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主　論　文　の　要　旨

論文題目　Numerical Investigation of Long-term Instability in Solution Growth of SiC Crystal
（数値解析による SiC 結晶の溶液成長における長時間不安定性の研究）

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論　文　内　容　の　要　旨

SiC grown by solution growth method has proven superior in crystal quality, but the mass production is still hindered by relatively low yield. The accurate description, understanding, and control of the unsteady phenomena in the growth system are essential to achieving a longer stable growth time and larger crystal thickness. This dissertation aims to numerically investigate the instabilities during long-term growth and provide engineering solutions.

Firstly, a 2D global CFD model was built to simulate the evolution of crucible configuration due to crystal growth, crucible dissolution, and polycrystal precipitation. This model could estimate the maximum available growth time for a given control recipe. A machine learning-based optimization system was subsequently constructed to optimize an adaptive control recipe, which corresponds to a thicker crystal with flatter growth front and longer available growth time.

Secondly, the evaporation and reaction of aluminum were simulated to study the instability of solution chemical composition during long-term growth. The detailed transport path of aluminum in the growth system was determined by thermodynamic calculation. The constructed model could predict the evolution of aluminum concentration inside the solution. Moreover, an improved geometric design was proposed to suppress evaporation and better preserve the aluminum in the solution during growth. The effect of the improved design was demonstrated both numerically and experimentally.

Finally, a simulation model was built that can predict the evolution of macrostep morphology on the entire crystal surface under the given control parameters. This model could be applied to investigate the effect of macroscopic control parameters on the step morphology, and the simulation results were validated by the experiments. Most importantly, through this model, a more sophisticated control pattern was designed and improved. The improved control pattern could result in uniform step morphology on the entire crystal surface, as well as freely-controlled step bunching level during the long-term growth process.