A THEORETICAL STUDY OF THE TEMPERATURE FIELD IN A PANCAKE CVD REACTOR

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For the pancake CVD reactor, a mathematical model for global analysis of heat transfer in the reactor was developed, and the effects of the geometry and location of the RF coil and the frequency of the RF current on the temperature distributions in the reactor, especially on the susceptor, were investigated.

It is found that the heat generation rate in the susceptor is strongly affected by the location of the RF coil and the current frequency, and that the temperature variation on the susceptor is large with the plane RF coil. Also, by modifying the geometry of the RF coil, the temperature distributions on the susceptor can be easily improved.

Introduction

Chemical vapor deposition (CVD) epitaxial processes are commonly used in microelectronics industries to form thin single-crystal films on semiconductor substrates. The quality of the devices depends on the uniformity in thickness and composition of the thin film grown by the CVD process, and the uniformity depends closely on the gas flow, and the heat and mass transfer, in the CVD reactor. Therefore, correct knowledge of the mechanism of transport phenomena in the reactor is indispensable for the design of the optimum reactor and the optimum operating conditions.

Recently, extensive studies^{1,2,4,6-8)} in the field of modelling of transport phenomena in the vertical and horizontal CVD reactor have been carried out. However, there have been few modelling studies⁵⁾ of the pancake or barrel CVD reactors which are mainly utilized in practical VLSI fabrication.

Figure 1 shows a schematic cross-sectional view of the pancake reactor which is commercially available for the CVD process of epitaxial silicon. The reactive gases diluted by carrier gas are introduced into the reactor, decompose and react at the substrates on the susceptor, which is heated with a radio-frequency (RF) coil. To grow the uniform thickness film on the substrates, it is essential to minimize the temperature distribution on the susceptor, especially under the surface-reaction controlled condition.

The object of this work is to develop a mathematical model for global analysis of heat transfer in the pancake CVD reactor, in order to determine the

optimum conditions for uniform temperature distribution on the susceptor.

1. Theory

We modeled an axi-symmetric pancake CVD reactor, shown in Fig. 1, which consists of a RF induction coil, a graphite susceptor coated with SiC, a gas-injection nozzle and a bell jar. All materials except the RF coil and the susceptor are made of quartz.

In the present work, the electromagnetic field induced by the RF coil was first computed, and the temperature distribution in the reactor based on the thermal power generated in the susceptor by the electromagnetic field were calculated. The gas flow

Fig. 1. Schematic diagram of the pancake CVD reactor, where the susceptor is 600 mm in diameter and 16 mm in thickness, and the bell jar is 700 mm in diameter and 920 mm height. Right side shows calculated isotherms, in which the conditions are the same as for Fig. 2, and the contour interval is 18.7 K.

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and mass transfer of the reactive species are not taken into account here.

1.1 Electromagnetic field

The electromagnetic field is expressed by the pre-Maxwell equations, Eqs. (1)–(5), provided that the media are linear, isotropic and stationary.

$$\text{rot}(\mathbf{B}/\mu) = \mathbf{J} \quad (1), \quad \text{rot}(\mathbf{E}) = -(\partial \mathbf{B}/\partial t) \quad (2)$$

$$\text{div}(\mathbf{B}) = 0 \quad (3), \quad \text{div}(\epsilon' \mathbf{E}) = \rho \quad (4)$$

$$\mathbf{J} = \sigma' \mathbf{E} \quad (5)$$

where μ , ϵ' and σ' are the permeability, permittivity and conductivity of each medium respectively. In this model, materials have no charge, i.e. $\rho = 0$ in Eq. (4), and σ' is zero in all materials except the conductors. The permeability of vacuum is used for μ , because there is no magnetic material in the system. Also, the displacement current term in Eq. (3) is neglected.

Introducing the vector potential $\mathbf{A}$ expressed by Eq. (6),

$$\mathbf{B} = \text{rot}(\mathbf{A}) \quad (6)$$

and assuming axi-symmetry, the pre-Maxwell equations, Eqs. (1)–(5), can be transformed into the following simple scalar equation,³⁾

$$\begin{aligned} &(\partial/\partial R)\{(1/R)(\partial\Psi/\partial R)\} + (\partial/\partial Z)\{(1/R)(\partial\Psi/\partial Z)\} \\ &= -\mu J_\theta \end{aligned} \quad (7)$$

in which Ψ is the magnetic stream function defined by $R\mathbf{A}_\theta$, where $\mathbf{A}_\theta$ is the azimuthal component of $\mathbf{A}$.

When the physical quantities such as vector potential and current density can be expressed as a time-harmonic function, i.e. $J_\theta = J_0 \cos \omega t$, the solution of Eq. (7) is expressed as follows.

$$\Psi = \Psi_i(R, Z) \cos \omega t + \Psi_o(R, Z) \sin \omega t \quad (8)$$

where Ψ_i and Ψ_o are respectively the in-phase and out-of-phase components of Ψ .

Substitution of Eq. (8) into Eq. (7) gives the equations for Ψ_i and Ψ_o , which are solved with the boundary conditions that $\Psi_i = \Psi_o = 0$ at the center line and at the far field.

The heat generation rate per unit volume in the conductor, i.e. the susceptor in the CVD reactor, is given as follows.

$$Q = \sigma' \omega^2 (\Psi_i^2 + \Psi_o^2) / (2R^2) \quad (9)$$

1.2 Temperature field

The dimensionless form of the conductive heat transfer equations for all materials in the system are expressed as follows, where R_0 , T_{ref} and k_{ref} are used for the characteristic values.

$$\text{div}\{\kappa_j^* \text{grad}(T_j^*)\} + Q_j^* = 0 \quad (10)$$

where Q_j^* is the volumetric heat generation rate in material j obtained by Eq. (9). In this model, Q_j^* is

Fig. 2. Distributions of (a) in-phase and (b) out-of-phase components of Ψ . The contour values of (*) are (a) 0.980×10^{-5} Wb and (b) 0.629×10^{-6} Wb, and the contour intervals are (a) 0.980×10^{-5} Wb and (b) 0.629×10^{-6} Wb.

zero except for the susceptor.

The boundary conditions are given by the following equations.

$$\text{At the base plate: } T_j^* = T_b^* \quad (11-1)$$

$$\text{At the RF coil surface: } T_j^* = T_c^* \quad (11-2)$$

At the outside wall of the bell jar, and the end of the gas nozzle and rotating supports:

$$-\kappa_j^* (\partial T_j^* / \partial n) = Bi_j (T_j^* - T_{a,j}^*) \quad (11-3)$$

Elsewhere:

$$-\kappa_j^* (\partial T_j^* / \partial n) = Ra_j \{ (T_j^*)^4 - (T_{eff,j}^*)^4 \} \quad (11-4)$$

It is assumed that the heat loss from the boundary surfaces other than the outside wall of the bell jar is caused only by radiation, and that $T_{eff,j}^*$ in Eq. (11-4) is defined by the following equation⁹⁾ with the aid of the assumption of diffuse-gray materials.

$$T_{eff,j}^* = \{ \sum \epsilon_k S_k G_{kj} T_k^{*4} / (\epsilon_j S_j) \}^{1/4} \quad (12)$$

This assumption is reasonable when the CVD reactor is operated at very low pressure and the effect of the surrounding gas flow on the heat transfer from the boundary surface is negligibly small.

To solve the electromagnetic and temperature fields in the CVD reactor, the Galerkin finite element method is used. The calculation domain shown in Fig. 1 is discretized by the quadrilateral elements, and Ψ_i and Ψ_o in the magnetic stream function and temperature are approximated with bilinear and biquadratic trial functions respectively.

2. Results and Discussion

In the computation of the pancake CVD reactor, the susceptor is 600 mm in diameter and 16 mm in thickness, and the bell jar is 700 mm in diameter and 920 mm in height. The distance between the upper surface of the susceptor and the base plate is 230 mm. The RF coil is a 10-turn spiral one. The physical properties (electric and thermal properties) and

Fig. 3. Effect of distance, a , on distributions of volumetric heat generation rate in the susceptor

Table 1. Physical properties and processing parameters used in the calculation

electric conductivity (σ)	
susceptor (graphite)	: 10^5 [$1/\Omega \cdot m$]
base plate (SUS)	: 4×10^6 [$1/\Omega \cdot m$]
permeability (μ)	: $4\pi \times 10^{-7}$ [H/m]
thermal conductivity (k)	
susceptor (graphite)	: 32.0 [W/m $\cdot$ K]
elsewhere (quartz)	: 3.0 [W/m $\cdot$ K]
emissivity (ϵ)	
susceptor (SiC coated)	: 0.85
base plate (SUS)	: 0.2
elsewhere (quartz)	: 0.5
RF coil (copper)	: 0.47
heat transfer coefficient	
outside bell jar	: 49.0 [W/m $^2 \cdot$ K]
end of gas nozzle and rotating support	: 34.0 [W/m $^2 \cdot$ K]
current density in RF coil (J_0)	: 2.25×10^6 [A/m 2]
frequency in RF coil (ω)	: 25 – 180 [kHz]
temperature at RF coil surface (T_c)	: 306 [K]
temperature at base plate (T_b)	: 306 [K]
temperature outside bell jar (T_a)	: 295 [K]
temperature at end of gas nozzle and rotating support	: 306 [K]

processing parameters are listed in Table 1.

Figure 2 shows typical results for the electromagnetic fields, i.e. the distributions of (a) the in-phase and (b) out-of-phase components of the magnetic stream functions, Ψ , defined by Eq. (8). In this case, the shape of the RF coil is flat, and the current density and frequency in the coil are 2.25×10^6 [A/m 2] and 180 [kHz], both typical values in the industry. The corresponding components of magnetic flux density B are the vector fields tangent to these curves. From Fig. 2, the in-phase component, Ψ_i , takes a maximum value on the RF coil, while the maximum value of the out-of-phase component, Ψ_o , appears in the susceptor. The contours drawn in Fig. 1 show the temperature profiles in the CVD reactor based on the heat generation rate calculated using the electromagnetic field in Fig. 2.

Fig. 4. Effect of distance, a , on temperature distributions at the upper surface of the susceptor

Fig. 5. Effect of distance, a , on total heat generation rate in the susceptor

Figures 3 and 4 show the effect of the distance between the lower surface of the susceptor and the RF coil, a , on the distributions of volumetric heat generation rate in the susceptor, Q , and on the radial temperature distribution at the upper surface of the susceptor respectively, where the current density and frequency in the RF coil are the same as those in Fig. 2. In Fig. 3, the heat generation rate in the radial direction has maximum value at the middle part of the susceptor. In the direction of thickness, Q decreases rapidly from the lower surface toward the upper one of the susceptor. This is due to the skin effect. The skin depth, δ , is calculated by the following equation.

Fig. 6. Effect of frequency of RF current on distributions of volumetric heat generation rate in the susceptor

$$\delta = (2/\mu\sigma\omega)^{1/2} \quad (13)$$

With high conductivity of the susceptor and high frequency of the RF current, the skin depth is small.

Also, Q is relatively large near the edge of the susceptor in Fig. 3. This fact is related to a large phase shift of the field near the edge of the susceptor where a large Ψ_o -value appears shown in Fig. 2.

It is apparent from Fig. 4 that the temperature on the susceptor shows the maximum value around the middle part according to the distributions of Q shown in Fig. 3, the large radiative heat loss from the periphery of susceptor, and the conductive heat loss to the rotating support shown in Fig. 1.

Figure 5 shows the relationship between the distance, a , and the total heat generation rate, Q_T , calculated by integration over the volume of the susceptor. It is found that Q_T decreases with a .

Figures 6 and 7 show the effect of the RF current frequency, ω , on the volumetric heat generation rate, Q , and on the temperature distribution at the upper surface of the susceptor respectively, where $a = 2.1$ cm. It is found from Fig. 6 that the magnitude of the heat generation rate and its gradient along the thickness of the susceptor decrease as ω decreases. The latter is due to the increase in skin depth with the frequency decrease. Then, as shown in Fig. 7, the temperature on the susceptor decreases with decrease of ω . Figure 8 shows the effect of ω on Q_T . It is found that Q_T increases with ω .

From the above results, it is concluded that the temperature changes considerably in the radial direction of the susceptor when the plane RF coil is used, and that a CVD reactor with such large temperature variation on the susceptor is not practically allowable, especially under the surface-reaction controlled condition. The object of the present work is to seek the optimum processing conditions to make the temperature distribution on the susceptor uniform.

Fig. 7. Effect of frequency of RF current on temperature distributions at the upper surface of the susceptor

Fig. 8. Effect of frequency of RF current on total heat generation rate in the susceptor

Fig. 9. Improvement of geometry of RF coil

To attain this, the geometry of the RF coil was investigated. The distance, a , and the coil interval were changed and the arrangement shown in Fig. 9 was found to be better.

Figure 10 shows (a) the distributions of Ψ_i and Ψ_o

Fig. 10(a). Distributions of (a) in-phase and (b) out-of-phase components of Ψ with the improved RF coil. The contour values of (*) are (a) 0.104×10^{-4} Wb and (b) 0.803×10^{-6} Wb, and the contour intervals are (a) 0.104×10^{-4} Wb and (b) 0.805×10^{-6} Wb.

Fig. 10(b). Distribution of volumetric heat generation rate in the susceptor with the improved RF coil

Fig. 10(c). Surface temperature distribution at the upper surface of the susceptor with the improved RF coil

components of Ψ , (b) the distribution of volumetric heat generation rate and (c) the temperature profile at the upper surface of the susceptor with the modified RF coil, where J_0 and ω are the same as those in Fig. 2. In Fig. 10(c) the dotted line shows the results with the plane coil. The distribution of the heat generation rate is remarkably improved by modification of the geometry of the RF coil, where Q at the middle position becomes relatively small in comparison with Q near the edge of the susceptor. Also, the temperature distribution on the susceptor can be much flattened in comparison to the plane RF coil.

In the case of a CVD process under the surface-

reaction controlled condition, it might be necessary to make the temperature distribution in the susceptor more uniform than that in Fig. 10(c), by modulating the distance, a , and the coil interval strictly. By calculations, however, it was confirmed that, in principle, modification of the coil geometry as shown in Fig. 9 is effective in achieving a uniform temperature distribution in the susceptor.

Conclusion

Finite element analyses of the electromagnetic and temperature fields in a pancake CVD reactor were carried out and the following conclusions were obtained.

- 1) The temperature variations in the susceptor are large with the plane RF coil.
- 2) The heat generation rate is strongly affected by the location of the RF coil and the current frequency.
- 3) Temperature distribution in the susceptor can be easily improved by modifying the geometry of the RF coil.

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Nomenclature

A	= vector potential	[Wb/m]
a	= distance between susceptor and RF coil	[m]
B	= magnetic flux density	[Wb]
Bi	= Biot number ($=hR_0/k_{ref}$)	[—]
E	= electric field strength	[V/m]
G_{kj}	= Gebhart's absorption factor	[—]
h	= heat transfer coefficient	[W/m ² K]
J	= current density	[A/m ²]
J_0	= current density of RF coil	[A/m ²]
k	= thermal conductivity	[W/m·K]
Q	= volumetric heat generation rate	[W/m ³]
Q^*	= $Qr_c^2/k_{ref}T_{ref}$	[—]
Q_T	= total heat generation rate	[W]
R	= radial distance in cylindrical coordinates	[m]
Ra	= radiation number ($=\epsilon\sigma'R_0T_{ref}^3/k_{ref}$)	[—]
R_0	= radius of bell jar	[m]
S	= surface area of boundary elements	[m ²]
T	= temperature	[K]
T_a	= ambient temperature	[K]
T_b	= temperature at base plate	[K]
T_c	= temperature at RF coil surface	[K]
T^*, T_a^*, T_b^*, T_c^*	= $T/T_{ref}, T_a/T_{ref}, T_b/T_{ref}, T_c/T_{ref}$	[—]
t	= time	[s]
Z	= axial distance in cylindrical coordinates	[m]
δ	= skin depth	[m]
ϵ	= emissivity	[—]
ϵ'	= permittivity	[H/m]
μ	= permeability	[F/m]
κ^*	= ratio of thermal conductivity ($=k/k_{ref}$)	[—]
ρ	= charge density	[A/m ³]

σ	= Stefan-Boltzman constant	[W/m ² K ⁴]
σ'	= electric conductivity	[1/ $\Omega \cdot m$]
ω	= frequency of RF current	[Hz]
Ψ	= magnetic stream function	[Wb]

<Subscripts>

i	= in-phase component
j, k	= material
o	= out-of-phase component
ref	= reference value
θ	= azimuthal component

Literature Cited

- 1) Bulsari, A. B., M. E. Orazem and J. G. Rice: *J. Crystal Growth*, **92**, 294 (1988).
- 2) Fotiadis, D. I., M. Boekholt and K. F. Fensen: *J. Crystal Growth*, **100**, 577 (1990).
- 3) Gresho, P. M. and J. J. Derby: *J. Crystal Growth*, **85**, 40 (1987).
- 4) Moffat, H. K. and K. F. Jensen: *J. Electrochem*, **135**, 459 (1988).
- 5) Oh, I., C. G. Takoudis and G. W. Neudeck: *J. Electrochem. Soc.*, **138**, 554 (1991).
- 6) Ouazzani, J., K. C. Chiu and F. Rosenberger: *J. Crystal Growth*, **91**, 497 (1988).
- 7) Ouazzani, J. and F. Rosenberger: *J. Crystal Growth*, **100**, 545 (1990).
- 8) Sato, T., T. Yuasa and N. Imaishi: *Kagaku Kogaku Ronbunshu*, **17**, 362 (1991).
- 9) Tsukada, T., N. Imaishi, M. Hozawa and K. Fujinawa: *J. Chem. Eng. Japan*, **20**, 146 (1987).