Numerical modelling of large diameter Cz-β-Ga_2O_3 crystal growth in reactive atmosphere

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The β-Ga_2O_3 crystal has received significant attention from the semiconductor industry due to its wide bandgap and high critical electric field, making it ideal for power electronics [1]. The Czochralski (Cz) growth method is favored for its structural properties and crystal orientation. However, growing high diameter Ga_2O_3 crystals using this method still poses some challenges. Increasing the substrate diameter to over 50 mm will further advance the development of this ultra-wide bandgap technology [2].

The shape of the solid/liquid interface is a critical factor that affects the thermal stress in the crystal and its quality. Other factors that impact the growth process include furnace and crucible design, rotating rates, growing atmosphere, and crystallization rate [1,3]. The decomposition of Ga_2O_3 if the oxygen concentration of the atmosphere is too low, and oxidation of the Iridium (Ir) crucible if the oxygen concentration is too high, are additional challenges in selecting the proper process parameters. Adding CO_2 to the Ar atmosphere can effectively reduce Ga_2O_3 evaporation without damaging the Ir crucible [1,4].

The simulation of crystal growth has become a vital tool in gaining insight into the physical processes that drive crystallization, defect generation, and temperature changes. Despite the challenges posed by the dynamic changes in gas composition in furnaces, modern CFD software has made remarkable progress in modeling the composition of the melt through chemical reactions at both the surface and gas-phase levels.

The objective of this framework is to create a robust numerical model that can accurately describe the conditions for growing bulk β-Ga_2O_3 crystals of large diameter using alternative reacting gas atmospheres. The model is established using CGSim software by STR. This novel quasi-steady state axisymmetric model with alternative sources of oxygen will provide valuable computational results which can be further used to generate training data for machine learning applications [5].

References:

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