OS10-1

逆算法に基づく PVT 法 AlN 結晶成長における 3D 温度場のシミュレーション

3D Temperature Field Simulation of Physical Vapor Transport for Aluminum Nitride Crystal Growth Based on an Inverse Algorithm

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This study presents a 3D thermal field simulation of aluminum nitride (AlN) physical vapor transport (PVT) process based on Simdroid, the general-purpose multiphysics simulation software. The electromagnetic simulation was conducted to determine the Joule heating distribution using FEM, after which the temperature distribution of the growth system was calculated with the thermal module of the software. The radiation heat transfer was calculated by the view factor method, considering only the surface-to-surface radiation. Additionally, an inverse algorithm was adopted to determine the required power inputs given specified temperature constraints. This simulation process is now seamlessly integrated into the Simdroid, which allows for the convenient simulation of PVT process. The established methodology provides an effective numerical tool for optimizing PVT process parameters, particularly in addressing the dimensional limitations inherent in conventional 2D simulations. This study provides the validation of Simdroid's applicability in PVT thermal design through coupled electromagnetic-thermal simulation, with the separately discussed framework to mass transport, growth kinetics, and thermal stress analysis for PVT process optimization.

Key Words : numerical simulation, physical vapor transport, aluminum nitride, inverse algorithm, thermal optimization

1. Introduction

Aluminum nitride (AlN), a wide-bandgap semiconductor material, holds significant application potential in deep-ultraviolet optoelectronic devices, high-power electronic devices, and other fields [1-2]. However, its ultra-high melting point (>2200° C) and lack of ambient-pressure liquid phase make traditional liquid-phase methods inapplicable. Additionally, at high temperatures, the raw material is prone to decompose into gaseous Al, leading to a complex gas-phase composition and making thermal field control highly challenging. Physical Vapor Transport (PVT) is currently the dominant method for AlN single-crystal growth. However, PVT process is directly influenced by thermal field parameters such as temperature gradients and heat flux distribution. Factors like source sublimation rate, gas-phase transport dynamics, and crystal crystallization quality are all closely tied to the thermal field. Therefore, accurately simulating the thermal field distribution during PVT growth is of critical importance for optimizing process parameters (e.g., crucible structure, heating power).

In this work, based on the low-frequency electromagnetic and thermal modules of Simdroid, the general-purpose multiphysics simulation software, we conducted a 3D thermal field simulation of the aluminum nitride physical vapor transport process. The model considers induction heating, surface-to-surface radiation, heat exchange between the AlN powder, furnace, and gas inside/outside the growth chamber. To determine the required power input under specified temperature conditions at target locations, we developed an efficient inverse algorithm. The thermal field analysis presented here serves as a first step for PVT process simulation.

2. Mathematical model

This section presents the mathematical equations of the AlN growth simulation. The induction heating based growth system is considered here. Global modeling of heat transfer in the furnace involves induction heating by an electromagnetic field, conductive heat transfer in all solid components and radiation heat transfer in all enclosures. The electromagnetic field generated by the induction coils is calculated by deriving and solving Maxwell’s equations. The volume density of the generated heat power can be computed by

$$J_e = \frac{1}{2}\sigma w^2 A A^* \tag{1}$$

Since the crystal growth rate is at the order of μm per hour, it can be assumed that the process be considered steady state. The heat conduction and convection in the solid, powder source and gas regions can all be described by the same equation.

$$\nabla \cdot \left(\rho_g c_p \vec{U} T\right) = \nabla \cdot \left(k_{eff} \nabla T\right) + Q_{th} + Q_r \tag{2}$$

where Q_{th} is the generated heat source by the induction heating. The heat convection term exists in the powder and gas regions, where the velocity in this study is assumed zero.

The specific heat and conductivity of the gas mixture is calculated using mole averaging method, and the conductivity of the powder region is computed by the following formula

$$k_{powder} = k_s(1-\varepsilon) + k_g\varepsilon + \frac{8}{3}\cdot\varepsilon_p\sigma 4T^3\cdot 2r\cdot\varepsilon \tag{3}$$

where the last term models the radiation effect in the internal porous region of the powder source region.

In the AlN crystal growth system, the temperature can be more than 2200℃, thus heat radiation is the most dominant factor for the heat transfer modeling. The radiation simulation implemented here is limited to surface-to-surface radiation, excluding volumetric effects such as absorption and scattering within the participating medium. The hemicube projection based view factor method is adopted in this study.

3. Numerical Algorithm

The thermal simulation of the PVT process involves two steps. Firstly, the electromagnets governing equations are solved by the finite element method for the magnetic field and induction heating power density in the crucible, then the temperature conservation equations for the solid, powder source and inner and outer gas regions are simultaneously solved using conjugate heat transfer boundary conditions. Also, the radiation calculation is coupled through an iteration process. The coupling between electromagnetic and thermal modules is achieved through file-based data transfer: Joule heat density calculated by the electromagnetic solver is projected onto the thermal mesh as a volumetric source term.

In numerical modeling of crystal growth processes, a critical requirement is to determine the input power by enforcing a target temperature at designated points. This is commonly referred as an inverse problem. This inverse problem can be formulated as a PDE constrained optimization problem, and a standard Gauss-Newton algorithm can be adopted [3]. In this study, we utilized a different method by treating the total power as unknown variables in the temperature equation assembling, in addition to the temperature field variables in the normal problem. The algorithm is briefly introduced as follows.

Firstly, the discretized temperature equation coupled conduction and radiation for the whole domain is expressed as follows.

$$[A_T]\{T\} - \lambda\{q_0\} = \{\hat{b}\} \tag{4}$$

where λ is the unknown power coefficient, q_0 is the guessed heating power vector. To determine the heating power, the temperature at some control point P is set as θ_{p}. This equation is regarded as constraint equation to add to the temperature equation (Equation (4)). Thus, the monolithic equation for both the power coefficient and temperatures is as follows.

$$\begin{bmatrix} A_T & -q \\ e_p^T & 0 \end{bmatrix} \begin{Bmatrix} T \\ \lambda \end{Bmatrix} = \begin{Bmatrix} \hat{b} \\ \theta_p \end{Bmatrix} \tag{5}$$

Solving the above monolithic equation using Newton iterations, the power coefficient and the temperature can be obtained simultaneously.

4. Results and Discussions

A typical conventional schematic of the PVT growth setup for the AlN crystal is shown in Fig. 1. The inverse problem mode is defined by setting the target temperature of 2373.15K at the central point of the crystal. The operation pressure is 101325 Pa. A convective heat transfer coefficient of 5.0 $W/m^2 \cdot K$ with an ambient temperature of 303.15 K was used at the furnace's external boundary. The induction heating frequency is 1000 Hz. Approximately 3.5 million elements are used in this simulation. The material properties and computational parameters employed in the simulations are documented in Ref. [4].

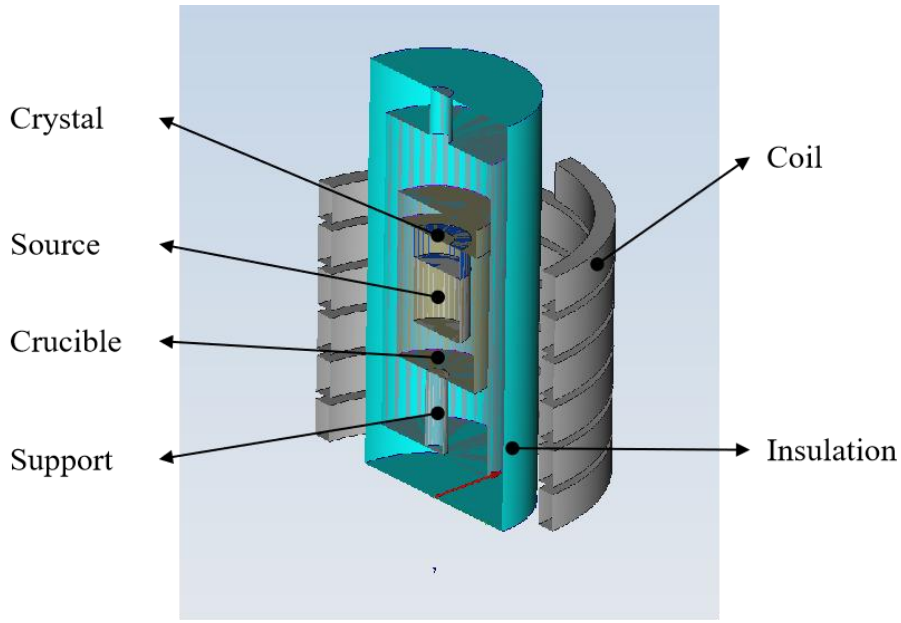
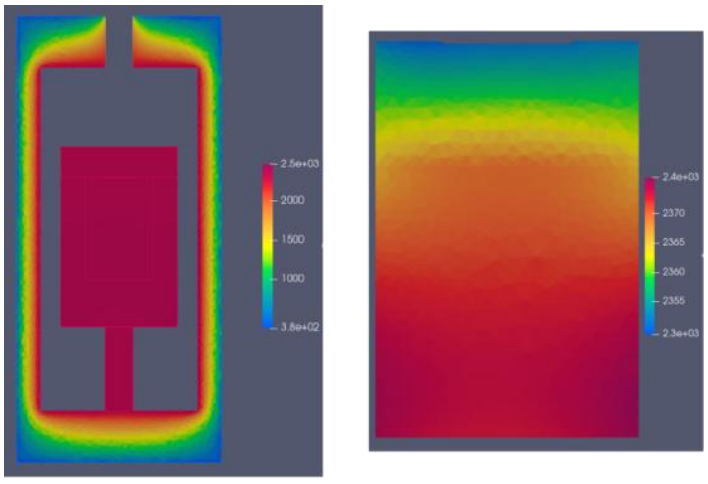


Figure 1 Schematic of the 3D growth system

The calculated temperature field is presented in Fig. 2. Fig 2(a) shows the whole temperature distribution of the whole growth system, while Fig 2(b) shows the temperature inside the chamber.



(a) (b)

Figure 2 Temperature distribution of this study: (a) whole growth system, (b) chamber

5. Conclusion

This study presents a 3D thermal simulation for aluminum nitride PVT crystal growth process within Simdroid, the general-purpose multi-physics simulation software. The related mathematical model and numerical method used in the software are briefly introduced. Besides, an inverse algorithm has been adopted to determine the required power inputs given specified temperature constraints. As the PVT process involves many physical and chemical behaviors, such as mass-flow transfer, chemical reaction, crystal shape evolution and thermal stress, these simulations will be discussed separately.

References

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