DA process at each temperature estimated by thermodynamic calculation using JANAF Thermochemical Tables. (b)-(e) SEM images of CMP-finished 4H-SiC substrates after the DA sublimation etching with different Si/C ratio at 1700°C and 1800°C.

Experiments

In the experiments, 4H-SiC (0001) 4°off-cut n-type substrates (10×25 mm^2 size) were used with different surface finishing processes (MP and CMP) to investigate the impact of the SSD layer on BPD propagation and IGSF formation during epitaxial growth. The CMP-finished substrates were cut from commercially available 6-inch production-grade wafers purchased by wafer vendors A, B, C, D, and E in 2021. The DA process was performed using an ultra-high temperature vacuum furnace (KGX-2000) manufactured by EpiQuest, Inc. DA sublimation etching was carried out first at 1700-1800°C for 10-120 min to control etching depth. The surface roughness (RMS) of substrates after the DA etching measured by AFM (10×10 μm^2) was 0.1-0.2 cm^{-2} regardless of the etching depth. Then, the epitaxial layer of about 15-20 μm was created by the DA sublimation growth at 1800°C (carrier concentration: 1.0-3.0×10^{17} cm^{-3}). The IGSF density in the grown layers was characterized by UV-PL imaging (Manufactured by PHOTON Design Corporation. Excitation wavelength: 313 nm using a high-pass filter of 750 nm for detection). Molten KOH etching was then performed at 500°C for 6 min 20 seconds to estimate BPD density from etch pits of the samples.

In addition, 6-inch production-grade 4H-SiC wafers without cutting into several pieces were etched by DA sublimation etching at 1800°C for 30-60 min. Subsequently, 30 μm-thick DA growth was conducted on the wafers at 1800°C and the defect densities in the epitaxial layer were observed by using UV-PL.

Results and Discussion

When DA sublimation growth was performed directly on MP-finished and CMP-finished substrates observed surface morphologies as shown in Figs. 3 (a), (b) without DA etching, a higher density in IGSF was clearly observed for the MP-finished one in the cross-sectional SEM images in Figs. 3 (c) and (d) due to its larger SSD. For the CMP-finished substrate in this case, however, a considerable number of IGSF still existed with a density of 30-150 cm^{-2} by using UV-PL. On the other hand, when DA sublimation etching was employed prior to DA growth on these substrates, IGSF was eliminated as shown in Figs. 3 (e) and (f). These results indicated that DA sublimation etching significantly suppressed the IGSF formation during DA growth process.

So, we verified the etching depth dependence of BPD propagation and IGSF formation to be suppressed on the CMP-finished substrate from vendor A. Fig. 4 shows the densities of the BPD and the IGSF after DA growth as a function of DA sublimation etching depth. CMP substrates purchased in 2021 were used as samples, and we employed DA growth at 1800°C after DA sublimation etching at 1700°C or 1800°C. When 15 μm-thick DA growth was conducted directly on CMP-finished substrates, the BPD and IGSF density were 5.5 cm^{-2} and 32.0 cm^{-2}, respectively. On the other hand, the substrate with a 0.7 μm etched by DA sublimation etching showed a BPD density of 1.5 cm^{-2} and an IGSF density of 10.0 cm^{-2}. Then, the substrate with an etching depth of more than 6 μm showed few BPDs and IGSFs in the epitaxial layer. Thus, both BPD and IGSF density were found to decrease exponentially with etching depth. From the fitting curves in Fig. 4, even the CMP-finished substrate purchased in 2021 required 2.2 μm and 3.4 μm etching depth to achieve BPD and IGSF density below 0.1 cm^{-2}, respectively.

We also investigated the etching depth dependence of the BPD propagation and the IGSF formation for the 6-inch production-grade SiC wafers. Fig. 5 shows the count maps of BPDs (red points) and

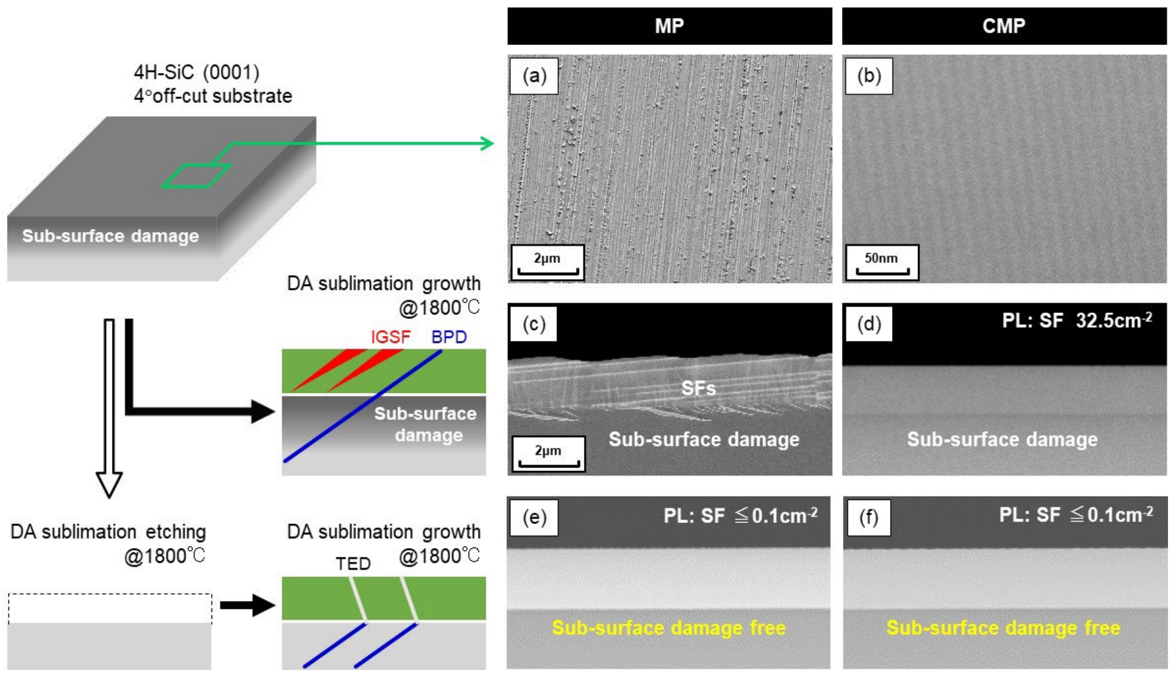

Fig. 3. (a), (b) SEM images of MP, CMP substrates. Cross-sectional SEM images after 1800°C DA growth without DA etching (c), (d) and with 1800°C DA etching (e), (f) for each substrate. The thickness and carrier concentration of the epitaxial layer are 2 μm and 1.0-3.0×10^{17} cm^{-3}.

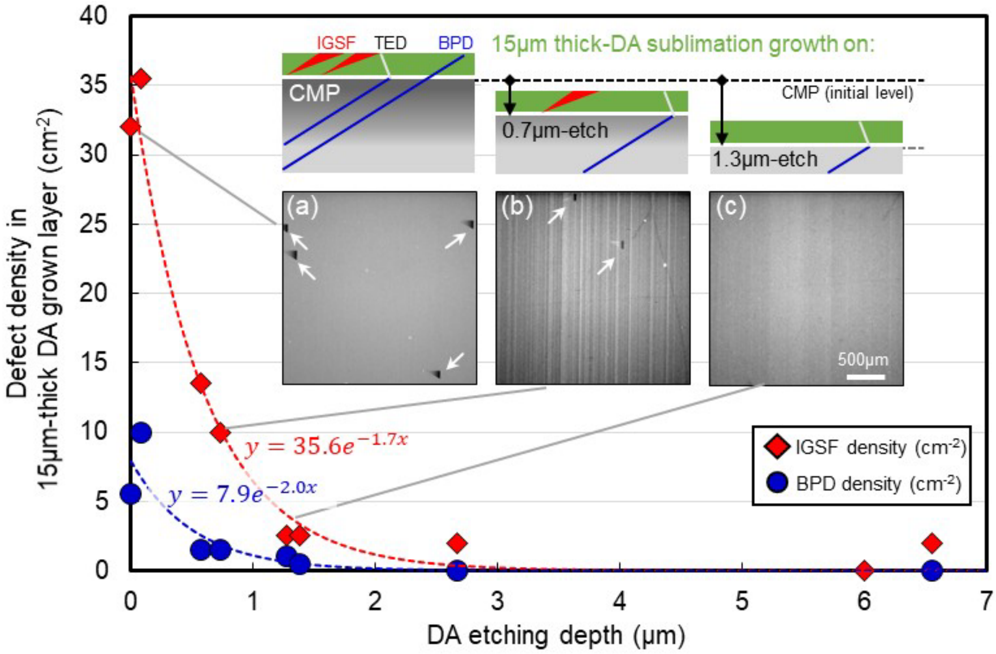

Fig. 4. BPD and IGSF density after 1800°C DA growth as a function of 1700 or 1800°C DA etching depth on CMP substrate. The thickness and carrier concentration of the epitaxial layer are 15µm and 1.0-3.0×10^{17} cm^{-3}. (a)-(c) PL images and each schematic diagram of samples grown on 4H-SiC substrates with different etching depths. The IGSFs generated in the growth layer are indicated by white arrows.

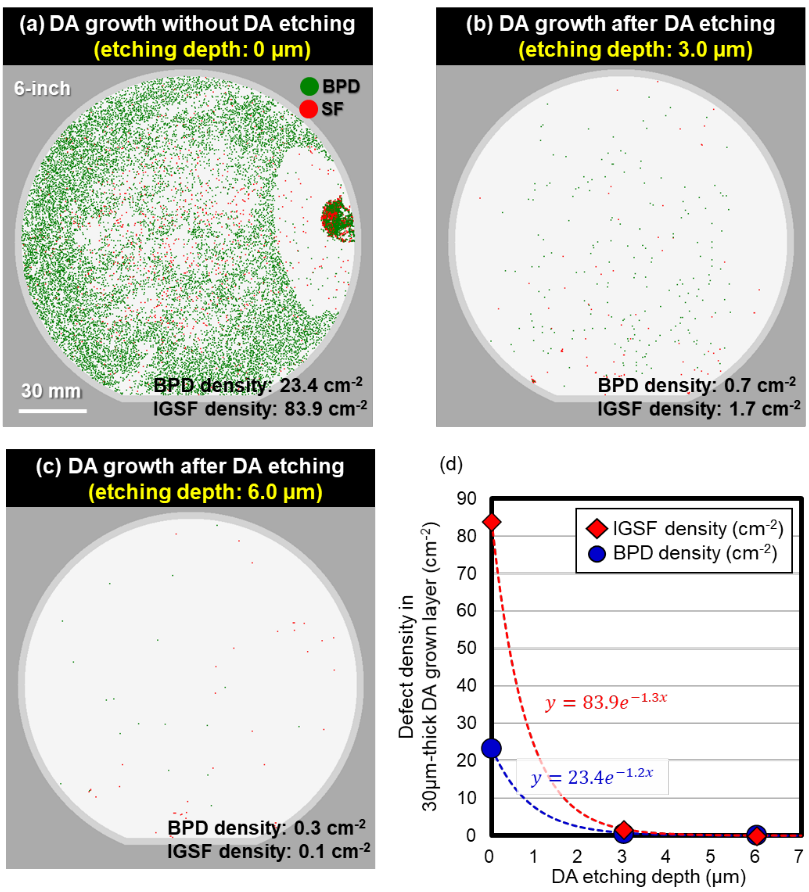

Fig. 5. Count maps of BPDs and IGSFs on the 6-inch wafers after DA sublimation growth (a) without DA sublimation etching, with (b) a 3.0 µm and (c) a 6.0µm etched by DA sublimation etching. The BPDs and IGSFs are represented by red and green points, respectively.

IGSFs (green points) on the epitaxial layer after DA sublimation growth observed by using UV- PL. As shown in Fig. 5 (a), the wafer in which DA growth was performed without DA sublimation etching had both BPD and IGSF density above 20 cm^{-2}. On the other hand, these defect densities were suppressed to 0.3 cm^{-2} and 0.1 cm^{-2}, respectively, when the amount of the DA etching was 6.0 µm, as shown in Figs. 5 (b) and (c). This tendency of decreasing exponentially BPD and IGSF density in the epitaxial layer as the etching depth increases was found to be valid not only for chip-size substrates, but also for 6-inch SiC wafers. However, in the case of this wafer, the defect densities could not be suppressed below 0.1 cm^{-2} with the SSD removal amount of 6.0 µm. Therefore, it is likely that the required etching depth may depend on the vendor of the CMP-finished SiC wafer.

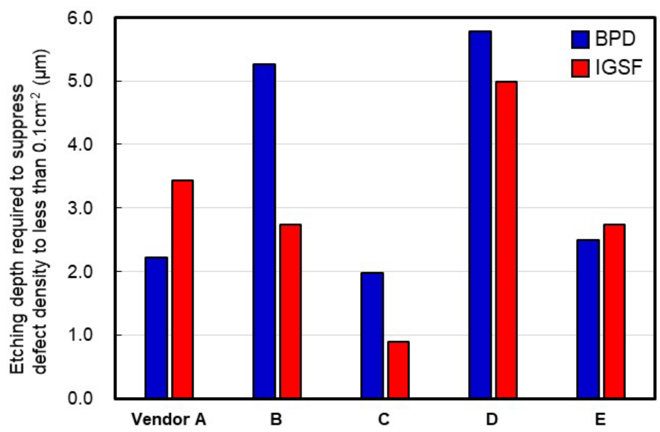

Fig. 6. Etching depth required to suppress the BPD and IGSF density of each CMP substrate from vendors A, B, C, D and E to less than 0.1 cm^{-2} after DA sublimation growth.

So, the same experiments were performed for the substrates (10×25 mm^2 size) cut out the CMP-finished wafers from vendors B, C, D, and E. For all samples, both BPD and IGSF density after DA growth also reduced exponentially with DA sublimation etching depth regardless of the wafer vendor. Based on fitting curves as shown in the broken line in Fig. 4, we determined the etching depth required to be less than 0.1 cm^{-2} for the BPD and IGSF density of the CMP substrate from each vendor. Fig. 6 revealed that the etching depth to suppress both BPD propagation and IGSF formation for each substrate varied in the wide range of 2.0-6.0 µm. It is assumed that the considerable variation is caused by the quality of the CMP process. H_2 etching in the conventional CVD growth process may not sufficiently remove SSD from the CMP substrate sub-surface.

Conventionally, the CMP-finished substrates have been etched about 100 nm prior to CVD epitaxial growth. However, this study indicates that a relatively large amount of etching is necessary to reduce BPD and IGSF density. It is also suggested that the SSD affecting BPD propagation and IGSF formation is not only localized as high-density defects of scratches but also extended as elastic strain regions deep into the substrate exponentially as shown in Fig. 7. Since DA sublimation etching can remove this elastic strain while maintaining surface flatness, the BPDs and IGSFs in the epitaxial layer could be suppressed. It should be noted that the required etching depth depends on the wafer vendor and mechanical process condition.

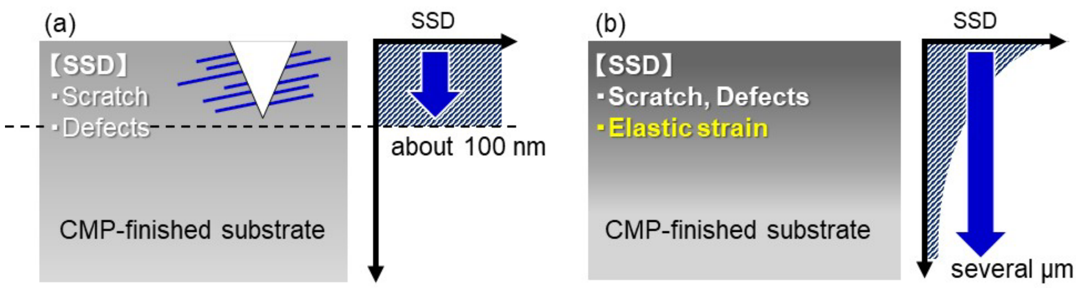

Fig. 7. Schematic models of (a) the conventional understanding that localized scratches and defects derived from mechanical contacts regard as SSD and (b) the new assumption that elastic strain is also defined as SSD which affects BPD propagation and IGSF formation.

Summary

We investigated whether sub-surface damage (SSD) on CMP-finished production-grade 4H-SiC substrate is a factor in both the BPD propagation and the IGSF formation during epitaxial growth. Each substrate with various amounts of SSD removal controlled by sublimation etching using Dynamic AGE-ing® (DA) at 1700-1800°C, was grown by DA growth to inspect the defect densities. The obtained results revealed the BPD and IGSF density of the epitaxial layer decreased exponentially as the etching depth increased. The grown layer with the BPD and IGSF density below 0.1 cm^{-2} requires an etching depth prior to the epitaxial growth in the wide range of about 2.0-6.0 μm depending on the amount of SSD on the substrates. Therefore, it is necessary to remove the damages according to the wafer vendor and the polishing quality to completely suppress BPDs and IGSFs.

Acknowledgments

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