

# Network Model Analysis of Poly-silicon Film Deposition on Wafers in CVD Reactor

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**Abstract-** We studied a simple reaction analysis technique using a network model (NM) to calculate the concentration distribution and deposition rate in a vertical hot-wall-type low-pressure chemical vapor deposition (LPCVD) reactor. We analyzed the deposition rates of poly-silicon film. The calculation results of the deposition rate using the NM analysis agreed with those of the FEM analysis within the difference of 10%. The computation of the NM analysis was 1000 times faster than that of the FEM analysis, indicating that the NM analysis model is effective for shortening computation time without increasing computation error.

**Keywords-** Chemical Vapor Deposition; Thin Film; Numerical Simulation; Network Model

## I. INTRODUCTION

In semiconductor processing, low-pressure chemical vapor deposition (LPCVD) process is indispensable to fabricate deposition films on wafers with a good step coverage rate. Most LPCVD processes are carried out in a batch-type furnace, where a row of many wafers is heated in a vertical hot-wall-type furnace at the same time, thus ensuring a high production rate. In order to fabricate thin films uniformly on wafers for high-density VLSI devices, it is important to know the concentration distribution of the process gas and the deposition rate of the film in the reactor by numerical simulation. It takes a long time to calculate the concentration distribution and the deposition rate in the reactor using a conventional numerical simulation code with the finite element method (FEM) or the finite differential method (FDM) because the flow velocity, the temperature, the concentration of the gas, and the chemical reaction at multiple node points must be calculated at the same time. In this work, we propose a simple simulation technique to calculate the concentration distribution and the deposition rate in the reactor using the network model (NM) in a vertical hot-wall-type LPCVD reactor to shorten the computation time without increasing computation errors.

There has been much previous research on the chemical vapor deposition (CVD) process. Roenigk et al. [1] reported a model of the deposition rate of silicon nitride ( $\text{Si}_3\text{N}_4$ ) film in the LPCVD process, while Sorita [2] reported a model of the deposition rate of silicon oxide ( $\text{SiO}_2$ ) film from tetraethyl orthosilicate (TEOS,  $\text{Si}(\text{OC}_2\text{H}_5)_4$ ) gas, and Shimogaki et al. [3] reported a model of the deposition rate of phosphorus doped poly-silicon (D-Poly) film. Lin et al. [4] studied a generic first principle process model of film growth in the LPCVD process, Sachs et al. [5] reported a model of poly-silicon film, Guo et al. [6] studied spatial uniformity manufacturing processes in the CVD process, Carlen et al. [7] studied spatial correlation in thin film deposition in the LPCVD process, Gumpher et al. [8] studied  $\text{Si}_3\text{N}_4$  film uniformity using adaptive temperature control, Morosanu et al. [9] studied the effect of parameters on the deposition rate of  $\text{Si}_3\text{N}_4$  film produced from the  $\text{SiH}_2\text{Cl}_2$  and  $\text{NH}_3$  gases, DePinto [10] reported a three-step approach to optimize the condition of the LPCVD process, Theodoropoulou [11] reported a model to optimize the rapid thermal CVD process, and He et al. [12] reported a thermal model to predict wafer temperature in the LPCVD process.

In this work we propose a simple simulation technique to calculate the concentration distribution and the deposition rate in a reactor using the network reaction analysis model in a vertical hot-wall-type LPCVD. We analyze the deposition rate of poly-silicon film using the network reaction analysis model and compare the results with those of the FEM analysis.

## II. NETWORK MODEL ANALYSIS IN LPCVD REACTOR

### A. Structure of LPCVD Reactor

Fig. 1 shows the cross-section of a vertical LPCVD reactor. The pressure inside the reactor is 1–100 Pa and temperature is 500–800°C. A row of near hundred wafers is placed in the reactor and thin film is deposited on the wafers by chemical reaction from raw material gas. The reactor contains both an outer quart tube and an inner quart tube. The wafers are set on a quart holder (not shown in the figure) with distance of several mm. There is a heater around the outer quart tube that heats the wafers by thermal radiation. There are insulating plates with the same diameter as the wafers placed below the wafers to reduce heat loss. The raw material gas is supplied from the lower end of the inner quart tube and flows around the wafers to create deposition film on the wafers. The remaining gas turns the flow direction at the top of the inner quart tube and it exits from the lower end of the outer quart tube. As the reactor is coaxial symmetric, the temperature, flow velocity, and concentration distributions are also coaxial symmetric.

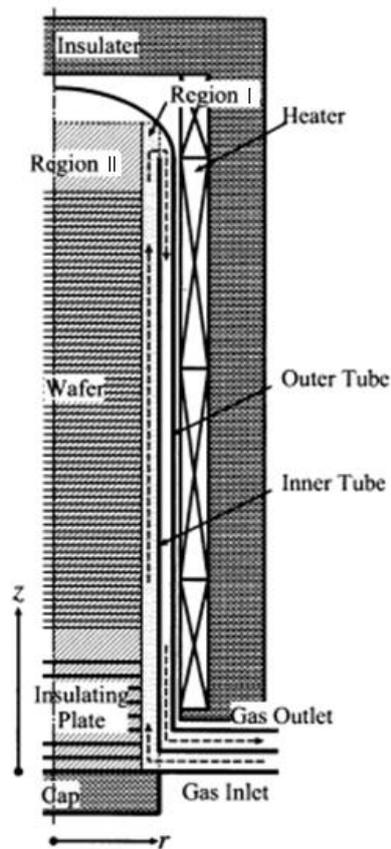


Fig. 1 Vertical LPCVD reactor

### B. Network Model Analysis

We calculate steady-state material transfer and chemical reaction in the LPCVD reactor using the network model (NM) analysis. The NM analysis is a simple calculation method with a rather small number of node points that is widely used in heat transfer analysis [13, 14]. In the NM analysis, the object is divided into ramps (node points) and the one-dimensional relations of material transfer among the node points are calculated. The calculation model of the reactor is divided into two regions I and II, as shown in Figs. 1 and 2. Region I is the main flow space of the gas between the periphery of the wafers and the inside wall of the inner quart tube, and region II is the space between wafers. The space between the insulating plates and the space between the top wafer and the ceiling wall of the outer quart tube are also treated as region II. The vertical direction from the lower end of the inner quart tube (the entrance of the raw material gas) is the coordinate  $z$  and the radial direction from the center axis is the coordinate  $r$ . In region I, the concentration of raw gas decreases along the  $z$  direction.

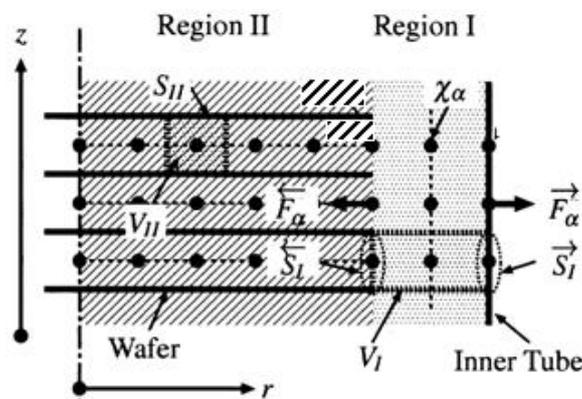


Fig. 2 Network model analysis

We used the following assumptions in our analysis: (1) Pressure in the reactor is constant. The volume expansion of the gas due to temperature change in the reactor is ignored. (2) Generation or absorption of heat and the volume change of gas due to chemical reaction are ignored. (3) Chemical reaction in the gas is one-dimensional and the surface reaction is a simple adhesion reaction.

Fig. 3(a) shows the calculation nodes and mesh for the NM analyses. We took 60 nodes in region I and 29 nodes for each area between wafers in region II for the NM analysis. The total number of nodes was 1800 ( $= 60 \times 30$ ). The calculation region was two-dimensional but the solving equations were simplified using the average mole fraction as shown next.

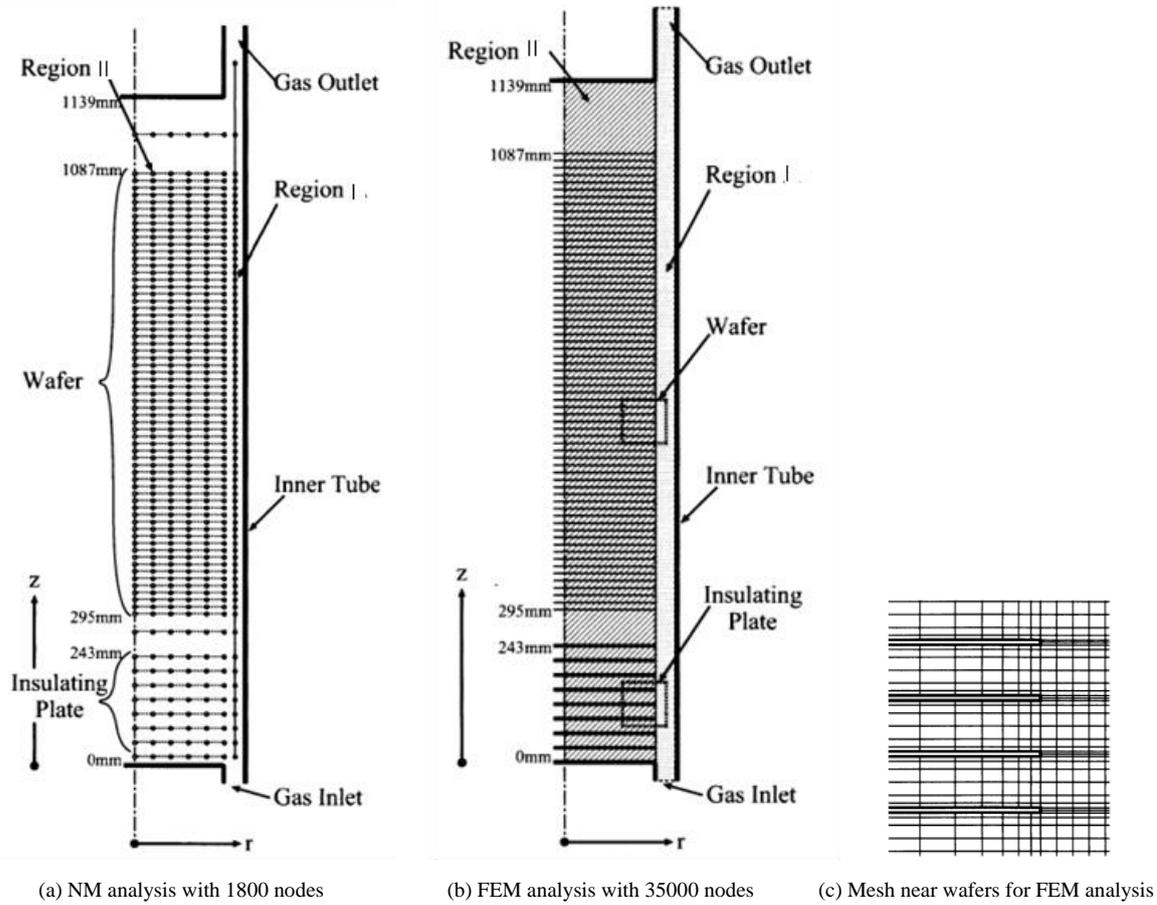


Fig. 3 Calculation nodes and mesh for NM and FEM analyses

We calculated the deposition rate of the D-Poly film using the NM analysis and then compared the results with those obtained by two-dimensional FEM analysis [15]. Figs. 3(b) and (c) show the calculation nodes and mesh for FEM analyses. The total number of nodes was 35000 in the FEM analysis.

### C. Governing Equations in Region I

We define the average mole fraction  $\bar{\chi}_\alpha(z)$  at each  $z$  position in region I, see Fig. 2. Distribution of the average mole fraction  $\bar{\chi}_\alpha(z)$  in region I is calculated with the following equation using the mass balance of gas  $\alpha$  in a small volume  $V_I$ .

$$u \frac{d\bar{\chi}_\alpha}{dz} = \frac{d}{dz} \left( D_\alpha \frac{d\bar{\chi}_\alpha}{dz} \right) - \bar{F}_\alpha \frac{\bar{S}_I}{V_I} - \bar{F}_\alpha \frac{\bar{S}_I}{V_I} - \sum_{\beta=1}^N k_{\alpha\beta} \bar{\chi}_\alpha + \sum_{\beta=1}^N k_{\beta\alpha} \bar{\chi}_\beta \quad (1)$$

where  $u$  is the velocity of gas,  $D_\alpha$  is the diffusion coefficient of gas,  $F_\alpha$  is the extinction rate,  $k_{\alpha\beta}$  is the chemical reaction constant in gas space,  $S_I$  is the wall surface area, and  $\alpha$  and  $\beta$  are kind of gases.

The left-hand term of Eq. (1) is convection, while on the right-hand side the first term is diffusion, the second and the third terms are extinction of the chemical concentration at the surface, the fourth term is extinction of the chemical concentration in the gas space, and the fifth term is generation of the chemical concentration in the gas space. The boundary conditions of Eq. (1) are the following equations, where " $\hat{\chi}_\alpha$ " means the given value.

$$\bar{\chi}_\alpha = \hat{\chi}_\alpha \quad (\text{at inlet}) \quad (2)$$

$$\frac{d\bar{\chi}_\alpha}{dz} = 0 \quad (\text{at outlet}) \quad (3)$$

The extinction rates  $\overline{F}_\alpha$  and  $\overline{F}_\alpha$  in Eq. (1) are defined as the following equations.

$$\overline{F}_\alpha = \frac{1}{4} v_\alpha \eta_\alpha \chi_\alpha \quad (\text{at periphery of wafers, } r = r_w) \quad (4)$$

$$\overline{F}_\alpha = \frac{1}{4} v_\alpha \eta_\alpha \chi_\alpha \quad (\text{at inside wall of inner quart tube, } r = r_i) \quad (5)$$

where  $\chi_\alpha$  is the local mole fraction,  $v_\alpha$  is the average molecular velocity of gas, and  $\eta_\alpha$  is the probability of the absorption.

As the radial distance between the periphery of the wafers ( $r = r_w$ ) and the inside wall of the inner quart tube ( $r = r_i$ ) is small, the change of the local mole fraction  $\chi_\alpha(r, z)$  to the  $z$  direction is negligibly smaller than the change to the  $r$  direction and the local mole fraction  $\chi_\alpha(r, z)$  at each  $z$  position in region I is calculated by the following equation.

$$D_\alpha \frac{1}{r} \frac{d}{dr} \left( r \frac{d\chi_\alpha}{dr} \right) - \sum_{\beta=1}^N k_{\alpha\beta} \chi_\alpha + \sum_{\beta=1}^N k_{\beta\alpha} \chi_\beta = 0 \quad (6)$$

The boundary conditions of Eq. (6) are the following equations.

$$\frac{1}{4} v_\alpha \eta_\alpha \chi_\alpha = D_\alpha \frac{d\chi_\alpha}{dr} \quad (\text{at } r = r_w) \quad (7)$$

$$\frac{1}{4} v_\alpha \eta_\alpha \chi_\alpha = -D_\alpha \frac{d\chi_\alpha}{dr} \quad (\text{at } r = r_i) \quad (8)$$

The average mole fraction  $\overline{\chi}_\alpha(z)$  is calculated by the following equation.

$$\overline{\chi}_\alpha = \int_{r_w}^{r_i} \chi_\alpha 2\pi r dr / \pi(r_i^2 - r_w^2) \quad (9)$$

#### D. Governing Equations in Region II

We define the average mole fraction  $\overline{\chi}_\alpha(r)$  at each  $r$  position in region II. Distribution of the average mole fraction  $\overline{\chi}_\alpha(r)$  in region II is calculated by the following diffusion equation using the mass balance of gas  $\alpha$  in a small volume  $V_{II}$ .

$$D_\alpha \frac{1}{r} \frac{d}{dr} \left( r \frac{d\overline{\chi}_\alpha}{dr} \right) - 2F_\alpha^* \frac{S_{II}}{V_{II}} - \sum_{\beta=1}^N k_{\alpha\beta} \overline{\chi}_\alpha + \sum_{\beta=1}^N k_{\beta\alpha} \overline{\chi}_\beta = 0 \quad (10)$$

The boundary conditions of Eq. (10) are the following equations, where  $\chi_\alpha(r_w)$  is the local mole fraction of the gas at the periphery of the wafers in region I.

$$\frac{d\overline{\chi}_\alpha}{dr}(0) = 0 \quad (\text{at } r = 0) \quad (11)$$

$$\overline{\chi}_\alpha(r_w) = \chi_\alpha(r_w) \quad (\text{at } r = r_w) \quad (12)$$

The extinction rate  $F_\alpha^*$  in Eq. (10) is defined as the following equation, where  $\chi_\alpha$  is the local mole fraction near the wafer surface.

$$F_\alpha^* = \frac{1}{4} v_\alpha \eta_\alpha \chi_\alpha \quad (\text{at wafer surface}) \quad (13)$$

As the distance between the wafers is small, the change to the  $r$  direction is negligibly smaller than the change to the  $z$  direction and the local mole fraction  $\chi_\alpha(r, z)$  at each  $r$  position in region II is calculated by the following equation.

$$D_\alpha \frac{d^2 \chi_\alpha}{dz^2} - \sum_{\beta=1}^N k_{\alpha\beta} \chi_\alpha + \sum_{\beta=1}^N k_{\beta\alpha} \chi_\beta = 0 \quad (14)$$

The boundary condition of Eq. (14) is the following equation.

$$\frac{1}{4} v_\alpha \eta_\alpha \chi_\alpha = D_\alpha \frac{d\chi_\alpha}{dz} \quad (\text{at wafer surface}) \quad (15)$$

The average mole fraction  $\overline{\chi}_\alpha(r)$  is calculated by the following equation, where  $W$  is the distance of wafers.

$$\overline{\chi}_\alpha = \int_0^W \chi_\alpha dz / W \quad (16)$$

### E. Calculation Scheme

The calculation scheme of the NM analysis is as following. We first generate the node data, initialize the variables, and then calculate the average mole fraction  $\overline{\chi}_\alpha(z)$  and the local mole fraction at the periphery of the wafers  $\chi_\alpha(r_w)$  in region I, the average mole fraction  $\overline{\chi}_\alpha(r)$  and  $\chi_\alpha(r_w)$  in region II by solving Eqs. (1)–(16), repeat the calculation until convergent, and finally obtain the deposition rate. We made a computational code using a finite difference method and an iterative method with the FORTRAN language and calculated with a personal computer.

### F. Calculation Condition of Poly-silicon Film Deposition Rate

The calculation conditions of the D-Poly film deposition rate are: the wafer diameter is 200 mm, wafer pitch is 6.4 mm, inner tube diameter is 300 mm, temperature is 580°C, pressure is 39 Pa, gas source and flow rate are 500 sccm of SiH<sub>4</sub> and 490 sccm of N<sub>2</sub>. In the analysis of the D-Poly film deposition rate, we assumed the model reported by Shimogaki et al. [3] and the raw material SiH<sub>4</sub> and the intermediate product SiH<sub>2</sub> deposited on the wafers. The reaction speed constant for SiH<sub>4</sub> and SiH<sub>2</sub> in the gas space ( $k_{\text{SiH}_4\text{-SiH}_2} = 3.0 \times 10^{16} (P/100)^{2.1} \exp(-3.4 \times 10^4/T)$ , where  $T$  is temperature and  $P$  is pressure) and their absorption probabilities of the surface reaction ( $\eta_{\text{SiH}_4} = 1.0 \times 10^{12} \exp(-3.4 \times 10^4/T)$ ,  $\eta_{\text{SiH}_2} = 9.0 \times 10^{-2}$ ) were determined by our experimental results.

## III. CALCULATION RESULTS

Figs. 4–7 show the calculation results of the mole fraction of SiH<sub>4</sub>, the mole fraction of SiH<sub>2</sub>, the D-Poly film deposition rate at the periphery of the wafers along the  $z$  direction, and the D-Poly film deposition rate along the  $r$  direction on the wafer at  $z = 0.65$  m. The difference of the mole fraction of SiH<sub>2</sub> is only near the exit  $z = 1$ – $1.2$  m. The reason is that the space between the top wafer and the ceiling of the outer quart tube is wide, and the assumption of no-convection in the NM analysis caused an error. The mole fraction of SiH<sub>4</sub> and SiH<sub>2</sub> of the NM analysis and the FEM analysis agreed within the difference of 1% and 15%, respectively. The D-Poly film deposition rate along the  $z$  direction and the  $r$  direction agreed with the difference of 5%.

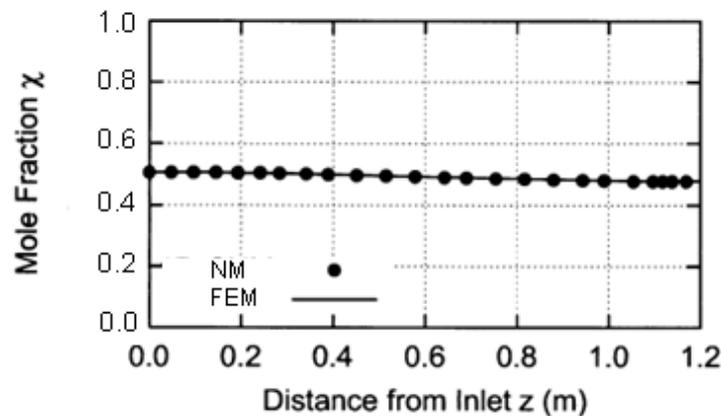


Fig. 4 Calculation result of mole fraction of SiH<sub>4</sub> along  $z$  direction

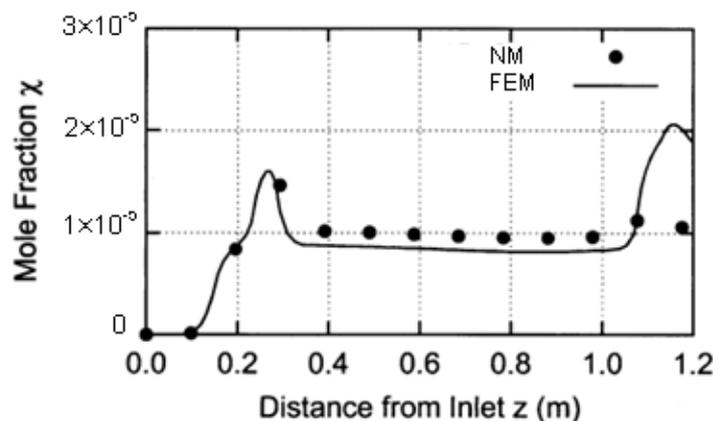


Fig. 5 Calculation result of mole fraction of SiH<sub>2</sub> along  $z$  direction

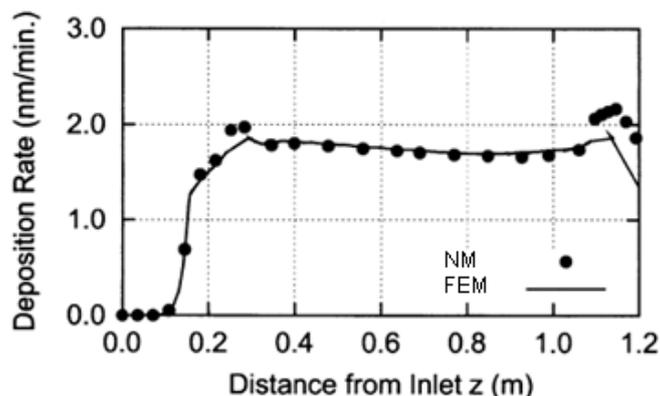


Fig. 6 D-Poly film deposition rate at periphery of wafers along  $z$  direction

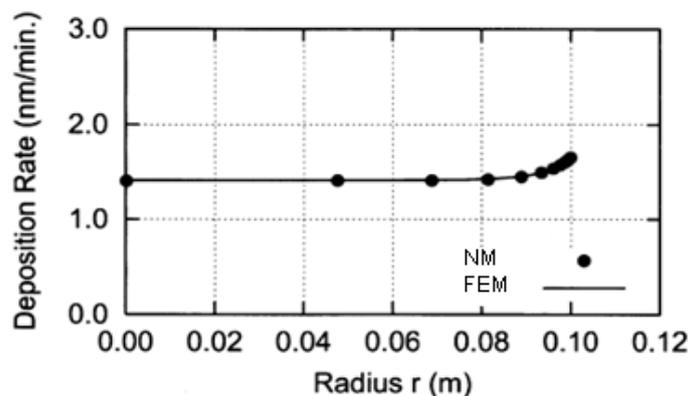


Fig. 7 D-Poly film deposition rate along  $r$  direction on wafer at  $z = 0.65$  m

We also calculated the deposition rate of the  $\text{Si}_3\text{N}_4$  film and the  $\text{SiO}_2$  film using the NM analysis. The calculation results of the deposition rate of the D-Poly film, the  $\text{Si}_3\text{N}_4$  film, and the  $\text{SiO}_2$  film using the NM analysis agreed with those of the FEM analysis within the difference of 10%. The computation time of the NM analysis was order of seconds and that of the FEM analysis was order of hours, so the computation of the NM analysis was 1000 times faster than that of the FEM analysis.

#### IV. SUMMARY

We analyzed the concentration distribution and deposition rate of the poly-silicon film using the network reaction analysis model (NM) in a vertical LPCVD reactor. Results showed the following. The calculation results of the deposition rate using the NM analysis agreed with those of the FEM analysis within the difference of 10% near the wafers. The computation of the NM analysis was 1000 times faster than that of the FEM analysis.

#### REFERENCES

- [1] K.F. Roenigk, and K.F. Jensen, "Low Pressure CVD of Silicon Nitride," *Journal of the Electrochemical Society*, vol. 134, iss. 7, pp. 1777-1785, 1987.
- [2] T. Sorita, "Model of Deposition of Dielectrics Thin Film using CVD method", Doctor Thesis of Tokyo University, pp. 135-136, 1995 (in Japanese).
- [3] K. Simogaki, et al., "Chemistry of Silane ( $\text{SiH}_4$ ,  $\text{SiH}_6/\text{C}_2\text{H}_2$ )," First Annual Report of Research Project on Basic CVD Engineering in Chemical Engineering Soc., pp. 95-114, 1991 (in Japanese).
- [4] K.K. Lin, and C.J. Spanos, "Statistical Equipment Modeling for VLSI Manufacturing: Application for LPCVD," *IEEE Transactions on Semiconductor Manufacturing*, vol. 3, iss. 4, pp. 216-229, 1990.
- [5] E. Sachs, G.H. Prueger, and R. Guerrieri, "An Equipment Model for Polysilicon LPCVD," *IEEE Transactions on Semiconductor Manufacturing*, vol. 5, iss. 1, pp. 3-13, 1992.
- [6] R.S. Guo, and E. Sachs, "Modeling, Optimization and Control of Spatial Uniformity in Manufacturing Processes," *IEEE Transactions on Semiconductor Manufacturing*, vol. 6, iss. 1, pp. 41-57, 1993.
- [7] E.T. Carlen, and C.H. Mastrangelo, "Statistical Model for Spatial Correlation in Thin Film Deposition and Reactive Growth," *IEEE Transactions on Semiconductor Manufacturing*, vol. 11, iss. 3, pp. 511-521, 1998.
- [8] J. Gumphier, W.A. Bather, and D. Wedel, "LPCVD Silicon Nitride Uniformity Improvement Using Adaptive Real-Time Temperature Control," *IEEE Transactions on Semiconductor Manufacturing*, vol. 16, iss. 1, pp. 26-35, 2003.
- [9] C.E. Morosanu, and D. Iosif, "Mechanism of  $\text{Si}_3\text{N}_4$  Films Prepared from  $\text{SiH}_2\text{Cl}_2$  and  $\text{NH}_3$  under Kinetically Controlled Conditions,"

*Thin Solid Films*, vol. 92, pp. 333-340, 1982.

- [10] G. DePinto, "A methodology for Optimizing a Constant Temperature Polysilicon Deposition Process," *IEEE Transactions on Semiconductor Manufacturing*, vol. 6, iss. 4, pp. 332-342, 1993.
- [11] A. Theodoropoulou, R.A. Adomaitis, and E. Zafiriou, "Model Reduction for Optimization of Rapid Thermal Chemical Vapor Deposition Systems," *IEEE Transactions on Semiconductor Manufacturing*, vol. 11, iss. 1, pp. 85-98, 1998.
- [12] Q. He, S.J. Qin, and A.J. Toprac, "Computationally efficient Modeling of Wafer Temperature in a Low-Pressure Chemical Vapor Deposition Furnace," *IEEE Transactions on Semiconductor Manufacturing*, vol. 16, iss. 2, pp. 342-350, 2003.
- [13] A. Radmehr, K.M. Kelkar, P. Kelly, S.V. Patankar, and S.S. Kang, "Analysis of the effect of bypass on the performance of heat sinks using Flow Network Modeling (FNM)," *Proceedings of 15th Annual IEEE Semiconductor Thermal Measurement and Management Symposium*, pp. 42-47, 1999.
- [14] SINDA/FLUINT, Cullimore & Ring Technologies, Inc., 2010, Available: <http://www.crtech.com/sinda.html>.
- [15] J. Kobayashi, N. Nakazato, and K. Hiratsuka, "Numerical Simulation for Gas Flow and Mass Transfer in a Dry Etching Chamber," *Journal of the Electrochemical Society*, vol. 136, iss. 6, pp. 1781-1786, 1989.

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