The Application of Generalized Predictive Control in the Radiant Heating Atomic Layer Deposition Reactor

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***Abstract*—Atomic layer deposition (ALD) technology is a self-limiting ultrathin film deposition method. In ALD reactions, the reaction temperature plays a key role. And generalized predictive control (GPC) algorithm is adopted to control the temperature of a radiant heating reactor. The mathematical model of the system's temperature uniformity is calculated with heat transfer theory. Since temperature control is affected by GPC parameters including soften factor, weighting coefficient, sample time etc, it is necessary to study the effect of these parameters. By experiments, the values of soften factor, weighting coefficient and sampling time could be optimized and then be applied in the process of ALD reactions. And conclusions can be draw that soften factor has the largest impact on the algorithm while the influences of weighting coefficient and sampling time are almost negligible. Efficient temperature control of the ALD reactor chamber using GPC algorithm with optimal parameters is demonstrated.**

Keywords* − *Atomic Layer Deposition (ALD) ; Generalized Predictive Control (GPC) ; CARMA model ; soften factor ; weighting coefficient ; radiant heating

I. Introduction

Atomic layer deposition (ALD) is an ultrathin film deposition method, where two or more precursors are alternately pulsed into the reactor, followed by an inert gas purge to remove excess precursors. These precursors form self-limited chemisorptions on the substrate surface, one layer (or sub-monolayer) per cycle. Thus the thickness of the deposited film can be precisely controlled by the number of ALD cycles [1-3]. The self-limiting nature of ALD makes it suitable for many applications in areas of microelectronics, complex nanostructures and energy conversion devices [4, 5]. Since the adsorption of the precursor to the surface is mainly thermally driven, there exists a so-called "ALD temperature window" [6] in which the ALD process takes place. The substrate temperature must be high enough to prevent condensation of the reactants, and exceed the reaction activation energy. On the other hand, if the temperature is too high, undesirable decomposition of reactants, gas phase re-evaporation, or CVD reactions will occur, which leads to an uncontrolled deposition of the film [7-9]. Thus maintaining the system in temperature window accurately is of crucial importance for ALD reactions.

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Generalized predictive control (GPC) - known for its on-line identification, multi-step prediction, and strong robustness - has been widely applied in many industrial processes [10]. GPC algorithm, which has been developed in linear/nonlinear and time varying system, is proposed by D.W.Clarke and etc. in 1987 [11, 12] based on the theory of minimum variance self-tuning control. GPC algorithm refers to the strategy of rolling optimization of model algorithm control (MAC) and dynamic matrix control (DMC). MAC, based on the model of impulse response, is initially studied by Rouhani and Mehra in 1982. DMC, based on the model of step response, is proposed by Cutler [13]. Both MAC and DMC need to build a highly precised mathematical model of the plant. Unfortunately, it is hard to determine parameters such as the dead time and the degree of the mathematical model for a given system. Hence it is necessary to explore the self-tuning control algorithm- GPC algorithm- which has little dependence on the model and strong robustness.

In this study, GPC has been implemented to control the ALD reactor temperature and demonstrate fast ramping rates and accuracy control.

II. Mathematical Model of System

The ALD reactor studied here is a radiant heating device under vacuum condition. In the following parts, structure of the reactor and the foundation of the algorithm will be described.

A. Hardware Structure

The sketch of the radiant heating reactor is shown in Fig.1.(a), where both the top and bottom surfaces of the reactor are heated by external heating sources, while the other four surfaces have little heat transfer with the atmosphere. The central plane inside the reactor is our target where ALD reaction takes place. The pressure of the reactor is maintained by the rotary vane pump.

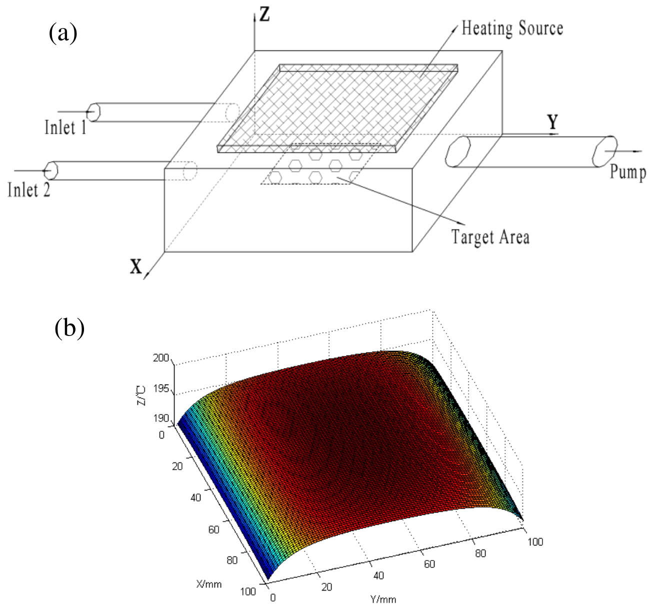

Fig. 1. (a) sketch of the radiant heating reactor of the radiated heating; (b) temperature distribution in the central plane inside the reactor

The radiant heating could provide a relatively uniform temperature environment which is beneficial to ALD reaction. The drawback is a relatively slow heating process, which lowers the efficiency and throughput. The temperature distribution of the target region is studied by considering only the radiation effect [14, 15]. In the calculation, the temperatures of two heating surfaces are set at 200℃, and temperatures for the other four surfaces are all equal to 150℃. Fig.1(b) demonstrates the theoretical calculation result, in which the temperature standard deviation is 0.0172℃ in the center square zone of 100mm side length. This means the target area has good temperature uniformity. It can be seen from the temperature contour that theoretically speaking, the system could meet the temperature requirement of ALD process.

B. Control Algorithm Model

GPC method calculates the future predictive control sequence by minimizing a multistage cost function basing on the controller auto regressive moving average (CARMA) model [16], which could be described by

$$A(z^{-1})y(k) = z^{-d}B(z^{-1})u(k-1) + C(z^{-1})\xi(k)/\Delta \quad (\Delta = 1 - z^{-1}) \qquad (1)$$

Where $y(k)$ is the output sequence (the temperature of the system), $u(k)$ is the control sequence (the control voltage of the system) and $\xi(k)$ is a white noise which will be ignored in this study. And d is the time-delay time of the system. Here $A(z^{-1})$, $B(z^{-1})$, $C(z^{-1})$ are the polynomial of the z^{-1}, where z^{-1} is the backward shift operator.

The cost function of the system which could be minimized to optimize the control regular is described in the following formula.

$$J(N_1, N_2, N_u) = \sum_{j=N_1}^{N_2} \delta(j)[\hat{y}(t+j|t) - w(t+j)]^2 + \sum_{j=1}^{Nu} \lambda(j)[\Delta u(t+j-1)]^2 \qquad (2)$$

Where $w(k+j) = \alpha^j y(k) + (1-\alpha^j) y_r(k)$ is the future reference sequence (3)

Here $y_r(k)$ is the set-point value which could be fixed and variable as well and α is the soften factor.

Considering the Diophantine equation

$$I = E_j(z^{-1})\Delta A(z^{-1}) + z^{-j}F(z^{-1}) \qquad (4)$$

The predictive output can be calculated as

$$\hat{y}(t+j|t) = G_j(z^{-1})\Delta u(t+j-1) + f_j \qquad (5)$$

With $G = \begin{bmatrix} g_0 & 0 & \cdots & 0 \\ g_1 & g_0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ g_{N-1} & g_{N-2} & \cdots & g_0 \end{bmatrix}$, $f_j = F_j(z^{-1})y(t) + G(z^{-1})\Delta u(t-1)$

Minimizing the formula (1.2), control increment can be described by $\Delta u = (G^T G + \lambda I)^{-1} G^T (w - f)$ (6)

So the control voltage in the k moment is $u(k) = u(k-1) + \Delta u$, which could be applied to control the heating source.

III. Experiments

GPC algorithm is applied to control a radiant heating ALD reactor's temperature for the experiments. The target temperature is set to 150℃ since it is a typical temperature for ALD process - depositing aluminum oxide thin film by trimethyl aluminum and water, and the pressure of the reactor is maintained at 100Pa in the experiments based on our ALD reaction requirement.

GPC parameters - including soften factor, weighting coefficient, sampling time - may affect the control process. So each parameter will be studied individually in detail.

A. Soften Factor

Compared with other parameters, the future reference trajectory is mainly affected by the soften factor as formula (3) shows. If the soften factor α is small, the future reference trajectory $w(k)$ will approach the target value rapidly, so that the system has good response time but poor robustness. When increasing α, the response time of system will become worse but with better robustness.

Fig.2 shows the temperature curves with different soften factors (0.50, 0.75, 0.80, 0.85 and 0.90), and it shows that the temperature overshoot decreases with the increase of soften factor. And the stabilization process decelerates correspondingly, which represents the poor tracking speed to the target temperature. When the soften factor is 0.80 or 0.85, the setting time is about 1300s under the accuracy of ±1℃, while the setting time is more than 3400s for other soften factor values. Since lower soften factor will lead to larger heating gain, it takes shorter time for the system to reach the target temperature, but it is unstable and larger overshoot consequently occurs. With the appearance of overshoot, the system needs some time to cool down so as to cost more time to stabilize finally. However, if the soften factor is too large, the system will spend much more time to track the future reference value to reach the desired value with minimum overshoot. Since soften factor is independent of temperature accuracy, the optimal soften factor can be determined by weighing overshoot and stabilization time. After experimenting with the radiant heating ALD system, the optimal soften factor range is chosen from 0.80~0.85.

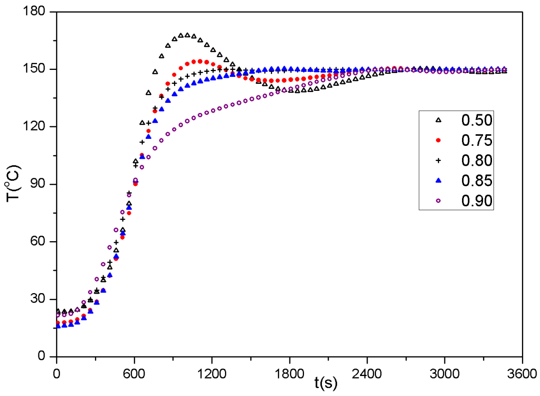

Fig.2. The temperature curves with different soften factors

B. Weighting Coefficient

The weighting coefficient is mainly used to restrain severe control increment, in case that the system is out of the limited range and appears oscillation as formula (2) has shown. After minimizing the cost function, the control increment is shown as formula (6). Then different values of the weighting coefficient λ are executed in the experiments, and the effect of the weighting coefficient will be analysed by comparing different temperature curves in Fig.3. On the whole, the temperaure curevs have the same heating gain, fluctuation, temperature overshoot and setting time. Further on from the inset figure, although it exists difference in the range of the overshoot, these differences show no certain law with weighting coefficients. Thus different weighting coefficient has little impact on the GPC performance in the radiant heating reactor.

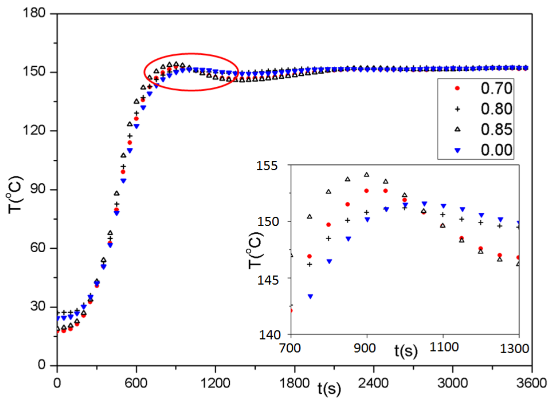

Fig.3. The temperature curves with weighting coefficient

C. Sampling Time

The reason of choosing optimal sampling time is that the sampling frequency should be at least twice of the cut-off frequency. In general, longer sampling time will cause the loss of some useful high frequency information, while shorter sampling time will result in large amount of computation and will lead to instability. Fig.4 shows the internal temperature under different sampling time (0.5s, 1s and 5s) with the soften factor of 0.80 and the pressure of 100Pa. Though sampling time of 5s results in longer heating time of total power heating and slower response of control increment variation in the experiment process, the difference between them is minimal. Thus, by combining the condition of the hardware and the temperature gain, 1s is the optimal sampling time in the experiments.

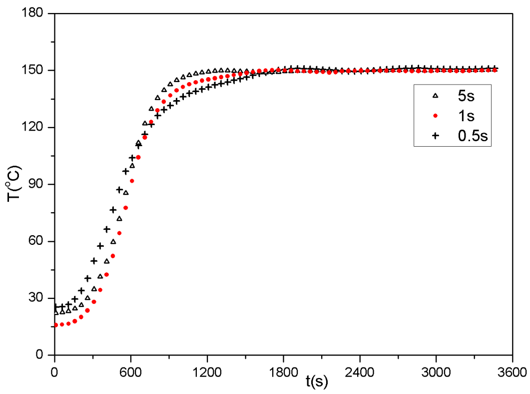

Fig.4. The temperature curves with the different soften factors

IV. CONCLUSIONS

An effective temperature control application has been achieved by implementing GPC algorithm control on a radiant heating ALD system. The internal temperature distribution of the radiant heating system is uniform. Among many GPC controlling parameters, soften factor has the most significant influence on the temperature overshoot, setting time and robustness, whose optimal value range is 0.80~0.85. Other parameters like weighting coefficient and sampling time only affect the temperature curve slightly. Lastly these experiments have demonstrated that GPC algorithm is quite effective in a radiant heating reactor.

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