SiC 溶液成長における経時変化のシミュレーションと最適化

Numerical investigation and optimization of time evolution in the solution during solution growth for SiC crystal

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Longer growth time and larger thickness are the essential targets for top-seed solution growth (TSSG) SiC crystal to achieve high-efficiency mass production. For long-term growth of SiC crystal in TSSG process, the unsteady factors including growth of single crystal, dissolution of carbon crucible wall, deposition of poly-SiC crystal at crucible bottom not only influence the thermal, flow and carbon concentration fields inside the solution, but also limit the maximum available growth time. However, most of the previous numerical studies of solution growth only focused on the steady condition under a fixed recipe, which can not reflect the time evolution of the growth process.

In the present study, firstly a quasi-unsteady 2D CFD simulation was conducted to investigate the evolution of crystal growth rate, crucible dissolution rate, polycrystals precipitation rate during a 50 hours 3-inch crystal growth process, under a recipe with constant controlling parameters which is commonly used in the current experiments. Then accordingly, a high-efficiency optimization system consisting of a machine learning prediction model and optimization algorithm was constructed (as shown in Fig. 1) to optimize the recipe with time-dependent controlling parameters in 5 timesteps (10 hours for each). The application of machine learning made the optimization process about 1600 times faster than the traditional optimization process using only CFD simulation. Finally, the growth under the optimized recipe was compared with the original growth process (as shown in Fig. 2). It was expected that under the optimized time variant controlling recipe, about 40% longer growth time as well as more stable growth condition can be obtained simultaneously.

The current study revealed the time evolution phenomena under long-term growth, and optimized the time variant recipe assisted by step-by-step machine learning model. The optimized recipe can be a qualitative guidance to the practical experiments and production.

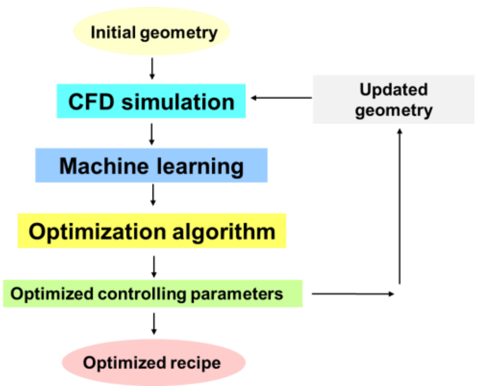

Figure 1. The flow chart of the high-efficiency optimization system.

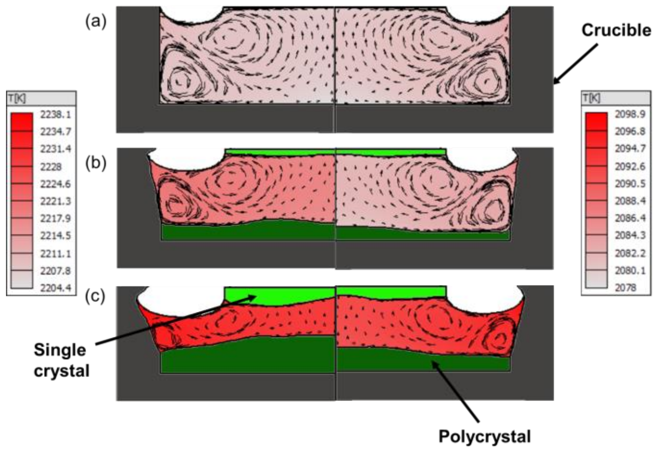

Figure 2. Time evolution of temperature, flow pattern and geometry in solution domain under the original recipe (left) and optimized recipe (right) after (a) 0 hour; (b) 20 hours; (c) 40 hours growth.