Optimization method of crystal growth conditions by tacit knowledge (for large-diameter SiC solution growth)

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The SiC solution growth method is expected to be a promising method for growing high-quality SiC bulk crystals [1]. In this method, precise control of flow distribution, concentration distribution, and temperature distribution inside the solution is important. However, it is difficult to optimize the growth conditions only using CFD simulation because the calculation speed is not fast enough. Therefore, we used machine learning techniques to construct a surrogate model for crystal growth simulation [2]. The predication speed is very fast and we can optimize the growth parameters in an inverse analytical manner using this model. However, we have a serious problem, that is, it is necessary to define an objective function that represents the desired distribution in a mathematical equation. However, it is not easy to express the distributions in solution by a mathematical expression. In this study, we developed a method to define an objective function in terms of latent variables and optimize it in a latent space, without converting the appropriate distribution of experimenter's tacit knowledge into an equation.

First, the tacit knowledge of the experimenter is extracted using the so-called AB test. Two of the various distributions are presented to the experimenter, who chooses which is more appropriate. By repeating this analysis, we obtain what the experimenter considers to be the appropriate distribution. Next, the various distributions are represented in latent space using Variable Auto Encoder in latent space. Figure 1 shows an example of a two-dimensional latent space of the various distributions. Each distribution is color-coded according to the score. In this distribution, states with relatively high scores are distributed in the lower right or upper region. The objective function is defined in terms of coordinates in the latent space. The distribution is calculated by the surrogate model by changing the growth conditions, and then it is expressed in terms of coordinates in the latent space. The growth condition is optimized to be as close to the target coordinate position as possible.

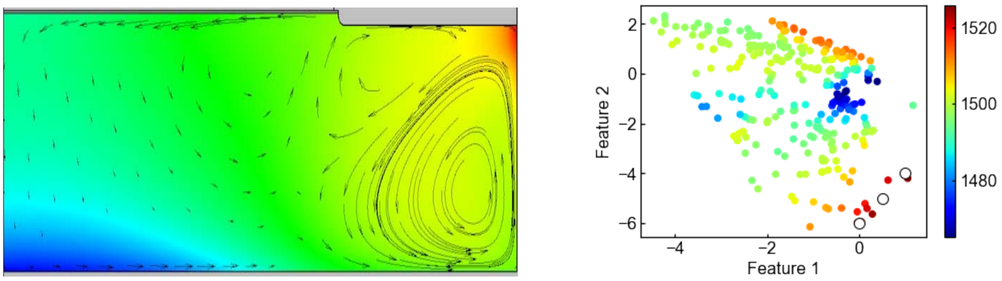

Fig. 1: Temperature and flow distribution (left), and the distributions in the latent space (right). Color bar means score according to tacit knowledge of experimenter.

References
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