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Crystal front shape control by use of an additional heater in a Czochralski sapphire single crystal growth system.

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## Abstract

The quality of sapphire single crystals used as substrates for LED production is largely influenced by two defects: dislocation density and bubbles trapped in the crystal. In particular, the dislocation density has a higher value in sapphire grown by the Czochralski(CZ) method than by other methods. In the present study, we predict a decreased value for the convexity and thermal gradient at the crystal front (CF) through the use of an additional heater in an induction-heated CZ system. In addition, we develop a solute concentration model by which the location of bubble formation in CZ growth is calculated, and the results are compared with experimental results. We further calculate the location of bubble entrapment corresponding with the use of an additional heater. We find that sapphire crystal growth with an additional heater yields a decreased thermal gradient at the CF, together with decreased CF convexity, improved energy efficiency, and improvements in terms of bubble formation location.

**Keywords:** A2. Czochralski method, B1. Sapphire, A2. Growth from melt, A2. Single crystal growth

## 1. Introduction

Recent increases in demand for LED's has led to a corresponding rise in the demand for materials used in LED production. Various materials may be employed as the substrate for LED's, such as sapphire, Si, SiC and GaN, but currently the most commonly used is sapphire single crystal. Sapphire single crystals may be obtained with good throughput through the CZ method with growth in the c-axis direction. However, sapphire c-axis growth using the CZ method leads to a high dislocation density within crystal, which is 20-100 times higher than for crystals grown by the Kyropoulos(KY) method. High dislocation densities can lead to substrate fracture during GaN deposition or diminished LED efficiency [1, 2].

Bubbles in sapphire single crystals are, along with dislocations, an important defect. Oversaturated O or CO in the melt can be trapped as bubbles at the crystal front(CF) during crystal growth and lead to diminished throughput. Studies regarding this issue have in the past mostly dealt with sapphire grown using the EFG method [3-7]. According to results of previous studies[3-6], bubble entrapment in the crystal is unavoidable during sapphire bulk crystal growth, and the only solution is to control the system in such a way that the bubbles are formed not at the crystal center but at the periphery. As the location of bubble entrapment is governed by the melt flow, controlling the melt flow is an essential aspect in determining sapphire single crystal quality.

In the present study we create a model of a CZ system in which a 4 inch boule is grown with induction heating, and the results are compared against experimentally measured values to evaluate the model effectiveness. We implemented additional heaters to decrease thermal gradient deviations at the CF and flatten the CF shape in order to decrease the dislocation density in the crystal, and obtained corresponding calculated results. We also calculated where bubbles will be trapped in the crystal as a result of the melt flow direction being altered by the additional heater.

## 2. Global modeling of CZ system

### 2.1. Numerical model

In this study, we developed a 2D axis-symmetric global simulation model of a 4 inch boule. As the sapphire single crystal growth is a very slow process, we assume quasi-steady state conditions in the

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