MPC Based Feedforward Trajectory for Pulling Speed Tracking Control in the Commercial Czochralski Crystallization Process

Kihong Lee, Dongki Lee, Jinguk Park, and Moonyong Lee*

Abstract: In this work, we propose a simple but efficient method to design a target temperature trajectory for pulling speed tracking control of the crystal grower in the Czochralski crystallization process. In the suggested method, the model predictive control strategy is used to incorporate the complex dynamic effect of the heater temperature on the pulling speed into the temperature trajectory design quantitatively. The feedforward trajectories designed by the proposed method were implemented on 200 mm and 300 mm silicon crystal growers in the commercial Czochralski process. The application results have demonstrated its excellent and consistent tracking performance of pulling speed along whole bulk crystal growth.

Keywords: Czochralski crystallization process, feedforward trajectory design, model predictive control, semi-conductor wafer, silicon crystal control.

1. INTRODUCTION

Czochralski (CZ) silicon-crystal technology has emerged as an indispensable technology for semiconductor wafer production and has shown continuous progress over the years in terms of crystal size and quality. Silicon wafers with diameters up to 200mm are now routinely used, while production of 300mm wafers with ultra high quality is rapidly expanding [1]. CZ crystal growth is accomplished by melting the material to be crystallized in an open crucible and then touching the melted surface with a seed crystal of the desired material and crystallographic orientation. In the CZ crystallization process, a single silicon-crystal is grown from the melt by pulling a seed crystal very slowly while maintaining a desired thermal environment in the furnace.

The important operational objectives of the CZ crystal grower are to attain a constant radius, with a low concentration of impurities and dislocations, and a uniform dopant distribution. To achieve the operation goal, the classical PID controllers in a cascade configuration combined with empirically derived feedforward trajectories are still the most widely utilized in commercial CZ crystal growers. Although there have been several research efforts to apply state of the art control techniques to the control of the CZ crystal growers [2-4], no open report for the real implementation of the advanced techniques on the commercial growers has been available thus far.

In the conventional control scheme of the CZ crystal grower, the crystal diameter is controlled by manipulating the pulling speed of the crystal. At the same time, concentration and distributions of point defects in the crystal are also mainly affected by the crystal growth rate of which optimal values vary along the crystal growth [1]. For this reason, the pulling speed itself should also track a target trajectory, which is predetermined by experiments, precisely along the whole bulk crystal growth. Tight and precise tracking control of the pulling speed is very crucial especially for wafer production with larger diameter and higher quality specification.

Tracking control of the pulling speed can be achieved by adjusting the heater power input to the crystal grower. However, complex dynamics with a large lag time through the heater, crucible, melt, meniscus, and crystal makes it quite difficult to achieve satisfactory tracking performance with the feedback control only. For this reason, a feedforward trajectory for the heater temperature is often added to the feedback control signal. In the real field, however, the feedforward trajectory has been typically designed and/or updated merely based on the intuition and experience of the process engineer, which often leads to poor and inconsistent tracking performance of the pulling speed and thus poor crystal quality.

In this work, we present a simple but efficient

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method to design the feedforward trajectory of the heater temperature for commercial CZ crystal growers. The proposed method utilizes the model predictive control technique to incorporate the complex dynamic effect into the feedforward trajectory design, quantitatively. Through the actual implementation on the commercial CZ crystal grower, the proposed method has been found to perform quite satisfactorily.

2. CONVENTIONAL CONTROL STRATEGY OF CZ GROWER

Major specifications of the silicon single crystal produced from the CZ process include various complex physical and chemical properties of crystal such as dislocation level, impurity content, and uniform radial and axial dopant distribution. However, since the online measurements of these properties are unavailable, only the crystal diameter and the pulling speed trajectory are normally chosen to be the main control variables to infer and affect the crystal properties.

Fig. 1 presents the conventional control scheme used in the commercial CZ crystal growers. First of all, control of the crystal diameter is essential not only to minimize the cutting waste but also to improve the quality of the crystal by reducing fluctuations in growing conditions. For this, as shown in Fig. 1, the crystal diameter adjacent to the melt surface is measured by the optical sensor and is controlled with the automatic diameter controller (ADC) by manipulating the pulling speed of the crystal. Fluctuations of crystal qualities including diameter during crystal growth are mainly caused by variations both in crystal pulling speed and thermal condition. The automatic temperature controller (ATC) adjusts the heater temperature to compensate the heater input against thermal disturbances.

The other main control variable is the pulling speed itself. Since it is closely related to the major crystal properties, the pulling speed should follow a predetermined target trajectory as closely as possible along

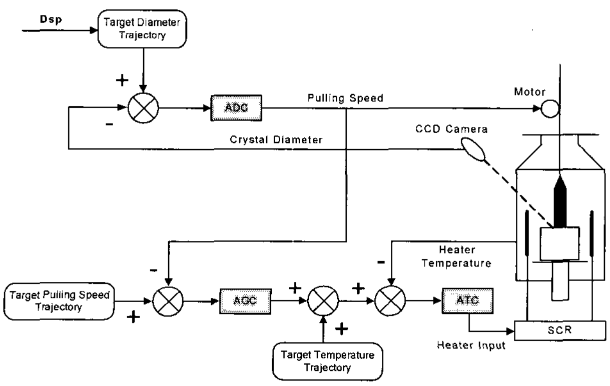


Fig. 1. Conventional control scheme of commercial CZ crystal growing process.

the whole bulk crystal growing process. Tight tracking control of the pulling speed becomes more essential as larger diameter and higher quality are required. To achieve this goal, the automatic growing controller (AGC) is used in a cascade configuration with the ATC. The AGC receives the pulling speed signal and compares with the pulling speed target to give the ATC the heater temperature required. Since variation of the target pulling speed is so wide along crystal growth and dynamic effect of the heater input to the crystal diameter is quite sluggish and complicated, a target temperature trajectory is often added to the AGC output as a feedforward control signal. If the target temperature trajectory is perfectly designed, the pulling speed would follow its target value closely enough with little feedback trim from the AGC.

3. APPLICATION OF MPC TECHNIQUE TO FEEDFORWARD TRAJECTORY DESIGN

It is well known that the quality of crystal product mainly depends on how accurately the target temperature trajectory is designed. However, because of its complex dynamic behaviors, it is very difficult to design the feedforward trajectory satisfactorily simply based on intuition and experience. One of the most proven ways for incorporating the complex dynamic effect into controller design is to use the model predictive control (MPC) technique. MPC is by far the most commonly applied advanced control technique for continuous operation in the chemical process industry. However, the CZ process is a typical batch process in which the operation proceeds along a time-varying reference trajectory over a finite period.

Recently, there has been extensive research effort to take advantage of the MPC to batch operation and some promising advances have been reported [5-7]. In this study, however, we exclude any attempt to replace the existing control strategy with the MPC because of practical difficulties in its actual implementation under commercial operation. Instead, we focused on utilizing the main principles of MPC to cope with the quantitative dynamic effect of heater temperature on the pulling speed into the design of the target temperature trajectory. By doing so, we could implement the advanced control strategy successfully with little change in the existing control scheme and algorithm.

Now, let us extend the MPC principles to batch-to-batch feedforward trajectory design for the CZ grower. Suppose that the input sequence over a specified operation horizon in the ith batch run is

$$\mathbf{u}^i = [u_0^i, u_1^i, u_2^i, \ldots, u_{n-1}^i]^T \quad (1)$$

and the input sequence results in the output sequence

$$\mathbf{y}^i = [y_1^i, y_2^i, y_3^i, \ldots, y_n^i]^T \quad (2)$$

while the setpoint trajectory is

$$\mathbf{y}^{sp} = [y_1^{sp}, y_2^{sp}, y_3^{sp}, \ldots, y_n^{sp}]^T. \tag{3}$$

In the CZ grower, the actual heater temperature, the actual pulling speed and the target pulling speed correspond to the input, the output and the setpoint of the proposed MPC method, respectively. Note that any batch run with the same input sequence as $\mathbf{u}^i$ would give the same output sequence as $\mathbf{y}^i$ if no change in disturbance conditions occurs through batch-to-batch runs.

Now consider that a step change is made at the *0*th time step in the *(i+1)*th batch run with no subsequent input changes, *i.e.*,

$$\Delta u_0^{i+1} = u_0^{i+1} - u_0^i = \cdots = u_{n-1}^{i+1} - u_{n-1}^i \neq 0$$
$$\textit{while } \Delta u_1^{i+1} = \Delta u_2^{i+1} = \cdots = 0.$$

Here, a net incremental step input change for the *j*th time step in the *(i+1)*th batch run, Δu_j^{i+1}, is defined as

$$\Delta u_j^{i+1} \equiv u_j^{i+1} - u_j^i - \sum_{k=0}^{j-1} \Delta u_k^{i+1}, \quad j = 1, \ldots, n-1. \tag{4}$$

Then the predicted output sequence of the *(i+1)*th batch run, $\hat{\mathbf{y}}^{i+1}$, can be calculated

$$\begin{aligned} \hat{y}_1^{i+1} &= y_1^i + a_1 \Delta u_0^{i+1}, \\ \hat{y}_2^{i+1} &= y_2^i + a_2 \Delta u_0^{i+1}, \\ &\vdots \\ \hat{y}_n^{i+1} &= y_n^i + a_n \Delta u_0^{i+1}, \end{aligned} \tag{5}$$

where a_j, j=1,…,n are the step response coefficients of the output obtained by making a unit step input change to a process.

Now suppose the general case where the net incremental input changes occur arbitrarily over whole time steps in the *(i+1)*th batch run. Then, according to the principle of superposition, the predicted output sequence of the *(i+1)*th batch run becomes

$$\begin{aligned} \hat{y}_1^{i+1} &= y_1^i + a_1 \Delta u_0^{i+1}, \\ \hat{y}_2^{i+1} &= y_2^i + a_2 \Delta u_0^{i+1} + a_1 \Delta u_1^{i+1}, \\ \hat{y}_3^{i+1} &= y_3^i + a_3 \Delta u_0^{i+1} + a_2 \Delta u_1^{i+1} + a_1 \Delta u_2^{i+1}, \\ &\vdots \\ \hat{y}_n^{i+1} &= y_n^i + a_n \Delta u_0^{i+1} + a_{n-1} \Delta u_1^{i+1} + \cdots + a_1 \Delta u_{n-1}^{i+1}, \end{aligned} \tag{6}$$

which can be re-written in matrix-vector notation as

$$\hat{\mathbf{y}}^{i+1} = \mathbf{A} \Delta \mathbf{u}^{i+1} + \mathbf{y}^i, \tag{7}$$

where

$$\hat{\mathbf{y}}^{i+1} = [\hat{y}_1^{i+1}, \hat{y}_2^{i+1}, \ldots, \hat{y}_n^{i+1}]^T, \tag{8}$$

$$\Delta \mathbf{u}^{i+1} = [\Delta u_0^{i+1}, \Delta u_1^{i+1}, \ldots, \Delta u_{n-1}^{i+1}]^T, \tag{9}$$

$$\mathbf{A} = \begin{bmatrix} a_1 & 0 & 0 & \cdots & 0 \\ a_2 & a_1 & 0 & \cdots & 0 \\ \vdots & & & & \vdots \\ a_n & a_{n-1} & a_{n-2} & \cdots & a_1 \end{bmatrix}. \tag{10}$$

The step response coefficient matrix **A** is often called the dynamic matrix in the dynamic matrix control [8].

The design objective of feedforward trajectory for the *(i+1)*th batch run is to find the best $\mathbf{u}^{i+1}$ that has the predicted output increment $\hat{\mathbf{y}}^{i+1} - \mathbf{y}^i$ to approach the current error $\mathbf{y}_{sp} - \mathbf{y}^i$ as closely as possible in a robust manner. The best solution for $\mathbf{u}^{i+1}$ can be obtained in the least-squares sense by minimizing the performance index

$$J[\Delta \mathbf{u}^{i+1}] = \hat{\mathbf{E}}^T \mathbf{W}_1 \hat{\mathbf{E}} + (\Delta \mathbf{u}^{i+1})^T \mathbf{W}_2 (\Delta \mathbf{u}^{i+1}), \tag{11}$$

where $\hat{\mathbf{E}} = \mathbf{A} \Delta \mathbf{u}^{i+1} - (\mathbf{y}_{sp} - \mathbf{y}^i)$; $\mathbf{W}_1$ and $\mathbf{W}_2$ are positive-definite weighting matrices for penalizing the predicted error and input movement, respectively.

The net incremental input sequence that minimizes *J* can be calculated by

$$\Delta \mathbf{u}^{i+1} = (\mathbf{A}^T \mathbf{W}_1 \mathbf{A} + \mathbf{W}_2)^{-1} \mathbf{A}^T \mathbf{W}_1 \mathbf{e}, \tag{12}$$

where $\mathbf{e} = \mathbf{y}_{sp} - \mathbf{y}^i$, *i.e.*, the error between the setpoint trajectory and the actual output of the *i*th run. Finally, $\mathbf{u}^{i+1}$ for the *(i+1)*th batch run can be calculated using (4) by

$$u_j^{i+1} = u_j^i + \sum_{k=0}^{j} \Delta u_k^{i+1} \quad , \; j = 0, \ldots, n-1. \tag{13}$$

4. IMPLEMENTATION ON THE COMMERCIAL CZ GROWER

The design of target temperature trajectory requires the step response model between the heater temperature and the pulling speed. However, the identification test to obtain the required step response model directly was practically disallowed during operation because the control structure needed alteration. To avoid this problem, we synthesized the required model by using the other step response models that can be obtained during operation easily: a step response of the crystal diameter to the pulling speed and a step response of the crystal diameter to the heater temperature. Crystal bulk growth period was divided into 5 representative regions based on the dynamic characteristics and the identification experiments were carried out at each region.

Figs. 2 and 3 show the examples for the open-loop responses of the crystal diameter to the step changes in the pulling speed and in the heater temperature, respectively. As seen in Fig. 2, the dynamics between the crystal diameter and the pulling speed can be modeled as an integrating plus time delay process. On the other hand, the dynamics between the crystal diameter and the heater temperature can be approximated to a first order plus time delay process.

Based on the two experimental models, the step response model between the heater temperature and the pulling speed can be derived in context with the conventional control scheme shown in Fig. 4. The dynamic models from Figs. 2 and 3 correspond to G_{p3} and G_{p4} in Fig. 4, respectively.

Fig. 5 indicates the unit step response derived. The dynamic matrix $\boldsymbol{A}$ in (10) can be obtained from the derived model straightforwardly. It is noted that the dynamic behavior of the pulling speed to the heater temperature shows zero gain with long time delay and lag. The zero gain indicates that a double integral action (or at least very strong integral action) is required to eliminate the tracking off-set in the pulling speed. However, the strong integral action in the AGC is not permitted because of large dead time and lag time. This confirms why the use of AGC only with the standard PID algorithm essentially gives poor performance and tracking off-set and the novel design of target temperature trajectory as a feedforward signal is so important.

The whole bulk crystal growth region from 100mm to 800mm in the ingot length range was considered as prediction and control horizons. The calculated input sequences were smoothed by the spline filter against excessive wiggle in the control action. The target temperature trajectory for the next batch was updated based on the calculated net incremental input change and the actual temperature trajectory of the previous batch.

Target temperature trajectories designed by the proposed method were implemented on 200mm commercial CZ crystal growers. Fig. 6 presents the target temperature trajectories by the proposed method and by the old run. The actual temperature trajectories (*i.e.*, sum of the AGC output and the target temperature trajectory) are also plotted in Fig. 6. In this application, $\mathbf{W}_1$ was chosen as the identity matrix $\mathbf{I}$. The move suppression matrix $\mathbf{W}_2$ was selected as $k\mathbf{I}$.

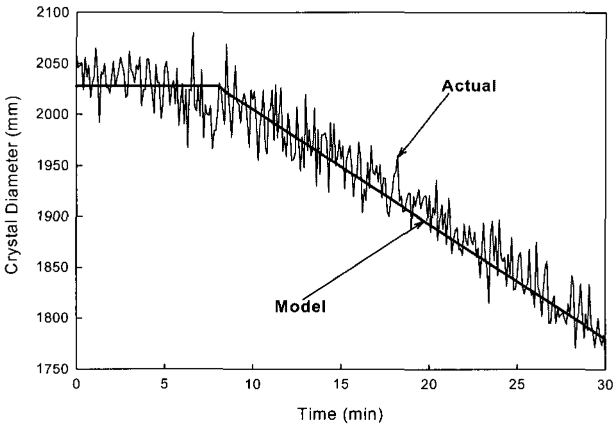


Fig. 2. Output response of the crystal diameter to 0.03mm/min step change in the pulling speed.

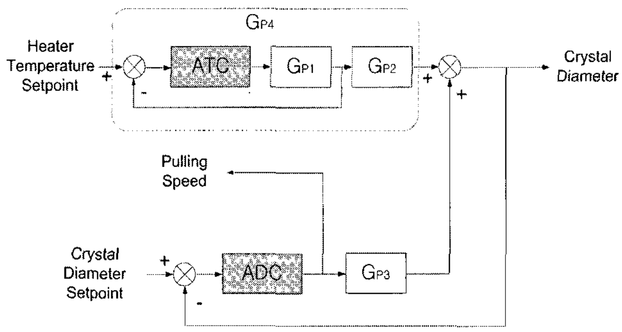


Fig. 4. Block diagram for derivation of step response model for the dynamic matrix $\boldsymbol{A}$: G_{p1}, G_{p2}, G_{p3} denote the transfer functions of heater input-heater temperature, heater temperature-crystal diameter, pulling speed - crystal diameter, respectively.

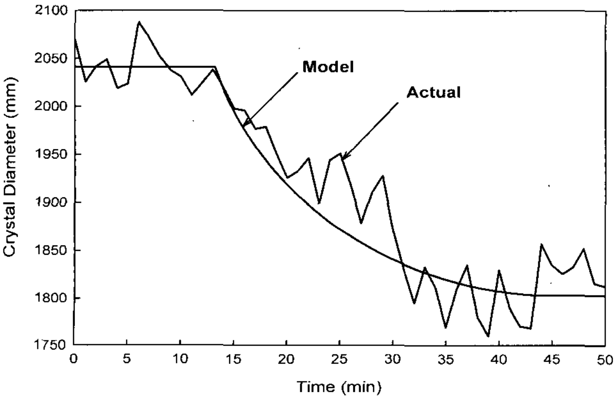


Fig. 3. Output response of the crystal diameter to 10□ step change in the heater temperature.

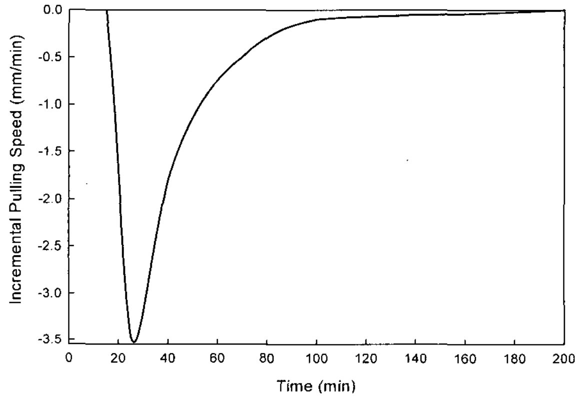


Fig. 5. Derived response of the pulling speed to the unit step change in the heater temperature.

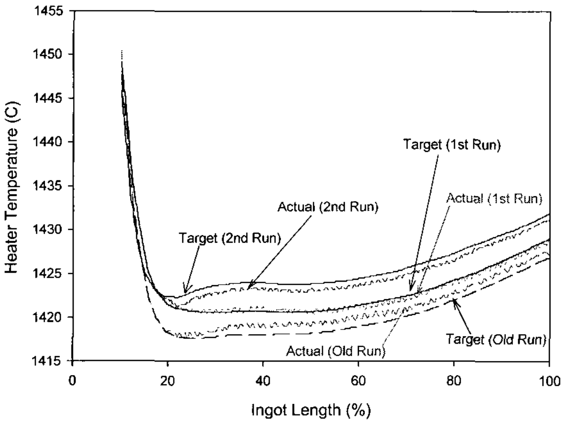
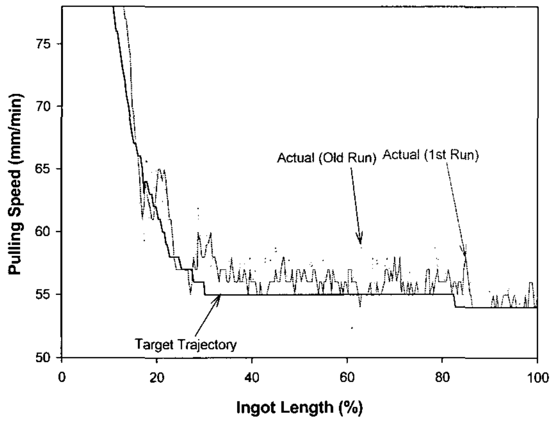


Fig. 6. Target and actual temperature trajectories in the new and old runs.



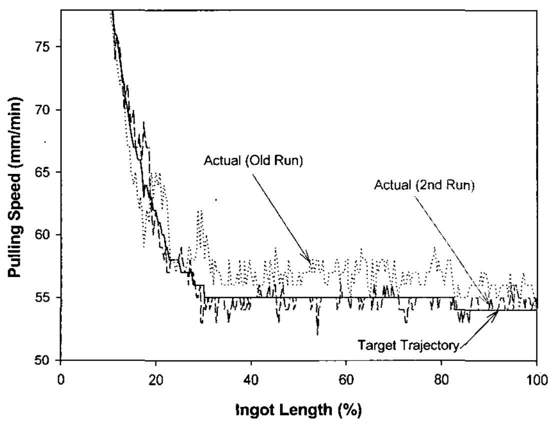


Fig. 7. Comparison of tracking performance of pulling speed before and after improvement of target temperature trajectory.

Fig. 7 presents the resulting tracking responses of the pulling speed by the corresponding target temperature trajectories in Fig. 6. As can be seen in Fig. 7, in the old run, there was a significant gap between the target and actual pulling trajectories due to inappropriate feedforward action. Based on the old run data, the target temperature trajectory was modified in the 1st run by using the proposed method. The move suppression factor k was 0.07. As a result, the actual pulling speed trajectory approaches the target trajectory somewhat more as seen in Fig. 7. To cut back the remaining gap further, additional modification of the target trajectory was carried out based on 1st run data and almost perfect tracking could be achieved as seen in Fig. 7. In the 2nd run, considering the magnitude of the remaining gap, the value of 0.02 was chosen as the move suppression factor to force the pulling speed onto the target trajectory more aggressively.

As a model based control technique, performance of the proposed method might sensitively depend on the model quality. However, the crude piece-wise linear model adopted in this study were found to be enough for satisfactory control performance, which demonstrated the robustness and practical usefulness of the method.

5. CONCLUSIONS

In this study, we applied the MPC technique to the feedforward trajectory design of the commercial CZ crystallization process. The method was aimed to incorporate the complex dynamic effect of the heater temperature on the pulling speed into the design of the target temperature trajectory. The proposed method was implemented on industrial CZ growers. The application results showed a significant improvement in tracking performance and thus crystal quality. The proposed method is now routinely used in the feedforward trajectory design of CZ crystal growers in the LG Siltron Company in Korea.

REFERENCES

[1] K. M. Kim, "Growing improved silicon crystals for VLSI/ULSI applications," *Solid State Technology*, Pennwell Publication Co., Nov. 1996.

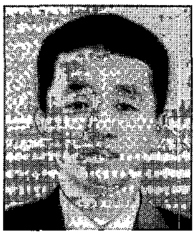
[2] M. A. Gevelber and G. Stephanopoulos, "Dynamics and control of the Czochralski process," *Journal of Crystal Growth*, vol. 84, no. 4, pp. 647-668, 1987.

[3] M. A. Gevelber, M. J. Wargo, and G. Stephanopoulos, "Advanced control design considerations for the Czochralski process," *Journal of Crystal Growth*, vol. 85, no. 1-2, pp. 256-263, 1987.

[4] R. I. Rivera and W. D. Seider, "Model predictive control of the Czochralski crystallization process," *Journal of Crystal Growth*, vol. 178, no. 4, pp. 593-611, 1997.

[5] K. S. Lee, J. H. Lee, I. Chin, and H. J. Lee, "A model predictive control technique for batch processes and its application to temperature tracking control of an experimental batch reactor," *AIChE Journal*, vol. 45, no. 10, pp. 2175-2187, 1999.

[6] K. S. Lee, J. Lee, I. Chin, J. Choi, and J. H. Lee, "Control of wafer temperature uniformity in rapid thermal processing using an optimal iterative learning control technique," *Industrial & Engineering Chemistry Research*, vol. 40, no. 7, pp. 1661-1672, 2001.
[7] K. S. Lee and J. H. Lee, "A generic framework for integrated quality and profile control for industrial batch processes," *Proc. of 6th IFAC Symp. on DYCOPS*, pp. 59-70, June 2001.
[8] C. R. Cutler and B. L. Ramaker, "Dynamic matrix control: a computer control algorithm," *Prof. of 86th AIChE National Meeting,* April 1979.



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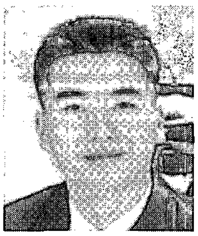

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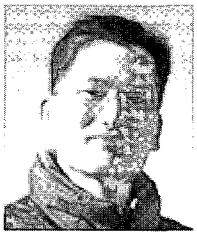

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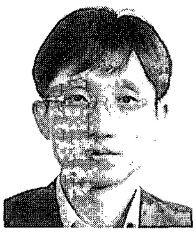

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