Machine Learning for SiC top-seeded solution growth
- Prediction, Optimization and Visualization -

Toru Ujihara*[1, 2, 3, 4], Yosuke Tsunooka[2, 3], Goki Hatasa[2], Can Zhu[1],
Kentaro Kutsukake[4], Taka Narumi[1], Shunta Harada[1, 2], Miho Tagawa[1, 2]

[1]Center for Integrated Research of Future Electronics (CIRFE), Institute of Materials and Systems for Sustainability (IMaSS), Nagoya University, Nagoya 464-8603, Japan
[2]Department of Materials Science and Engineering, Nagoya University, Nagoya 464-8603, Japan
[3]GaN Advanced Device Open Innovation Laboratory (GaN-OIL), National Institute of Advanced Industrial Science and Technology (AIST), Nagoya 464-8601, Japan
[4]Center for Advanced Intelligence Project, RIKEN, Nagoya 464-8603, Japan
* e-mail: ujihara@nagoya-u.jp

Keywords: SiC, Crystal Growth, Machine Learning, Optimization, Visualization

Abstract

We are developing solution growth technique for high-quality SiC bulk crystal. In actual, we have achieved high-quality crystal with very-low-density of threading dislocations grown by controlling the surface morphology. In order to apply this technique to large-scale crystal growth, it is necessary to control supersaturation at growth surface, flow rate and flow direction of solvent in detail. However, there are many growth parameters which should be optimized. Simulation technique based on computational fluid dynamics (CFD) is often used. However, it is still difficult to optimize growth condition by utilizing simulation technique since the calculation speed of CFD simulation is not enough to optimize the growth conditions, exhaustively. In recent, informatics including machine learning is applied to various fields including materials science. In this study, we tried to apply machine learning to the analysis of the results of CFD. We could make the model to optimize the crystal growth parameters based on a neural network model. Using the model, the optimization time became 10000 times faster. This is just a trial of "Process Informatics".

Large-diameter crystal growth is a big issue to establish the semiconductor bulk crystal growth technology. Generally speaking, we must spend much time to optimize the growth condition for the large-diameter bulk crystal. For example, over 30 years was necessary to enlarge from 1 inch to 300 mm in silicon wafer. In addition, the silicon bulk crystal growth depends on craftmanship, yet.

We have developed the growth technique of ultra-high quality SiC crystals in top-solution growth method [1]. Unfortunately, the crystal size is still small. In order to enlarge the size to 2-inch, 3-inch and over, it is necessary to control temperature, concentration, fluid velocity spatial distributions to achieve ultra-high quality SiC (to reduce dislocations) by optimization of many growth parameters. We must spend much time.

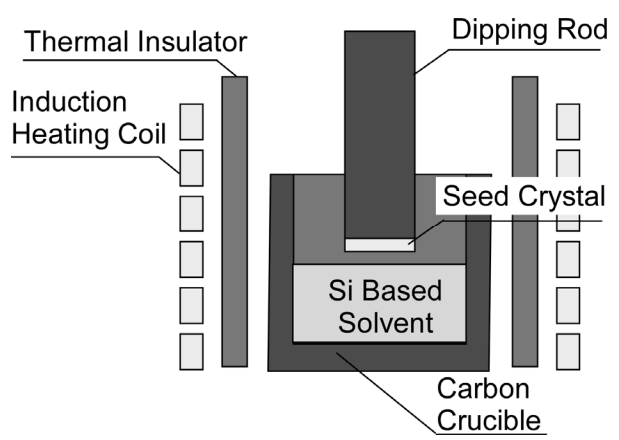

Fig. 1. Outline of SiC solution growth.

In the field of the development of motor cars, "model-based development" is used, now. In this method, the early stage of development is carried out on the model in cyber-space (simulation). This method speeded up the development. We hope to apply this method to the crystal growth. However, we do not have high-speed and accurate simulation because computational fluid dynamics (CFD) technique is very powerful tool but CFD simulation spends long time. In this study, we developed the high-speed and accurate prediction model of CFD simulation result by using machine learning [2]. In addition, we built visualization system for SiC crystal growth process using this prediction model. This means that we established the primitive model-based development in crystal growth.

Figure 1 shows the configuration of solution growth. In this method, a seed crystal is dipped into a Si-based solvent in a carbon crucible at high temperature around 1900-2000 deg. C. The seed crystal grows from carbon-saturated solvent. In order to control temperature distribution, concentration

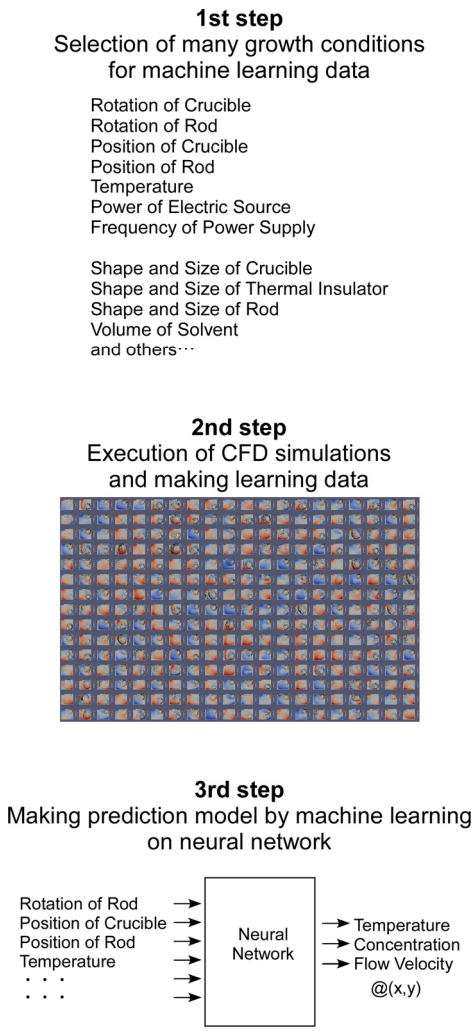

Fig.2. Sequence of construction of prediction model.

distribution, and flow velocity distribution, we carry out CFD simulation. The calculation time is too long to optimize all of growth parameters. So, we made a regression model of simulation result based on neural network by machine learning. Figure 2 shows the sequence of making prediction model.[2, 3] Firstly, we prepared 300 results of CFD simulations as training data for machine learning. The prediction model was made on neural network by using simulation data as big data.

Figure 3 shows the simulation result of supersaturation distribution and fluid velocity distribution and the predicted result based on the prediction model. Both results are very similar to each other. The calculation times of the simulation and the prediction model are about 3000 s and 0.0003 s, respectively. Using this prediction model, it is also possible to optimize growth conditions.

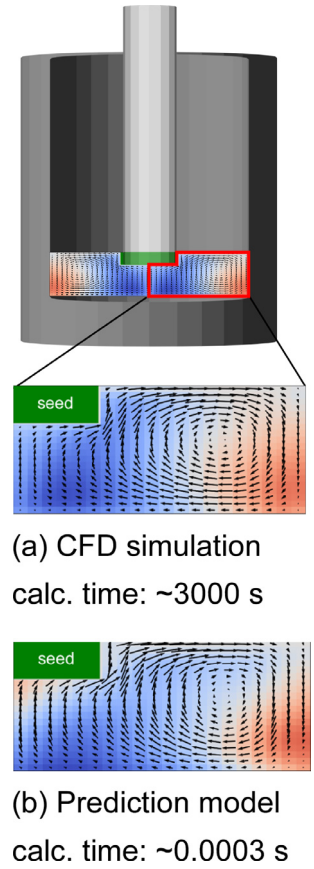

Fig.3. Supersaturation distributions (color contrast) and flow velocity (arrows) distributions in the solvent in SiC solution growth calculated by (a) CFD simulation and (b) the prediction model constructed by machine learning.

This work was partly supported by Council for Science, Technology and Innovation (CSTI), Cross-ministerial Strategic Innovation Promotion Program (SIP), "Next-generation power electronics/ Consistent R&D of next-generation SiC power electronics" (funding agency: NEDO), JSPS KAKENHI Grant Number 18H03839, RIKEN Center for Advanced Intelligence Project.

References

[1] K. Murayama, T. Hori, S. Harada, S. Xiao, M. Tagawa, T. Ujihara, J. Cryst. Growth **468**, 874-878 (2017).

[2] Y. Tsunooka, N. Kokubo, G. Hatasa, S. Harada, M. Tagawa, T. Ujihara, CrystEngComm, **20**, 6546-6550 (2018).

[3] T. Ujihara, Y. Tsunooka, G. Hatasa, K. Kutsukake, A. Ishiguro, K. Murayama, T. Narumi, S. Harada, M. Tagawa, Vacuum and Surface Science, (2019) in press.