Numerical modeling of the macrostep formation in SiC solution growth by phase field method

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Introduction

In solution growth of 4H-SiC by TSSG method, crystal quality is highly related to step growth behavior.[1] The growth process of steps bunching from small steps into large steps directly influences the formation of defects and the growth rate. [2][3] Therefore, to improve both the growth rate and quality of the crystal, controlling macrostep formation is essential. So this study aims to achieve better control of step growth by understanding the formation process of macrostep.

Experimental Procedures

To reveal the mechanism of step formation in SiC solution growth, a phase field model coupled with the C diffusion near the growth interface is proposed. First, we set the simulation scenario within a stagnant flow layer range of 200-300 micrometers on the crystal growth surface, a mesoscale range that closely aligns with the real step scales observable in experiments. Then, we introduce different flow conditions to observe the changes in supersaturation and step behavior under varying flow intensities and directions.

Results and Discussion

The Fig. 1 illustrates the process by which basic steps under parallel flow conditions gradually form macrosteps from smaller steps. From this, we can observe that the change in macrostep size begins with the initial bunching of adjacent basic steps, which then grows into larger macrosteps as the number of steps within bunched structure increases.

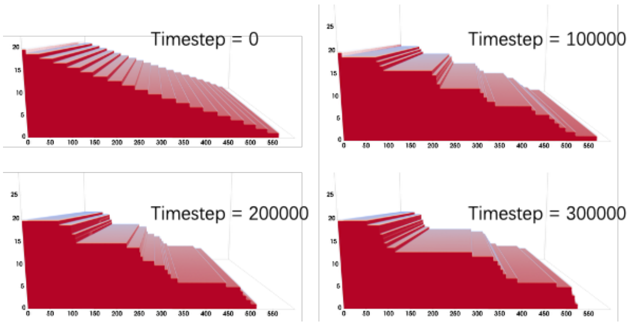

Fig. 1 Step bunching formation process under parallel flow conditions.

From Fig. 2, we can observe that the formation of a macrostep involves smaller step catching up to the bunched steps ahead. Under parallel flow, when the left-side step approaches, the undersaturated concentration region tends to shrink. Because the flow moves from left to right, causing the small steps on the left to capture the concentration that would otherwise be supplied to the steps on the right. When a step joins a bunched group of steps, they become a unified structure sharing the same undersaturated region. The region on the left-side individual step remains smaller, so it appears as a larger step.

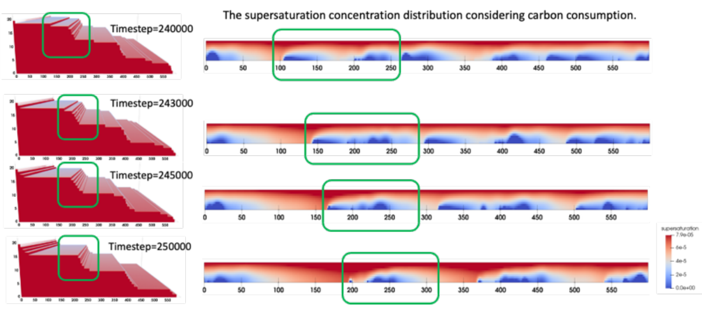

Fig. 2 Movement of small steps and changes in supersaturation during step bunching process.

The above illustrates the expansion process of macrostep. We believe that formation of larger macrostep is related to uneven supersaturation in the adjacent step regions, which is influenced by the flow.

References

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