Numerical Modeling on spiral formation of Cz-β-Ga2O3 crystal growth considering solidification kinetic effect

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Recently, we have presented the results of a numerical simulation of the β-Ga_2O_3 crystal growth using Czochralski (Cz) method to investigate the cause of spiral formation (twisting) of doped crystal occurs during the crystal growth [1]. In the previous study, we proposed that the onset of the spiral formation is related to that the melt temperature over the melt free surface near the tri-junction point becomes lower than that on the melt/crystal interface, so called melt supercooling. To overcome this challenge, an accurate temperature prediction near the melt/crystal interface is necessary. It it is known that the single crystal growth from the melt can be limited by the heat removal from the melt/crystal interface to the crystal and the solidification kinetic effect on its interface. In particular, the solidification kinetic effect is crucial for a compound crystal such as oxide crystal. Therefore, it is important to consider the kinetic effect to predict the temperature accurately for β-Ga_2O_3 crystal growth. However, this effect has not been considered the previous study.

In this study, we have developed numerical modeling considering the solidification kinetic effect for β-Ga2O3 crystal growth from the melt. In our developed numerical modeling, the growth rate is determined by the heat balance equation (Stephan problem) and the crystallization rate equation ($V_{cryst}=K\Delta T$). Here, K and ΔT mean the solidification kinetic coefficient and the supercooling degree on the growth interface, respectively. The kinetic coefficient was theoretically estimated from thermodynamic parameters and material properties of β-Ga2O3. The developed kinetic model has been implemented into CGSim^{TM} software developed by STR [2]

We performed 2D steady and 3D unsteady coupling simulation for β-Ga2O3 crystal growth by Cz method using the kinetic model in CGSim. As for coupling simulation, we performed 2D axisymmetric modeling of global heat transfer in the whole Cz furnace. The obtained heat flux by 2D axisymmetric modeling was used in detailed 3D unsteady modeling of crystallization zone.
We will show the results of crystal growth stability depending on the crystal transparency related to doping level with considering solidification kinetics effect.

References

[1] Masaya.Iizuka, Yuji Mukaiyama and Vladimir Artemyev, The 4th International Workshop on Gallium Oxide and Related Materials, IWGO (2022)
[2] https://www.str-soft.com/products/CGSim