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VELOCITY PROFILE AND TEMPERATURE DISTRIBUTION IN THE HORIZONTAL EPITAXIAL REACTOR

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The cross-sectional and axial velocity profiles and temperature distributions in a horizontal epitaxial reactor were calculated numerically from fundamental equations under certain assumptions. Streamlines in the cross-section showed similar pattern over the whole range of Gr , but the value of stream function was affected by Gr . The axial velocity profiles were quite different from that of parabolic flow when Gr was larger than 10^4 . The temperature distributions in a cross-section of the channel became uniform when Gr was large.

In order to check the calculated results, the axial velocity profile and the temperature distribution were measured in this reactor under the same conditions as those of this calculation. The calculated velocity and temperature were a good approximation of the experimental ones.

Introduction

The epitaxial reactor (chemical vapor deposition reactor) has been widely used for production of semiconductor high purity crystals and dielectric films, and for the treatment of material surface. This reactor has been recently used for the treatment of sensitive film surface in photographic technology.

In an epitaxial reactor, a susceptor heated up in

700–1200°C is placed at the bottom in the channel, and vigorous three-dimensional free convective flow is generated by the buoyancy force induced by a large temperature difference. This phenomenon is pronounced in a horizontal epitaxial reactor, which has been generally used. Therefore, velocity distributions are not easily calculated from fundamental equations, and only temperature distributions have been investigated experimentally^{2,6,10}.

Recently, along with the remarkable development of electronic computers, a few numerical solutions have been obtained for the three-dimensional laminar

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Fig. 1 Coordinate system for a horizontal rectangular channel

Table 1 Logic diagram for computer calculation

natural convective heat transfer in a horizontal tube^{3,11)}. However, these theoretical calculations were restricted to the case of large Pr and low Gr for the reason of instabilities of numerical calculation. Thus it seemed that the calculated results of these papers did not well express the phenomena in a horizontal epitaxial reactor. Furthermore, the laminar natural convection in the horizontal flow tube, of which a part of the bottom is heated, has not been studied up to this time.

In this paper, the cross-sectional and axial velocity profiles and temperature distributions in a horizontal epitaxial reactor were calculated numerically from fundamental equations under some suitable assumptions.

To check these calculated results, axial velocity components and local temperature distribution in the reactor were investigated.

1. Fundamental Equations and Numerical Calculation Procedure

Let us consider phenomena on the steady heat transfer in a three-dimensional flow with laminar natural convection in a horizontal rectangular channel,

of which a part of the bottom is heated and the other walls are kept at low constant temperature, as shown in Fig. 1. From the observed flow pattern in this reactor, the following assumptions are made to calculate the velocity component and temperature.

1) Since the gas is well preheated before entering the reaction zone, the temperature distribution and flow pattern in the reactor are established and not affected by its axial length, i.e.,

$$\frac{\partial u}{\partial z} = \frac{\partial v}{\partial z} = \frac{\partial w}{\partial z} = \frac{\partial t}{\partial z} = 0$$

$$\frac{\partial^2 u}{\partial z^2} = \frac{\partial^2 v}{\partial z^2} = \frac{\partial^2 w}{\partial z^2} = \frac{\partial^2 t}{\partial z^2} = 0$$

2) The physical properties of the fluid, such as viscosity, thermal conductivity, etc., are independent of temperature, but buoyancy force is dependent upon the temperature difference.

Furthermore, dimensionless variables as shown in Eq. (1) are introduced, and the dimensionless stream function ψ and vorticity ζ are defined as Eqs. (2) and (3), respectively.

$$\left. \begin{aligned} (U, V, W) &= (u, v, w)H/\nu \\ (X, Y, Z) &= (x, y, z)/H \\ T &= (t - t_w)/(t_H - t_w), \quad P = pH^2/\rho\nu^2 \\ Gr &= g\beta H^3(t_H - t_w)/\nu^2, \quad Pr = C_p\mu/\lambda \end{aligned} \right\} \quad (1)$$

$$U = -\partial\psi/\partial Y, \quad V = \partial\psi/\partial X \quad (2)$$

$$\zeta = \partial V/\partial X - \partial U/\partial Y = (\partial^2\psi/\partial X^2 + \partial^2\psi/\partial Y^2) \quad (3)$$

After some manipulations the nondimensional fundamental equations are written as Eqs. (4)–(6), and the boundary conditions become Eq. (7).

$$U \frac{\partial \zeta}{\partial X} + V \frac{\partial \zeta}{\partial Y} = \left(\frac{\partial^2 \zeta}{\partial X^2} + \frac{\partial^2 \zeta}{\partial Y^2} \right) + Gr \frac{\partial T}{\partial X} \quad (4)$$

$$U \frac{\partial T}{\partial X} + V \frac{\partial T}{\partial Y} = \frac{1}{Pr} \left(\frac{\partial^2 T}{\partial X^2} + \frac{\partial^2 T}{\partial Y^2} \right) \quad (5)$$

$$U \frac{\partial W}{\partial X} + V \frac{\partial W}{\partial Y} + \frac{\partial P}{\partial Z} = \left(\frac{\partial^2 W}{\partial X^2} + \frac{\partial^2 W}{\partial Y^2} \right) \quad (6)$$

$$\left. \begin{aligned} X=0; \quad \psi &= \partial^2\psi/\partial X^2 = \partial W/\partial X = \partial T/\partial X = 0 \\ X=L/H; \quad \psi &= \partial\psi/\partial X = W = T = 0 \\ Y=0, \quad \left\{ \begin{array}{l} 0 \leq X \leq x_A/H; \quad \psi = \partial\psi/\partial Y = W = 0, \quad T = 1 \\ x_A/H < X \leq L/H; \quad \psi = \partial\psi/\partial Y = W = T = 0 \end{array} \right. \\ Y=1; \quad \psi &= \partial\psi/\partial Y = W = T = 0 \end{aligned} \right\} \quad (7)$$

These equations can not be solved analytically, because Eqs. (2)–(7) are second-order simultaneous partial differential equations. In this study Eqs. (2)–(7) were solved numerically. Table 1 shows the computer logic diagram for this calculation.

The calculation procedure is as follows. At first each equation was written in a finite difference form with “upwind method”^{1,8,9)} which exhibited good numerical stability. This method was quite suitable

for the calculation of this reactor in the case of large Gr ($Gr=10^4-10^5$). Then, Eqs. (3)–(5) and (7) were solved numerically with relaxation method. U and V were obtained from Eq. (2). After establishing the velocity components in X and Y directions, and specifying the axial pressure gradient from the flow rate of gas, the axial velocity component, W , was calculated numerically from Eqs. (6) and (7) with the relaxation method as the function of X and Y .

The calculation was carried out for $D_e=3.24, 3.86, 5.0$ cm, $L/H=0.827, 1.204, x_A/H=0.25-0.87, Pr=0.69, Gr=10^3-10^5$ and $Re=12.8-52.7$.

In this calculation ΔX and ΔY were 1.03×10^{-1} and 9.09×10^{-2} , respectively. The computer used was HITAC 8800/8700, and computer time for a condition needed about 20 seconds.

2. Experimental Apparatus and Procedure

To check the calculated results, temperature distributions and axial velocity profile in a horizontal epitaxial reactor were measured.

Figure 2 shows the schematic diagram of the experimental apparatus. Rectangular channel with the cross sectional area of 2.6×4.3 cm² ($L/H=0.827$)* and 170 cm long was made of transparent quartz glass. A silicon carbide heating element (130 cm long) was placed on the bottom of the channel and was heated by electricity. The temperatures of the heating element and the channel wall were measured by a micropyrometer and Pt-PtRh thermocouples (0.3 mm ϕ), respectively. Sizes of the channel and the heating element were equal to those in the case of numerical calculation.

A suction pyrometer was used to measure the gas temperature. Pt-PtRh thermocouples (0.3 mm ϕ) were inserted into this pyrometer, and suction rate was adjusted in order not to disturb the flow pattern in the channel. Axial velocity was measured by a Pitot tube, and the pressure difference for the Pitot tube was measured by an extremely precise pressure difference meter which was able to measure the pressure difference up to 0.001 mmAq.

Air from a compressor was passed through a dehydration tower filled with silica-gel and a CO₂-absorption tower filled with KOH–CaO, and then passed into the reactor.

To investigate the local velocity and the temperature distribution, the Pitot tube or the suction pyrometer was put into a channel where the velocity profile and the temperature distribution had already been established.

Surface temperatures of the heating element were in

* Another size of rectangular channel, 2.3×5.5 cm² ($L/H=1.204$), was also used for this experiment.

** W is calculated from Eq. (6) under the condition of $U=V=0$.

Fig. 2 Schematic diagram of the experimental apparatus

the range of 900 to 1100°C. Feed rates of air were in the range of 1.2 to 4.9 l/min (at 20°C, 1 atm). Under these flow rates, steady spiral flow was established in this channel⁷⁾.

3. Calculated Results

3.1 Velocity profile

Since velocity and temperature distributions were symmetrical about the Y axis in a horizontal epitaxial reactor, these distributions were calculated in the right-hand half of the cross-section.

Figures 3 and 4 show some typical streamlines to the cross-sectional direction and axial velocity profile, W , in the cross-section of the channel with Gr as a parameter. In Figs. 3(a) and 4(a) the similar pattern of streamlines is found at all over the range from $Gr=10^3$ to 10^5 , but the value of the stream function is strongly affected by Gr . As Gr increases, the streamlines extend toward the upper wall, and the center of the circulating streamlines moves upward. In Fig. 3(b) dotted lines and solid lines show dimensionless axial velocity profile for $U=V=0$ (parabolic flow)** and $Gr=10^3$, respectively. In both cases, the axial velocity profiles are almost the same pattern and the axial velocity is the largest at the center of the channel. However, when Gr is larger than about 10^4 , the axial velocity profile shown in Fig. 4(b) is quite different from that of parabolic flow. That is, the axial velocity becomes the largest in the center of the right and left half cross-section of the channel. When Gr is larger than 10^5 , this tendency becomes pronounced.

Figure 5 shows some typical experimental results of the axial velocity across the channel under the same conditions as those of the numerical calculation for $Gr=3.54 \times 10^4$. From these values, the calculated velocities agree approximately with the measured ones.

The shapes of axial velocity profiles are not changed by the feed rate of air, Q , of 1.2 and 4.9 l/min. The shapes of the streamlines and the axial velocity profiles are not affected by the width of heating element. However, the values of stream function are somewhat increased with increase in width.

3.2 Temperature distribution

(a) Stream function

(b) Axial velocity

Fig. 3 Contour maps of streamline and axial velocity with $Gr=0$ and 10^3 for $L/H=0.827$, $x_A/H=0.310$, $Pr=0.69$ and $Re=26.8$ ($Re'=35.8$)

(a) Stream function

(b) Axial velocity

Fig. 4 Contour maps of streamline and axial velocity with $Gr=1.5 \times 10^4$ and 10^5 for $L/H=0.827$, $x_A/H=0.310$, $Pr=0.69$ and $Re=26.8$ ($Re'=35.8$)

Fig. 5 Comparison of calculated axial velocities with experimental ones

Figures 6 to 8 show some typical dimensionless temperature distributions in the cross-section. Figures 6 and 7 show the effect of Gr upon the temperature distribution in the channel. It appears that, as Gr is increased, the intensity of vortex flow in the channel becomes vigorous and then the temperature distributions become uniform.

Fig. 6 Temperature distributions with $Gr=10^3$ and 10^5 for $L/H=0.827$, $x_A/H=0.310$, $Pr=0.69$ and $Re=12.8$ ($Re'=17.2$)

Fig. 7 Comparison of calculated temperature distributions with experimental ones for $Gr=1.5 \times 10^4$, $L/H=0.827$, $x_A/H=0.310$, $Pr=0.69$ and $Re=12.8$ ($Re'=17.2$)

In Fig. 7 the numerical values written near the experimental point are the dimensionless local temperatures obtained by the experiment under the same conditions as those of this numerical calculation. As can be seen from these values, the calculated temperature is a sufficiently good approximation to the measured one. Furthermore, a good agreement between the calculated results and experimental ones was also obtained in other cases ($L/H=1.204$ ($H=2.30$ cm, $L=2.77$ cm), $x_A/H=0.43-0.87$).

Figure 8 shows the temperature distribution in the cases where x_A/H are 0.517 and 0.724, respectively. Comparing Fig. 8 with Fig. 7, if the width of heating element is increased, the temperature in the channel becomes large.

4. Discussion

4.1 Fluid flow characteristics

Usually, a horizontal epitaxial reactor is operated

Fig. 8 Temperature distribution with $x_A/H=0.517$ and 0.724 for $L/H=0.827$, $Pr=0.69$ and $Re=12.8$ ($Re'=17.2$)

Fig. 9 Contour maps of fluid speed $(U^2 + V^2)^{1/2}$ with $Gr=5 \times 10^4$ and 10^5 for $L/H=0.827$, $x_A/H=0.310$, $Pr=0.69$ and $Re'=80-190$

under conditions such as $Re'=10-200$ and $Gr=10^4-10^5$ ⁴⁾. Under these conditions, stable two symmetrical spiral flows with the same pitch length towards the axial direction were generated, and axial velocity components were a slightly changed across the cross-section of the reactor⁵⁻⁷⁾. This means that the vigorous vortex flow makes the axial velocity distribution uniform.

Figure 9 shows the cross-sectional local speed $(U^2 + V^2)^{1/2}$ in the cases where $Gr=5 \times 10^4$ and 10^5 . As shown in Fig. 9, the cross-sectional local speed is comparatively slow near the walls and in the central part of the right and left half cross-sections of the channel and the local speed is the largest in the central part of the channel.

In the horizontal epitaxial reactor, if Re' is smaller than 80, a stable spiral flow is generated, and when Re' is larger than 80, its spiral flow is gradually disturbed, and when Re' is larger than 190, no spiral flow is generated⁷⁾. Figure 10 shows the axial velocity profiles for $Re'=80$ and 190. Figures 9 and 10 suggest that the values of cross-sectional velocities are almost equal to those of axial velocity. Therefore, the forma-

Fig. 10 Axial velocity profiles with $Re'=80$ and 190 for $L/H=0.827$, $x_A/H=0.310$, $Pr=0.69$ and $Gr=5 \times 10^4, 10^5$

Fig. 11 Vertical temperature gradient at $X=0.3$ in the channel

tion of the stable spiral flow may be caused by the cross-sectional velocity being the same order of magnitude as the axial velocity.

4.2 Temperature distribution

Temperature distribution in a horizontal epitaxial reactor was measured⁸⁾, and its distributions was quite uniform except near the walls and the heating element. The large cross-sectional vortex flow makes gas temperature uniform across the reactor.

Figure 11 shows the calculated temperature distribution toward cross-sectional direction with Gr as a parameter. From Fig. 11, the temperature distribution is quite uniform except near the wall and the heating element when Gr is larger than 1.5×10^4 . The calculated results agree approximately with the experimental ones.

4.3 Pitch length

As mentioned above, there are two symmetrical spiral flows in this reactor in the case where Re' is smaller than 190. The authors pointed out the pitch length of the spiral flow as one of the most important factors which characterize the flow pattern in this reactor, and obtained the empirical equation for estimation of the pitch length⁸⁾.

In this study the axial and cross-sectional velocity components in this reactor were calculated from the

Fig. 12 Relation between computed pitch length and stream function for $Gr = 1.5 \times 10^4$ with Q as parameter

Table 2 Comparison of measured pitch length with estimated one

D_e [cm]	Q [l/min]	Pitch length [cm]	
		Measured	Estimated
3.24	1.2	4.5	4.7
	2.5	10.1	9.8
	4.9	21.4	19.1
3.86	2.07	3.8	3.6

fundamental equations. The pitch length of the spiral flow was approximately estimated from these components. The pitch length is considered as the distance moved by the axial velocity W when the fluid takes one round in the channel with the cross-sectional velocity components U and V . If the length of any solid streamline in Fig. 4 is expressed as l_N , this streamline is divided into small compartment Δd_k ($\sum_{k=1}^N \Delta d_k = l_N$). Average cross-sectional velocity in Δd_k is expressed as,

$$S_k = (u_k^2 + v_k^2)^{1/2}$$

and the time taken for the fluid to move through Δd_k is

$$\Delta \theta_k = \Delta d_k / S_k$$

Therefore the pitch length is calculated from,

$$\text{Pitch length} = \sum_{k=1}^N \left\{ \Delta \theta_k \left(\frac{w_k + w_{k+1}}{2} \right) \right\}$$

where w_k is the axial velocity component.

Figure 12 shows the relationship between the computed pitch length and the stream function in the case of $D_e = 3.24$ with Q as a parameter. From Fig. 12, the pitch length decreases a little with an increase of stream function. That is, the pitch length becomes the smallest in the centers of the right and left half cross-sections of the channel.

In the previous paper, the pitch length of spiral flow was measured as follows⁶⁾. The tracer gas was put into the bulk gas flow near the wall by a narrow tube and the concentration of tracer gas in the downstream was measured by sampling the gas near the wall with a narrow tube.

Now, some typical comparisons of the measured pitch length with the computed one under the same condition are shown in Table 2. From this table, the

calculated results are a sufficiently good approximation to the experimental ones. This means the axial and the cross-sectional velocity components obtained by this calculation are approximately equal to those in the real reactor.

Conclusion

The velocity and temperature distributions in the horizontal epitaxial reactor were calculated numerically from the fundamental equations under certain assumptions and following results were obtained.

(1) Streamlines to the cross-sectional direction show a similar pattern over the range from $Gr = 10^3$ to 10^5 , but the value of stream function is affected by Gr . The axial velocity profiles are quite different from that of parabolic flow when Gr is larger than 10^4 and the axial velocity profiles are not changed by the feed rate of gas.

(2) The calculated axial velocity profiles agreed approximately with the measured ones.

(3) As Gr is increased, the intensity of vortex flow becomes vigorous and the temperature distributions become uniform across the cross-sectional direction. The calculated temperature distributions agreed well with the measured ones.

(4) The shapes of streamlines and the axial velocity profiles are not affected by the width of the heating element, but the values of the stream function are somewhat increased with an increase in the width. If the width of the heating element is increased, the temperature in the channel becomes large.

(5) The value of the cross-sectional velocities are almost equal to those of the axial velocity under ordinary operating conditions.

(6) The pitch length of the spiral flow estimated from the computed flow pattern agrees well with the experimental results.

Nomenclature

C_p	= heat capacity at constant pressure	[cal/g·°C]
D_e	= equivalent diameter of tube ($= 4LH/(2L+H)$)	[cm]
G	= mass velocity of gas	[g/cm ² ·sec]
Gr	= Grashof number ($= g\beta H^3(t_H - t_W)/\nu^2$)	[—]
g	= gravitational acceleration	[cm/sec ²]
H	= channel height	[cm]
L	= half width of channel	[cm]
P	= dimensionless pressure	[—]
p	= fluid pressure	[g/cm·sec ²]
Pr	= Prandtl number ($= C_p\mu/\lambda$)	[—]
Q	= volume flow rate of gas	[l/min]
Re	= Reynolds number based on channel height ($= Q\rho/2L\mu$)	[—]
Re'	= Reynolds number based on equivalent diameter ($= D_e G/\mu$)	[—]
S	= dimensionless cross-sectional local speed ($(U^2 + V^2)^{1/2}$)	[—]
T	= dimensionless temperature	[—]

t	= temperature	[°C]
U	= dimensionless velocity in X -direction	[—]
u	= velocity in x -direction	[cm/sec]
V	= dimensionless velocity in Y -direction	[—]
v	= velocity in y -direction	[cm/sec]
W	= dimensionless velocity in Z -direction	[—]
w	= velocity in z -direction	[cm/sec]
X, Y, Z	= dimensionless rectangular co-ordinates	[—]
x_A	= half width of reaction zone	[cm]
x, y, z	= rectangular co-ordinates	[cm]
α	= thermal diffusivity	[cm ² /sec]
β	= volumetric coefficient of expansion	[1/°C]
ζ	= dimensionless vorticity	[—]
λ	= thermal conductivity	[cal/cm·sec·°C]
μ	= viscosity	[g/cm·sec]
ν	= kinematic viscosity	[cm ² /sec]
ρ	= density	[g/cm ³]
ϕ	= dimensionless stream function	[—]
<Subscripts>		
H	= reaction zone	
W	= wall	

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CHARACTERISTICS OF THE HORIZONTAL EPITAXIAL REACTOR — IN CASE OF MASS TRANSFER RATE CONTROL —

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Concentration distributions of reactant and mass transfer coefficient in a horizontal epitaxial reactor were numerically calculated from fundamental equations under some assumptions in the case of mass transfer rate control. The concentration distribution in the cross-section of the channel became uniform when Gr and the distance from the leading edge were increased or the feed rate of gas was decreased. To check the calculated results, carbon plates were burned in this reactor under the mass transfer rate control and local concentration of carbon dioxide was measured. The calculated concentration and mass transfer coefficient were a sufficiently good approximation to the experimental ones.

Introduction

In an epitaxial reactor (chemical vapor deposition reactor), deposition reaction occurs on the surface of a susceptor heated up in 700–1200°C. Thickness and purity of reaction products must be controlled for the application purpose. Especially, in the case of production of semiconductor material, the thickness must be

as strictly uniform as possible. Thickness and purity of reaction products are influenced by the concentration distribution of reactants in the reactor.

In a horizontal epitaxial reactor, which has been generally used, vigorous three-dimensional free convective flow is generated by the buoyancy force induced by large temperature differences. Therefore, velocity distributions are not easily calculated from fundamental equations, and concentration distributions of reactant gas and temperature distributions have been determined experimentally^{1,3–6,8,13,14}. There are few

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