Elucidation of the Origin of Polycrystals Adhering to the Growth Interface during SiC Solution Growth

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Introduction

The solution growth method for 4H-SiC has been reported to enable the fabrication of crystals with low dislocation densities. However, a persistent challenge is the formation of "polycrystals" - crystals with different facet orientations or polytypes - on the surface of the grown crystal. While techniques such as the meniscus method have been reported for their suppression, complete inhibition remains difficult and stands as an obstacle to achieving higher crystal quality. To resolve this issue, it is essential to identify the fundamental factors governing polycrystal formation. Therefore, this study aims to elucidate the formation mechanism through a comparative analysis of polycrystals generated on the crystal surface and within the crucible [1,2].

Experimental Procedures

An 8-inch SiC crystal was grown for 30 hours using a 58at%Si-40at%Cr-2at%Al solvent. The fabricated crystal was sliced parallel to the step-flow direction and subsequently polished into a thin plate for observation via transmission optical microscopy. Polycrystal samples were also collected from the crucible wall and bottom retrieved after the growth. Raman spectra from all samples were then compared and classified using a Variational Auto-Encoder (VAE). Specifically, each Raman spectrum was mapped by the VAE into a low-dimensional feature space, and quantitative similarity was evaluated based on the proximity of the data points within that space.

Results and Discussion

Figure 1 shows the transmission image of a polycrystal observed in a thin-plate sample from the grown crystal surface. In the figure, the blue and white striped areas correspond to the bulk single crystal grown from the seed, while the polygonal-shaped parts, such as those colored blue or brown, are polycrystals. A distinct, dark, streak-like boundary layer is observed between the bulk single crystal and the polycrystals. These results strongly suggest that the polycrystals did not form directly on the bulk single crystal surface but were instead incorporated at the growth interface after nucleating heterogeneously within the solution.

Next, to identify the origin of these incorporated polycrystals, a comparative classification of their Raman spectra was performed. As a result of the comparison, the spectra of polycrystals from the crystal surface and those from the vicinity of the crucible bottom exhibited a high degree of similarity in their primary optical phonon modes (TA and TO). This was confirmed by the fact that their respective data sets formed closely located clusters in the VAE-mapped feature space. Furthermore, it was confirmed that the similar spectra tended to be obtained from polycrystals collected from below a certain height on the crucible bottom.

Integrating the hypothesis of incorporated floating microcrystals, suggested by the cross-sectional observation, with the results of the comparative Raman spectral analysis, it is concluded that the polycrystals on the grown surface are predominantly caused by the adhesion of microcrystals formed at the crucible bottom and subsequently transported through the solution. This finding will contribute to the establishment of a new process design guideline for the fundamental suppression of polycrystal formation.

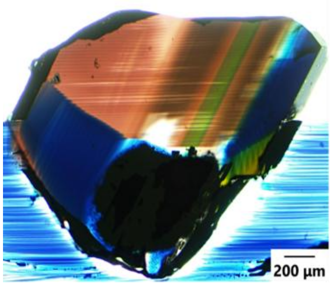

Figure 1 Transmission image of polycrystals on the grown crystal surface

References

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