Efficient Re-Optimization Method using VAE to Transfer Growth Conditions between Crystal Growth Systems

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Introduction

To grow high-quality crystals, it is essential to create an appropriate growth condition (such as the temperature and flow fields) through optimal process conditions. However, such optimal conditions are often specific to each crystal growth furnace, making it difficult to directly apply them to furnaces with different structure. Therefore, every time the furnace structure is changed, a search for optimal process conditions through experiments is required.

In this study, we propose an efficient method to transfer an optimized growth condition from furnace A to furnace B by combining a Variational Autoencoder (VAE) with optimization algorithm. This concept borrows from recent studies that demonstrate the transfer of growth condition between different crystal-growth systems [1,2].

Experimental Procedures

The proposed method uses a Genetic Algorithm (GA), and the solution individuals are the process conditions of furnace B. The process conditions proposed by the GA are input into a surrogate model of a CFD simulation of furnace B and transformed into temperature and flow field. The similarity between the obtained temperature and flow fields and the optimal temperature and flow field of furnace A is then evaluated using VAE. VAE is a machine learning method that can extract features from images and represent them as low-dimensional latent variables. Since images with similar features are transformed into similar latent variables, the distance between them can be used as the similarity between images. This similarity is defined as the objective function, and the evolutionary strategy of GA is used to search for process conditions that maximize the similarity.

The proposed method is applied to the growth of 200 mm 4H-SiC crystals using solution growth method. An optimal temperature and flow fields was transferred from furnace A to furnace B with a modified insulation layout.

Results and Discussion

Compare the temperature and flow fields and crystal surface photographs obtained from crystal growth experiments under the three process conditions. Figure 1 (a), (d) are the results of furnace A, which was the optimization target. High quality crystals without polycrystal formation were obtained. (b), (e) are the results of furnace B under the optimal process conditions of furnace A. The area on the right side of the image is locally heated, and several small vortices are generated. Many polycrystals have formed on the crystal surface, confirming that the optimal process conditions changed due to the change in the insulation arrangement. (c) is the temperature and flow fields of furnace B under the conditions obtained by optimization, which is similar to (a) in terms of the number and shape of vortices. In (f), it is confirmed that polycrystal deposition is suppressed as in (d).

This method is generally applicable to crystal growth processes that require control of the temperature and flow fields in the furnace and is considered to be effective for rapid condition search in materials development.

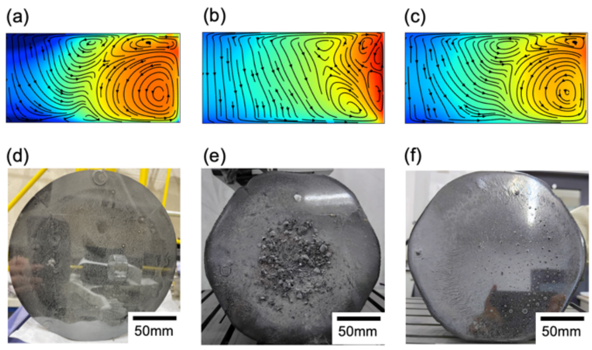

Figure 1 Comparison of temperature and flow fields and crystal surface images: Furnace A optimized (a, d), Furnace B before optimization (b, e), and Furnace B after optimization (c, f).

References

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