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Model Predictive Control Using Thermal Inputs for Crystal Growth Dynamics

Takashi Shimizu, Tomoaki Hashimoto

***Abstract*—**Recently, crystal growth technologies have made progress by the requirement for the high quality of crystal materials. To control the crystal growth dynamics actively by external forces is useful for reducing composition non-uniformity. In this study, a control method based on model predictive control using thermal inputs is proposed for crystal growth dynamics of semiconductor materials. The control system of crystal growth dynamics considered here is governed by the continuity, momentum, energy, and mass transport equations. To establish the control method for such thermal fluid systems, we adopt model predictive control known as 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 establish a model predictive control method for crystal growth dynamics of semiconductor materials.

***Keywords*—**Model predictive control, optimal control, crystal growth, process control

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I. Introduction

In recent decades, the requirement for the high quality of crystal materials has driven extensive research and development in crystal growth technologies. To grow semiconductor crystals with high quality, the control of mass transport phenomena in thermal fluid dynamics becomes crucial. The crystal growth technology is related with the control of heat flow and mass transfer during phase transformation. Controlling the crystal growth actively by external forces is necessary, especially for suppressing unsteady flow and reducing composition non-uniformity.

Model predictive control (MPC) is a well-established control method 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, model predictive 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. So far, several MPC methods have been proposed for fluid systems [1]-[4], spatiotemporal dynamic systems [5]-[10], Schrödinger systems [11], [12], stochastic systems [13]-[15], and probabilistic constrained systems [16]-[18].

The objective of this study is to propose a model predictive control method using thermal inputs for crystal growth dynamics of semiconductor materials. Crystal growth dynamics are governed by not only continuity, momentum, energy equations but also mass transport equations. Therefore, the objective of this study is to propose a model predictive control method to achieve the uniform concentration in thermal fluid systems with taking mass transport phenomena into consideration.

This paper is organized as follows. In Section II, we introduce some notations and define the system model. In Section III, we consider the model predictive control problem for mass transport phenomena in thermal fluid systems with boundary control inputs. 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.

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T. Shimizu and T. Hashimoto are with the Department of Mechanical Engineering, Osaka Institute of Technology, Asahi-ku 535-8585, Japan (e-mail: info@thashi.net).

TABLE I
System Parameters

$v(t,s)$	velocity
$p(t,s)$	pressure
$\theta(t,s)$	temperature
$c(t,s)$	concentration
$u(t,s)$	thermal input
ρ	density
ν	kinematic viscosity
θ_0	standard temperature
c_0	standard concentration
β_θ	thermal expansion coefficient
β_c	solute expansion coefficient
α_θ	thermal diffusivity
α_c	solute diffusivity
g	gravitational acceleration

II. Notation and System Model

Let $s = [s_1, s_2]^{\mathrm{T}}$ and t denote a spatial vector and temporal variable, respectively. For a matrix A, the transpose of A is denoted by A^{T}.

In this study, we restrict our attention to the range $0 \leq s_i \leq \ell$ for $i = 1, 2$.

Let Ω be the set defined by $\Omega := \prod_{i=1}^{2} \{s_i | 0 \leq s_i \leq \ell\}$.

Crystal growth dynamics of semiconductor materials are governed by continuity, momentum, energy, and mass transport equations. Thus, the system equations considered here are described as follows:

- Continuity equation:

$$\frac{\partial v_1}{\partial s_1}(t,s) + \frac{\partial v_2}{\partial s_2}(t,s) = 0 \tag{1a}$$

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- Momentum equations:

$$\frac{\partial v_1}{\partial t}(t,s) = -\left(v_1\frac{\partial v_1}{\partial s_1}(t,s) + v_2\frac{\partial v_1}{\partial s_2}(t,s) + \frac{1}{\rho}\frac{\partial p}{\partial s_1}(t,s)\right) + \nu\left(\frac{\partial^2 v_1}{\partial s_1^2}(t,s) + \frac{\partial^2 v_1}{\partial s_2^2}(t,s)\right) \tag{1b}$$

$$\frac{\partial v_2}{\partial t}(t,s) = -\left(v_1\frac{\partial v_2}{\partial s_1}(t,s) + v_2\frac{\partial v_2}{\partial s_2}(t,s) + \frac{1}{\rho}\frac{\partial p}{\partial s_2}(t,s)\right) + \nu\left(\frac{\partial^2 v_2}{\partial s_1^2}(t,s) + \frac{\partial^2 v_2}{\partial s_2^2}(t,s)\right) + g\beta_\theta\left(\theta(t,s) - \theta_0\right) - g\beta_c\left(c(t,s) - c_0\right) \tag{1c}$$

- Energy equation:

$$\frac{\partial \theta}{\partial t}(t,s) = -\left(v_1\frac{\partial \theta}{\partial s_1}(t,s) + v_2\frac{\partial \theta}{\partial s_2}(t,s)\right) + \alpha_\theta\left(\frac{\partial^2 \theta}{\partial s_1^2}(t,s) + \frac{\partial^2 \theta}{\partial s_2^2}(t,s)\right) \tag{1d}$$

- Mass transport equation:

$$\frac{\partial c}{\partial t}(t,s) = -\left(v_1\frac{\partial c}{\partial s_1}(t,s) + v_2\frac{\partial c}{\partial s_2}(t,s)\right) + \alpha_c\left(\frac{\partial^2 c}{\partial s_1^2}(t,s) + \frac{\partial^2 c}{\partial s_2^2}(t,s)\right) \tag{1e}$$

The system parameters used in (1) are listed in Table I. In this study, the fluid is assumed to be an incompressible and Newtonian liquid in two-dimensional square domain Ω as shown in Fig. 1.

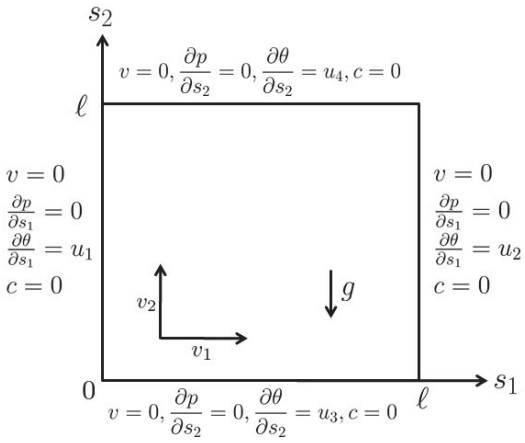


Fig. 1 A schematic view of system model

We adopt the Boussinesq approximation, in which density differences are neglected except when they induce the buoyancy. The equation of continuity (1a) implies the mass conservation. The momentum equations (1b) and (1c), also called the Navier-Stokes equations, implies the momentum conservation law. These two equations describe the motion of the incompressible flow. The equations of energy (1d) and mass transport (1e) govern temperature and concentration changes in the flow, respectively.

The boundary conditions are given as follows:

$$v = 0,\ \frac{\partial p}{\partial s_1} = 0,\ \frac{\partial \theta}{\partial s_1} = u_1,\ c = 0 \quad \text{for } s_1 = 0 \tag{2a}$$

$$v = 0,\ \frac{\partial p}{\partial s_1} = 0,\ \frac{\partial \theta}{\partial s_1} = u_2,\ c = 0 \quad \text{for } s_1 = \ell \tag{2b}$$

$$v = 0,\ \frac{\partial p}{\partial s_2} = 0,\ \frac{\partial \theta}{\partial s_2} = u_3,\ c = 0 \quad \text{for } s_2 = 0 \tag{2c}$$

$$v = 0,\ \frac{\partial p}{\partial s_2} = 0,\ \frac{\partial \theta}{\partial s_2} = u_4,\ c = 0 \quad \text{for } s_2 = \ell \tag{2d}$$

Note that the gradient of temperature in the boundary region is considered as the control input $u = [u_1\ u_2\ u_3\ u_4]^{\mathrm{T}}$. Let x be defined by $x := [v_1\ v_2\ \theta\ c]^{\mathrm{T}}$. For notational simplicity, we introduce $f(x,p)$ such that system equations (1b)-(1e) can be rewritten as

$$\frac{\partial x}{\partial t}(t,s) = f(x,p). \tag{3}$$

III. Model Predictive Control

In this section, we consider the model predictive control problem for crystal growth dynamics governed by system equation (1). 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 integration by parts that plays an important role in this study.

The control input at each time t is determined so as to minimize the performance index given by

$$J = \int_0^\ell\int_0^\ell \varphi\left(c(t+T,s)\right) ds_1 ds_2 + \int_t^{t+T}\int_0^\ell\int_0^\ell L\left(c(\tau,s), u(\tau,s)\right) ds_1 ds_2 d\tau.$$

$$\varphi := \frac{w_1}{2}\left(c(t+T,s) - c_f\right)^2 \tag{4a}$$

$$L := \frac{w_2}{2}\left(c(\tau,s) - c_f\right)^2 + \frac{w_3}{2}u^{\mathrm{T}}(\tau,s)u(\tau,s) \tag{4b}$$

where T is the evaluation interval of the performance index, c_f is the desired concentration, w_i $(i = 1,2,3)$ are weight coefficients, φ is the terminal cost function, and L is the cost function over the prediction horizon.

The minimization problem of performance index (4) subject to system equation (1) can be reduced to the minimization of the following performance index introduced using the costate $\lambda := [\lambda_1\ \lambda_2\ \lambda_3\ \lambda_4]^{\mathrm{T}}$ and Lagrange multiplier η associated with system equation (3) and equality constraint (1a), respectively:

$$\bar{J} = \int_0^\ell\int_0^\ell \phi\left(x_4(t+T,s)\right) ds_1 ds_2 + \int_t^{t+T}\int_0^\ell\int_0^\ell \Big\{ L\left(x_4(\tau,s), u(\tau,s)\right) + \lambda^{\mathrm{T}}(\tau,s)\left(f(x,p) - \frac{\partial x}{\partial \tau}(\tau,s)\right) + \eta(\tau,s)\left(\frac{\partial x_1}{\partial s_1}(\tau,s) + \frac{\partial x_2}{\partial s_2}(\tau,s)\right)\Big\} ds_1 ds_2 d\tau \tag{5}$$

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For notational simplicity, we introduce the Hamiltonian H defined by

$$H = L\left(x_4(\tau,s), u(\tau,s)\right) + \lambda^{\mathrm{T}}(\tau,s) f(x,p) + \eta(\tau,s)\left(\frac{\partial x_1}{\partial s_1}(\tau,s) + \frac{\partial x_2}{\partial s_2}(\tau,s)\right). \tag{6}$$

Furthermore, we adopt the following notations:

$$x_s(i,j) := \frac{\partial x_i}{\partial s_j}(\tau,s),$$
$$x_{ss}(i,j) := \frac{\partial^2 x_i}{\partial s_j^2}(\tau,s)$$
$$H_{x_s(i,j)} := \frac{\partial H}{\partial x_s(i,j)}(x,p,\lambda,\eta),$$
$$H_{x_{ss}(i,j)} := \frac{\partial H}{\partial x_{ss}(i,j)}(x,p,\lambda,\eta)$$

Let δ denote the variation (infinitesimal change). It is well known that $\delta\bar{J} = 0$ must be satisfied for performance index $\bar{J}$ to be minimized. Note that we must perform the following integration by parts for the computation of $\delta\bar{J}$. It is important to note that we can obtain the following equations using integration by parts.

$$\begin{aligned}&\int_0^\ell \int_0^\ell \left(H_{x_s(i,j)} \frac{\partial \delta x_i}{\partial s_j}(\tau,s)\right) ds_1 ds_2 \\ &= \int_0^\ell \left[H_{x_s(i,j)} \delta x_i(\tau,s)\right]_0^\ell ds_{\{1,2\}\setminus\{j\}} \\ &- \int_0^\ell \int_0^\ell \left(\frac{\partial H_{x_s(i,j)}}{\partial s_j} \delta x_i(\tau,s)\right) ds_1 ds_2 \end{aligned} \tag{7}$$

$$\begin{aligned}&\int_0^\ell \int_0^\ell \left(H_{x_{ss}(i,j)} \frac{\partial^2 \delta x_i}{\partial s_j^2}(\tau,s)\right) ds_1 ds_2 \\ &= \int_0^\ell \left[H_{x_{ss}(i,j)} \frac{\partial \delta x_i}{\partial s_j}(\tau,s) - \frac{\partial H_{x_{ss}(i,j)}}{\partial s_j} \delta x_i(\tau,s)\right]_0^\ell ds_{\{1,2\}\setminus\{j\}} \\ &+ \int_0^\ell \int_0^\ell \left(\frac{\partial^2 H_{x_{ss}(i,j)}}{\partial s_j^2} \delta x_i(\tau,s)\right) ds_1 ds_2 \end{aligned} \tag{8}$$

It is also important to note that we can obtain the following equation using integration by parts.

$$\begin{aligned}&\int_t^{t+T} -\lambda^{\mathrm{T}}(\tau,s) \frac{\partial \delta x(\tau,s)}{\partial \tau} d\tau \\ &= \left[-\lambda^{\mathrm{T}}(\tau,s)\delta x(\tau,s)\right]_t^{t+T} + \int_t^{t+T} \left(\frac{\partial \lambda(\tau,s)}{\partial \tau}\right)^{\mathrm{T}} \delta x(\tau,s) d\tau \\ &= -\lambda^{\mathrm{T}}(t+T,s)\delta x(t+T,s) + \int_t^{t+T} \left(\frac{\partial \lambda(\tau,s)}{\partial \tau}\right)^{\mathrm{T}} \delta x(\tau,s) d\tau \end{aligned} \tag{9}$$

In the above equation, we set $\delta x(t,s) = 0$ because $x(\tau,s)$ is fixed at $\tau = t$ as the present state.

From boundary conditions (2a)–(2d), we can obtain the following equations:

$$\begin{bmatrix} \delta x_1(\tau,s) \\ \delta x_2(\tau,s) \\ \delta x_4(\tau,s) \end{bmatrix} = 0, \quad \text{for } s_j = 0,\ell, \quad j = 1,2 \tag{10a}$$
$$\frac{\partial p}{\partial s_j}(\tau,s) = 0 \quad \text{for } s_j = 0,\ell, \quad j = 1,2 \tag{10b}$$
$$\frac{\partial \delta x_3}{\partial s_1}(\tau,s) = \delta u_1(\tau,s) \quad \text{for } s_1 = 0 \tag{10c}$$
$$\frac{\partial \delta x_3}{\partial s_1}(\tau,s) = \delta u_2(\tau,s) \quad \text{for } s_1 = \ell \tag{10d}$$
$$\frac{\partial \delta x_3}{\partial s_2}(\tau,s) = \delta u_3(\tau,s) \quad \text{for } s_2 = 0 \tag{10e}$$
$$\frac{\partial \delta x_3}{\partial s_2}(\tau,s) = \delta u_4(\tau,s) \quad \text{for } s_2 = \ell \tag{10f}$$

Using (7)-(10), we compute the variation in J. On the basis of the variational principle, we obtain the necessary conditions $\delta\bar{J} = 0$ for a stationary value of J over the horizon $(t \le \tau \le t+T)$ as follows.

- The governing equations of x and p:

$$\frac{\partial x}{\partial \tau}(\tau,s) = f(x,p) \tag{11a}$$
$$\frac{\partial x_1}{\partial s_1}(\tau,s) + \frac{\partial x_2}{\partial s_2}(\tau,s) = 0 \tag{11b}$$

- Terminal condition

$$\lambda(t+T,s) = \begin{bmatrix} 0 \\ 0 \\ 0 \\ w_1\left(x_4(t+T,s) - c_f\right) \end{bmatrix} \tag{12}$$

- The governing equations of λ and η:

$$\begin{aligned}\frac{\partial \lambda_1}{\partial \tau}(\tau,s) = &-\nu\left(\frac{\partial^2 \lambda_1}{\partial s_1^2}(\tau,s) + \frac{\partial^2 \lambda_1}{\partial s_2^2}(\tau,s)\right) \\ &+ \lambda_1 \frac{\partial x_1}{\partial s_1}(\tau,s) + \lambda_2 \frac{\partial x_2}{\partial s_1}(\tau,s) \\ &- \left(x_1 \frac{\partial \lambda_1}{\partial s_1}(\tau,s) + x_2 \frac{\partial \lambda_1}{\partial s_2}(\tau,s)\right) \\ &+ \lambda_3 \frac{\partial x_3}{\partial s_1}(\tau,s) + \lambda_4 \frac{\partial x_4}{\partial s_1}(\tau,s) + \frac{\partial \eta}{\partial s_1}(\tau,s)\end{aligned} \tag{13a}$$

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$$\frac{\partial \lambda_2}{\partial \tau}(\tau,s) = -\nu\left(\frac{\partial^2 \lambda_2}{\partial s_1^2}(\tau,s) + \frac{\partial^2 \lambda_2}{\partial s_2^2}(\tau,s)\right) + \lambda_1 \frac{\partial x_1}{\partial s_2}(\tau,s) + \lambda_2 \frac{\partial x_2}{\partial s_2}(\tau,s) - \left(x_1 \frac{\partial \lambda_2}{\partial s_1}(\tau,s) + x_2 \frac{\partial \lambda_2}{\partial s_2}(\tau,s)\right) + \lambda_3 \frac{\partial x_3}{\partial s_2}(\tau,s) + \lambda_4 \frac{\partial x_4}{\partial s_2}(\tau,s) + \frac{\partial \eta}{\partial s_2}(\tau,s) \tag{13b}$$

$$\frac{\partial \lambda_3}{\partial \tau}(\tau,s) = -\alpha_\theta\left(\frac{\partial^2 \lambda_3}{\partial s_1^2}(\tau,s) + \frac{\partial^2 \lambda_3}{\partial s_2^2}(\tau,s)\right) - \left(x_1 \frac{\partial \lambda_3}{\partial s_1}(\tau,s) + x_2 \frac{\partial \lambda_3}{\partial s_2}(\tau,s)\right) - g\beta_\theta \lambda_2(\tau,s) \tag{13c}$$

$$\frac{\partial \lambda_4}{\partial \tau}(\tau,s) = -\alpha_c\left(\frac{\partial^2 \lambda_4}{\partial s_1^2}(\tau,s) + \frac{\partial^2 \lambda_4}{\partial s_2^2}(\tau,s)\right) - \left(x_1 \frac{\partial \lambda_4}{\partial s_1}(\tau,s) + x_2 \frac{\partial \lambda_4}{\partial s_2}(\tau,s)\right) + g\beta_c \lambda_2(\tau,s) - w_2\left(x_4(\tau,s) - c_f\right) \tag{13d}$$

$$\frac{\partial \lambda_1}{\partial s_1}(\tau,s) + \frac{\partial \lambda_2}{\partial s_2}(\tau,s) = 0 \tag{14}$$

- Boundary conditions for λ and η:

$$\lambda(\tau,s) = 0, \quad \frac{\partial \eta}{\partial s_j}(\tau,s) = 0 \ \text{ for } \ s_j = 0, \ell, \ \ j = 1,2 \tag{15}$$

- Optimality conditions:

$$w_3 u_1(\tau,s) - \alpha_\theta \lambda_3 = 0, \ \text{ for } \ s_1 = 0 \tag{16a}$$
$$w_3 u_2(\tau,s) + \alpha_\theta \lambda_3 = 0, \ \text{ for } \ s_1 = \ell \tag{16b}$$
$$w_3 u_3(\tau,s) - \alpha_\theta \lambda_3 = 0, \ \text{ for } \ s_2 = 0 \tag{16c}$$
$$w_3 u_4(\tau,s) + \alpha_\theta \lambda_3 = 0, \ \text{ for } \ s_2 = \ell \tag{16d}$$

Equations (11)–(16) are called the stationary conditions or KKT conditions that must be satisfied for performance index (5) to be minimized. Equations (11a) and (11b) are the time-evolutionary equations of the state x and the equality constraint of the pressure p, respectively. Equation (12) is called the terminal condition. Equations (13) and (14) are the time-evolutionary equations of the costate λ and the equality constraint of the Lagrange multiplier η, respectively. Equations in (15) are the boundary conditions of the costate λ and the Lagrange multiplier η. The remaining condition (16) is called the optimality condition.

A well-known difficulty in solving nonlinear optimal control problems is that the obtained stationary conditions cannot be solved analytically in general.

IV. Numerical Solution

Although we have analytically derived the exact stationary conditions in Section III, we need a numerical algorithm to solve the stationary conditions. In this section, we provide a framework so that the fast algorithm called the contraction mapping method [8] is applicable for solving the model predictive control problem of crystal growth dynamics.

In the following, we provide a brief description of the numerical method for solving stationary conditions (11)–(16). Several numerical algorithms are applicable to solving equations (11a) and (11b). In general, the solution obtained by simply integrating time-evolutionary equation (11a) does not satisfy continuity equation (11b). Note that $f(x,p)$ in (11a) contains unknown variable p. Hence, we can consider p as the flexible parameter to be adjusted for satisfying continuity equation (11b). We adopt here the simplified marker and cell (SMAC) method, in which p is updated through the integration of (11a) so as to satisfy (11b). Hence, using the SMAC method, we can determine $x(\tau,s)$ and $p(\tau,s)$ over the prediction horizon $(t \le \tau \le t+T)$ from $\tau = t$ to $\tau = t+T$.

Furthermore, the terminal costate $\lambda(t+T,s)$ is determined by (12). Note that there is a duality between equations (11a), (11b) and (13), (14). Hence, the SMAC method also can be applied to solve (13), (14) using the boundary conditions in (15). Then, $\lambda(\tau,s)$ and $\eta(\tau,s)$ can be calculated from $\tau = t+T$ to $\tau = t$ using (13)–(15). Fig. 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 λ is backward.

Consequently, for the present state $x(t,s)$ and a given solution candidate $u(\tau,s)$, $x(\tau,s)$, $p(\tau,s)$, $\lambda(\tau,s)$, and $\eta(\tau,s)$ are determined over the prediction horizon $(t \le \tau \le t+T)$. Then, the optimization problem can be reduced to solving single condition (16).

For the present state $x(t,s)$ and a given solution candidate $u(\tau,s)$, the optimality condition (16) is not necessarily satisfied. If optimality condition (16) is not satisfied, the solution candidate $u(\tau,s)$ needs to be suitably updated so as to satisfy optimality condition (16). Here, we adopt the contraction mapping method [8] for updating $u(\tau,s)$ so as to satisfy optimality condition (16).

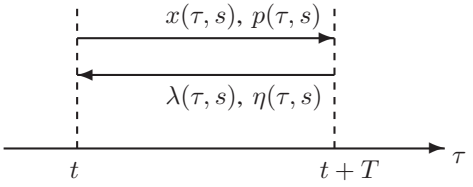


Fig. 2 Procedure used for obtaining numerical solutions

V. Conclusion

This paper proposed the model predictive control method using thermal inputs for crystal growth dynamics of semiconductor materials. The system model considered here is described by the continuity, momentum, energy, and mass transport equations. For this system, we first formulated the model predictive control problem for 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 algorithm for solving the obtained stationary conditions. To conduct numerical simulations for verifying the effectiveness of the

proposed method is an important future work. It is known that time delays may cause instabilities of the closed-loop system and lead to more complex analysis [19]-[24]. The control problem of the system with time delays is also a possible future work.

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