Machine learning applications for crystal growth

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Machine learning is a method to inductively derive useful rules from a large amount of data. Once a machine learning model is obtained, we can instantly predict the results for any given condition within the parameter range of the data, accelerating research and development significantly. Machine learning has been applied in various research fields and has been spreading particularly in recent years. In this talk, machine learning applications to crystal growth will be briefly reviewed as well as its introduction. Then, machine learning applications for Czhocralski growth of Si using actual experimental data and solution growth of SiC using simulation data will be presented.

In the application to Czhocralski growth of Si, a neural network model was constructed to predict interstitial oxygen concentration in Si ingots from the process conditions of crystal growth. A real-time prediction system was developed using the model online connecting to the growth furnace [1]. Furthermore, the influence of process parameters on the interstitial oxygen concentration was evaluated by analyzing the learned model [2].

In the application to solution growth of SiC, we made a machine learning model having the input and output parameters the same as the simulation. This surrogate model can predict the simulation results with significantly small computational costs [3]. Thus, we can obtain an appropriate condition in a reasonable computation resource using optimization algorisms, such as genetic algorism [4]. Furthermore, a combination of machine learning and crystal growth simulation realized the adaptive optimization of process conditions considering the time development of crystal and crucible shapes [5] and the optimization of flow patterns in a crucible using topological analysis [6].

At the end of the talk, future prospects will be discussed. It is expected that machine learning will be increasingly applied to more practical applications in all research fields, including crystal growth science and technology. In such situations, it is important to use machine learning appropriately, based on the scientific knowledge of crystal growth.

References

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