Optimal Feedback Control Method using Magnetic Force for Crystal Growth Dynamics

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Abstract - This paper proposes the optimal feedback control method using magnetic force for crystal growth dynamics of semiconductor materials. The system model considered here is described by the continuity, momentum, energy, mass transport, and magnetic induction equations. Receding horizon control is a kind of optimal feedback control in which the control performance over a finite future is optimized with a performance index that has a moving initial time and terminal time. The objective of this study is to propose a receding horizon control method for crystal growth dynamics of semiconductor materials.

Keywords - Optimal control, crystal growth, process control

I. INTRODUCTION

In recent years, the requirement for the high quality of crystal materials has increased dramatically, with the rapid growth of electronic industry. The demand for better crystals has driven extensive research and development in crystal growth technologies. To grow semiconductor crystals with high quality, i.e. with low defect density and good dopant uniformity, the control of mass transport phenomena in thermal fluid dynamics becomes crucial. The crystal growth technology is linked closely with the control of heat flow and mass transfer during phase transformation.

Most of bulk crystals are grown from melt or solution. A number of melt growth technologies have been developed so far. They can be grouped into three configurations, namely, the Czochralski, Bridgman, and zone-melting method. Recent studies on the melt growth technologies have been reviewed in [1]. In contrast, several solution growth technologies have also been developed. One of the most important solution growth technologies is the travelling heater method which is a technique for growing and synthesizing binary and ternary compound semiconductors. Recently, the crystal growth by travelling heater method has attracted much attention in this research field [2–3].

In addition to the development of the crystal growth technologies, controlling the growth actively by external forces is necessary in crystal growth, especially for suppressing unsteady flow and reducing composition non-uniformity. In [4], a mathematical approach to achieve vertical gradient freeze growth of crystals under optimized thermal conditions is provided. Therein, the temperature control is determined by minimizing the tracking errors for prescribed reference trajectories. Thus, the control method in [4] is not based on the feedback approach but feedforward approach.

The research on optimal control of fluid systems can be classified into feedforward control method and feedback control method. That means control methods can be classified into open-loop control methods with off-line optimization and closed-loop control methods. Most studies consider the open-loop control problems because conventional algorithms for solving the optimal control problems of fluid systems are computationally expensive. In general, however, feedback control methods are more robust against disturbance and model errors than feedforward control methods. Therefore, this paper focuses on the optimal feedback control problem of the crystal growth dynamics of semiconductor materials.

Receding horizon control, also known as model predictive control, is a well-established control method [5–12] in which the current control input is obtained by solving a finite-horizon open-loop optimal control problem using the current state of the system as the initial state, and this procedure is repeated at each sampling instant. Thus, receding horizon control is a type of optimal feedback control in which the control performance over a finite future is optimized with a performance index that has a moving initial time and terminal time.

Recently, we have proposed a design method of receding horizon controller for thermal fluid systems governed by continuity, momentum, and energy equations [13–15]. However, the control method for crystal growth dynamics governed by not only continuity, momentum, energy equations but also mass transport, magnetic induction equations. Therefore, the objective of this study is to propose the receding horizon control method using magnetic force for crystal growth dynamics of semiconductor materials.

This paper is organized as follows. In Section II, we introduce some notations and define the system model. In Section III, we consider the optimal control problem for crystal growth dynamics of semiconductor materials. Using the variational principle, we derive the stationary conditions that must be satisfied for a performance index to be optimized. In Section IV, we provide a brief description of the algorithm for numerically solving the obtained stationary conditions. Finally, some concluding remarks are given in Section V.
II. NOTATION AND SYSTEM MODEL

A schematic description of the crystal growth system modeled in this study is shown in Fig. 1. Without loss of generality, we consider the 3-dimensional square spatial domain $\Omega = [0, \ell]^3$. The melt is assumed to be an incompressible and Newtonian metallic liquid. The well-known Boussinesq approximation was adopted, i.e., the melt density was assumed constant everywhere except in the gravitational body force term in the momentum equations. The Lorentz force components due to the applied magnetic field are included in the field equations. Under these assumptions, the governing equations of the melt are given as follows:

Continuity equation
$$\nabla \cdot \mathbf{v} = 0$$ (1)

Momentum equation
$$\frac{\partial \mathbf{v}}{\partial t} = \frac{1}{\rho} \nabla p - \frac{1}{\rho} (\mathbf{v} \cdot \nabla \mathbf{v} + \nabla p) + \frac{1}{\mu_0} (\nabla \times \mathbf{B}) \times \mathbf{B} + \mathbf{g} \left( \beta_T (T - T_i) - \beta_s (C - C_i) \right)$$ (2)

Energy equation
$$\frac{\partial T}{\partial t} = \alpha \nabla^2 T - \mathbf{v} \cdot \nabla T$$ (3)

Mass transport equation
$$\frac{\partial C}{\partial t} = d \nabla^2 C - \mathbf{v} \cdot \nabla C$$ (4)

Magnetic induction equation
$$\frac{\partial \mathbf{B}}{\partial t} = \frac{1}{\mu_0 \sigma} \nabla \mathbf{B} + \nabla \times (\mathbf{v} \times \mathbf{B})$$ (5)

Throughout this paper, let bold and normal notation denote a vector and a scalar, respectively. Thus, $\mathbf{v}$, $\mathbf{B}$, and $\mathbf{g}$ are vectors that denote fluid velocity, magnetic field induction, and acceleration due to gravity, respectively. More precisely, $\mathbf{v}$, $\mathbf{B}$, and $\mathbf{g}$ are defined by
$$\mathbf{v} = \begin{bmatrix} v_1 \\ v_2 \\ v_3 \end{bmatrix}, \quad \mathbf{B} = \begin{bmatrix} B_1 \\ B_2 \\ B_3 \end{bmatrix}, \quad \mathbf{g} = \begin{bmatrix} 0 \\ 0 \\ g \end{bmatrix}.$$ (6)

Let $v_1$, $v_2$, and $v_3$ be velocities along the coordinates $s_1$, $s_2$, and $s_3$, respectively. Let $B_1$, $B_2$, and $B_3$ be magnetic field induction along the coordinates $s_1$, $s_2$, and $s_3$, respectively. Let $g$ denote gravity acceleration along the coordinate $s_3$. For a vector $\mathbf{s}$, let $\mathbf{s}'$ denote its transpose vector.

Boundary region $\partial \Omega_i$ is defined by $\partial \Omega_i = \{ \mathbf{s} \mid s_i = 0, \ell \}$.

Then, boundary conditions are defined as follows. For each $i = 1, 2, 3$, and $s_i = 0, \ell$,
\( \mathbf{v} = 0, \ T = T_b, \ C = C_b, \ \frac{\partial p}{\partial s_j} = 0, \) \hspace{1cm} (7)

where \( T_b \) and \( C_b \) are given constants. For each \( i = 1, 2 \) and \( s_i = 0, \ell, \)

\[ \mathbf{B} = 0. \] \hspace{1cm} (8)

For \( i = 3 \) and \( s_i = 0, \ell, \)

\[ \mathbf{B} = \begin{bmatrix} 0 \\ 0 \\ u \end{bmatrix}. \] \hspace{1cm} (9)

In this study, the perpendicular magnetic field induction \( \mu \) along with \( s_3 \) is considered as the external control input. Here, we introduce the system state \( \mathbf{x} \) defined by

\[ \mathbf{x} = \begin{bmatrix} \mathbf{v} \\ \mathbf{B} \\ T \\ C \end{bmatrix}. \] \hspace{1cm} (10)

For notational convenience, we introduce the following notations:

\[ \mathbf{x}_i(s,t) = \frac{\partial \mathbf{x}(s,t)}{\partial t} = \begin{bmatrix} \frac{\partial x_1(s,t)}{\partial t}, \ldots, \frac{\partial x_n(s,t)}{\partial t} \end{bmatrix} \] \hspace{1cm} (11)

\[ \mathbf{x}'_i(s,t) = \frac{\partial}{\partial s_j} \frac{\partial \mathbf{x}_i(s,t)}{\partial t} = \begin{bmatrix} \frac{\partial'}{\partial s_j} \frac{\partial x_1(s,t)}{\partial t}, \ldots, \frac{\partial'}{\partial s_j} \frac{\partial x_n(s,t)}{\partial t} \end{bmatrix} \] \hspace{1cm} (12)

\[ \int_{s_0}^{s_1} \ldots \int_{s_0}^{s_2} \ldots \int_{s_0}^{s_3} (\cdot) ds_3 ds_2 ds_1 \] \hspace{1cm} (13)

Moreover, let \( \mathbf{F}(\mathbf{x}, \mathbf{x}', \mathbf{x}''') \) be a vector valued function that consists of right hand sides of Eqs. (2)-(5). Using \( \mathbf{F}(\mathbf{x}, \mathbf{x}', \mathbf{x}''') \) in a general form, we can rewrite the system model (1)-(5) as a single time-evolutionary equation and a state constraint shown below.

\[ \mathbf{x}_t = \mathbf{F}(\mathbf{x}, \mathbf{x}', \mathbf{x}'') \] \hspace{1cm} (14)

\[ \nabla \cdot [x_1 \ x_2 \ x_3] = 0 \] \hspace{1cm} (15)

Note that the crystal growth dynamics considered in this paper can be described by Eqs. (14) and (15).

### III. Optimal Control Method

In this section, we consider the optimal control problem for crystal growth dynamics governed by Eqs. (14) and (15). Using the variational principle, we analytically derive the stationary conditions that must be satisfied for a performance index to be optimized. For this purpose, we exploit integrations by parts, which play an important role in this study.

The control input at each time \( t \) is determined so as to minimize the following performance index:

\[ J = \int_\Omega \phi(\mathbf{x}(s,t+T))ds + \int_{t-T}^{t} \int_\Omega L(\mathbf{x}(s,t),u(s,t))dtds, \] \hspace{1cm} (16)

where \( T \) is the evaluation interval of the performance index, \( w_i \) for \( i = 1, 2, 3, \) are weight coefficients, and \( C_r \) is the desired concentration. \( \phi \) is called the terminal cost function, and \( L \) is called the stage cost function.

The minimization problem of (16) subject to constraints (14) and (15) can be reduced to minimization problem of the following performance index introduced using the costate \( \lambda \) associated with (14) and the Lagrange multiplier \( \eta \) associated with (15):

\[ \overline{J} = \int_\Omega \phi(\mathbf{x}(s,t+T))ds + \int_{t-T}^{t} \int_\Omega \left[ H(\mathbf{x}(s,t),u(s,t)) - \lambda(s,t) \frac{\partial \mathbf{x}}{\partial t} \right] dtds, \] \hspace{1cm} (17)

where \( H \) denotes the Hamiltonian defined by

\[ H = L + \lambda \cdot \mathbf{F} + \eta \left( \nabla \cdot \mathbf{v} \right). \] \hspace{1cm} (18)

Let \( \delta \overline{J}, \delta \mathbf{x}, \delta \mathbf{x}', \delta p, \delta u, \delta \lambda, \) and \( \delta \eta \) denote the variations (infinitesimal changes) in \( \overline{J}, \mathbf{x}, \mathbf{x}', \mathbf{x}''', \mathbf{p}, \mathbf{u}, \lambda, \) and \( \eta, \) respectively. Since the optimal solution must satisfy the stationary condition \( \delta \overline{J} = 0, \) we need to consider the variation \( \delta \overline{J} \) due to the variations \( \delta \mathbf{x}, \delta \mathbf{x}', \delta \mathbf{x}''', \delta \mathbf{p}, \delta \mathbf{u}, \delta \lambda, \) and \( \delta \eta. \) Then, we need to calculate the following equation:
\[ \delta \tilde{J} = \int_{\Omega} \left( \frac{\partial \phi}{\partial x_i} \right) \delta x_i (s, t + T) ds + \int_{0}^{t+T} \int_{\Omega} \left[ \frac{\partial H}{\partial x_i} \right] \delta x_i (s, \tau) + \frac{\partial H}{\partial u} \delta u (s, \tau) \delta \lambda (s, \tau) + \frac{\partial H}{\partial \eta} \delta \eta (s, \tau) \right] ds d\tau \]

(23)

Applying the Taylor expansion into the first term of the right hand side in the above equation and neglecting the high order terms of each variation, we can compute the variation in \( \tilde{J} \). Thus, \( \delta \tilde{J} \) can be given as follows:

\[ \delta \tilde{J} = \int_{\Omega} \left[ \frac{\partial H}{\partial x_i} \right] \delta x_i (s, t + T) ds \]

(24)

From boundary condition (9), we have

\[ \delta x_6 = \delta u \quad \text{for } s \in \partial \Omega. \]

(25)

Applying Eqs. (22)-(25) to the computation of \( \delta \tilde{J} \) in (20) and using the variational principle, we obtain the necessary conditions for a stationary value of \( \tilde{J} \) over the evaluation interval as follows. For \( s \in \Omega \), we obtain

\[ x_i = F(x, x_i, x_i). \]

(26)

\[ \nabla \cdot v = 0, \]

(27)

\[ \lambda (s, t + T) = \begin{bmatrix} 0 \\ \vdots \\ 0 \end{bmatrix}, \]

(28)

\[ \frac{\partial \lambda_B}{\partial \mu} = -\frac{1}{\mu^2} \nabla^2 \lambda_B + \frac{1}{\rho} \left( \lambda_B \frac{\partial v}{\partial \lambda_B} - \frac{\partial \lambda_B}{\partial \lambda_B} \right) \]

(29)

\[ \frac{\partial \lambda_B}{\partial \mu} = -\frac{1}{\mu_0 \sigma} \nabla^2 \lambda_B - \left( \nabla \cdot \lambda_B \right) \times v \]

(30)

\[ \frac{\partial \lambda_B}{\partial \lambda_B} = -\frac{1}{\mu_0 \sigma} \nabla^2 \lambda_B - \left( \nabla \cdot \lambda_B \right) \times v \]

(31)
\[ \frac{\partial \lambda}{\partial \tau} = -d \nabla^2 \lambda + g \beta \lambda - w_2 (C - C_r) \]  
\[ \nabla' (\lambda \nu), \]  
\[ \nabla \cdot \lambda = 0. \]  
\[ \lambda = 0, \quad \eta = 0. \]  
\[ w_1 u - h(s_j) \left( \frac{1}{\mu} \frac{\partial \lambda}{\partial \delta} - \lambda v_1 - \lambda v_2 \right) = 0. \]  
In the above, the following notations are adopted.

\[ A \otimes B := \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \otimes \begin{bmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{bmatrix} = \begin{bmatrix} a_{11} b_{11} & a_{12} b_{12} \\ a_{21} b_{21} & a_{22} b_{22} \end{bmatrix} \]  
\[ \lambda = \begin{bmatrix} \lambda_1 \\ \lambda_2 \\ \lambda_3 \end{bmatrix}, \quad \lambda_B = \begin{bmatrix} \lambda_4 \\ \lambda_5 \\ \lambda_6 \end{bmatrix} \]  
\[ E_j := \begin{bmatrix} \lambda_1 & \lambda_2 & \lambda_3 \\ \lambda_1 & \lambda_2 & \lambda_3 \\ \lambda_1 & \lambda_2 & \lambda_3 \end{bmatrix} \]  
\[ h(s_j) = \begin{cases} 1 & (s_j = 1) \\ -1 & (s_j = 0) \end{cases} \]  
Conditions (26)-(35) are called the stationary conditions, which must be satisfied for the performance index (17) to be minimized. A well-known difficulty in solving nonlinear optimal control problems is that the obtained stationary conditions cannot be solved analytically in general.

IV. NUMERICAL ALGORITHM

Although we have analytically derived the exact stationary condition in Section III, we need a numerical algorithm for solving the stationary conditions. In the following, we provide a framework in which a fast on-line algorithm is applicable for solving the receding horizon control problem of crystal growth dynamics.

Here, note that the stationary conditions contain two time-evolutionary equations with respect to \( x \) and \( \lambda \). The others are algebraic equations, and (34) is considered as the boundary conditions for the time-evolutionary equation of \( \lambda \). For a given initial solution candidate \( u(s, \tau), (t \leq \tau \leq t + T) \) and the present state \( x(t) \), we first determine \( x(s, \tau), (t \leq \tau \leq t + T) \) and \( p(s, \tau), (t \leq \tau \leq t + T) \) by numerically solving (26) and (27) with boundary conditions (7)-(9) from \( \tau = t \) to \( \tau = t + T \). Then, terminal costate \( \lambda(s, t + T) \) is determined from the obtained terminal state \( x(s, t + T) \) by (28). Then, \( \lambda(s, \tau), (t \leq \tau \leq t + T) \) and \( \eta(s, \tau), (t \leq \tau \leq t + T) \) are also determined by numerically solving (29)-(33) with boundary conditions (34) from \( \tau = t + T \) to \( \tau = t \). Figure 2 shows that the procedure for solving the time-evolutionary equation of \( x \) is forward, whereas the one for solving the time-evolutionary equation of \( \lambda \) is backward.

For given \( u(s, \tau), (t \leq \tau \leq t + T) \) and \( x(t), x(s, \tau) \) and \( \lambda(s, \tau) \) for \( t \leq \tau \leq t + T \) are determined so as to satisfy the stationary conditions (26)-(34). However, the remaining stationary condition (35) is not necessary satisfied for determined \( u(s, \tau), x(s, \tau) \), and \( \lambda(s, \tau) \). If the stationary condition (35) is satisfied for determined \( u(s, \tau), x(s, \tau) \), and \( \lambda(s, \tau) \), then we can obtain the solutions that satisfy all the stationary conditions (26)-(35). Several algorithms have been developed such that the norm of left hand side of (35) can be decreased by suitably updating \( u(s, \tau), (t \leq \tau \leq t + T) \).

A conventional way of updating \( u(s, \tau) \) is to replace \( u(s, \tau) + \alpha h, \) which is known as the steepest descent method, where \( h \) is the steepest descent direction and \( \alpha \) is the step length satisfying Armijo condition. For Newton’s method, \( h \) is given by the Hessian instead of the gradient. However, these methods are computationally expensive. Recently, we have developed a more efficient algorithm called the contraction mapping method [16]. The contraction mapping method provides a satisfactory tradeoff between computational burden and error performance through the selection of design parameter. More detailed information about the implementation of the contraction mapping method is provided in [16].

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V. CONCLUSION
This paper proposed the optimal feedback control method using magnetic force for crystal growth dynamics of semiconductor materials. The system model considered here is described by the continuity, momentum, energy, mass transport, and magnetic induction equations. For this system, we first formulated the optimal control problem for suppressing unsteady flow and reducing composition non-uniformity. Next, we analytically derived the stationary conditions that must be satisfied for the performance index to be minimized. Finally, we established a fast on-line algorithm for solving the obtained stationary conditions. To conduct numerical simulations for verifying the effectiveness of the proposed method is an important future work.

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