HEAT AND MASS TRANSFER IN A VERTICAL EPITAXIAL REACTOR.

2. NONSYMMETRICAL HEATING OF THE REACTOR

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A numerical investigation yields the distribution of dimensionless deposition rate along an epitaxial reactor in the form of a vertical plane channel with heated and cooled walls.

The first part of this study [1] described heat and mass transfer in an epitaxial reactor in the form of a symmetrically heated vertical channel. In another type of reactor which is widely used, the walls are cooled and their temperature is considerably below the temperature of the deposition surface. These differences account for the differences in heat and mass transfer in the given reactor and the reactor described in [1].

Reactors with "cold" walls are usually made in the form of a cooled vertical segment of a tube (quartz or metal) enclosing a coaxially-positioned substrate holder in the form of a polyhedral pyramid [2]. In commercial reactors, the width of the annular gap between the reactor wall and the substrate holder is much smaller than the diameter of the reactor. For purposes of simplification, this allows us to represent the gap as a plane channel. It is shown schematically in Fig. 1.

The thin plate-substrates 1 are located on the flat substrate holder 2 and heated to the deposition temperature. The wall of the reactor 3 is cooled to a temperature considerably below the deposition temperature. The gas mixture is fed downward into the reactor as shown by the arrow.

In the boundary-layer approximation, the equations describing heat and mass transfer in the given reactor are the same as Eqs. (2-5) in [1]. The boundary conditions have the form:

$$\begin{gathered}\tilde{x}=0,\ \ 0<\tilde{y}<1,\ \tilde{u}=1,\ \tilde{T}=1,\ c_1=c_{01};\ \tilde{x}\geqslant 0,\ \ y=y_{\mathrm{s}},\ \ \tilde{u}=0,\\ \tilde{v}=\tilde{v}_{\mathrm{s}}\ \ \tilde{T}=\tilde{T}_{\mathrm{s}},\ c_1=0;\ \tilde{x}\geqslant 0,\ \ \tilde{y}=1,\ \ \tilde{u}=\tilde{v}=0,\ \ \tilde{T}=\tilde{T}_{\mathrm{w}},\\ \frac{\partial c_1}{\partial\tilde{y}}+\frac{\alpha_T c_1(1-c_1)}{\tilde{T}_{\mathrm{w}}}\frac{\partial\tilde{T}}{\partial\tilde{y}}=0.\end{gathered}\tag{1}$$

The geometric characteristics of the reactor and the space coordinates (h, α, x, y, y_S) are shown in Fig. 1, while the remaining notation coincides with that used in [1].

At α = 0°, the deposition angle decreases with increasing distance from the reactor inlet (see Fig. 2) due to depletion of silane from the gas mixture. However, this relation is monotonic. As in a symmetrically heated channel [1], the presence of a maximum or an inflection point on the curve $Nu_{0D}(\tilde{x}_T)$ is connected with a reduction in the contribution of free convection and thermodiffusion.

The effect of these factors — which is to decrease deposition rate — diminishes toward the end of the initial thermal section. The role of free convection increases with a decrease in wall temperature. The effect of free convection is smaller in a convergent channel and disappears at a smaller value of $\tilde{x}_T$ than in a parallel channel (Fig. 2).

As is shown in Fig. 2, free convection reduces silicon deposition rate to the greatest extent in the region of small $\tilde{x}_T$. Meanwhile, the value of the ratio of the numbers Nu_{0D}

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TABLE 1. Critical Values of the Complex Ga/Re for Different Conditions of Silicon Epitaxy

Number of regime	T_s	T_w	T_0	u_0, m/sec	h_0, m	α, deg	Ga/Re
	K						
1	13 23	573	293	0,22	0,03	0	391
2	13 23	573	573	0,20	0,05	0	199
3	13 23	573	293	0,21	0,03	3	410
4	13 23	573	293	0,18	0,03	5	478
5	14 23	323	293	0,45	0,05	0	531
6	14 23	323	293	0,35	0,05	2	683

determined with and without allowance for free convection depends only slightly on $\tilde{x}_T$ in the range $0.005 \le \tilde{x}_T \le 0.03$.

As in the symmetrically heated channel, the effect of free convection on Nu_{0D} is characterized by the ratio Ga/Re. At constant T_s, T_0, and T_w, the values of Nu_{0D} obtained with different Ga/Re are generalized by a single straight line (Fig. 3). A change in T_0 and T_w is accompanied by a change in Nu_{0D} and the slope of the curves Nu_{0D} (Ga/Re). At $T_s = 1323$ and $T_w = 573$ K, an increase in T_0 from 293 to 573 K leads to a reduction in Nu_{0D} and an increase in the dependence of this quantity on Ga/Re. In contrast to Nu_{0D}, the dimensional rate of deposition increases with an increase in T_0.

The increase in the dependence of Nu_{0D} on free convection (the increase in the slope of the curve Nu_{0D} (Ga/Re)) is evidently connected with weakening of the effect of thermodiffusion.

A reduction in reactor temperature leads to a reduction in Nu_{0D} (Fig. 3), which can be attributed to the role of free convection and thermodiffusion.

At high values of Ga/Re, a reverse flow develops along the deposition surface. With a decrease in Ga/Re, the separation point moves from the inlet farther into the channel. The distance to this point cannot exceed the length of the zone in which free convection plays an important role, i.e. $\tilde{x}_T = 0.1\text{-}0.15$ (see Fig. 2). Thus, at Ga/Re lower than a certain critical value $(Ga/Re)_{cr}$, recirculation does not occur for any value of $\tilde{x}_T$.

The value of $(Ga/Re)_{cr}$ is given in Table 1 for certain combinations of conditions typical of the deposition of silicon from a mixture of SiH_4 and H_2. It follows from this data that the critical values of Ga/Re are lower in a reactor with "cold" walls than in a symmetrically heated reactor with "hot" walls [1]. Meanwhile, $(Ga/Re)_{cr}$ increases with a decrease in T_0, T_s, and T_w and an increase in the angle α. It does not follow from this that the flow becomes more stable in the reactor with a decrease in gas temperature at its inlet. Conversely, an increase in T_0 leads to a decrease in Ga/Re and stabilizes the flow.

Since $Ga/Re \sim P^2$, this criterion is small at reduced pressures in the reactor and the laminar flow is stable.

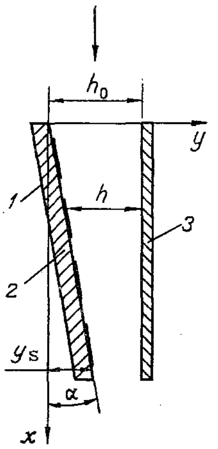

Fig. 1. Scheme of the reactor.

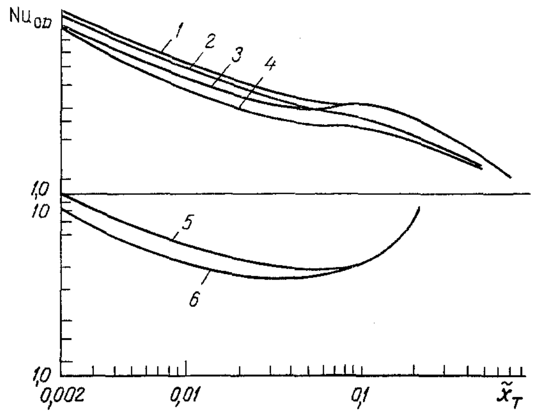

Fig. 2. Dependence of Nu_{0D} on $\tilde{x}_T$ (P = 101 kPa, X_{01} = 0.002, T_0 = 293 K, T_s = 1323 K, Re = 117.1): T_w = 323 (2, 4, 5, 6) and 573 K (1, 3); α = 0 (1-4) and 3° (5, 6); Ga = 0 (1, 2, 5) and 25,180 (3, 4, 6).

At small values of the criterion Ga/Re, free convection can be ignored. As can be determined from Fig. 3, free convection reduces Nu_{0D} by no more than 5% if Ga/Re does not exceed a certain value. This value is found within the range 35-65 and depends on T_0 and T_w. Such values are several times lower than in the case of a symmetrically heated channel [1]. However, the low values of Ga/Re can be realized in practice with small values of h_0, heating of the gas mixture at the reactor inlet, or a reduction in pressure. For example, with P = 101 kPa, h_0 = 0.02 m, T_0 = 573 K, and T_s = 1373 K, the criterion $Ga/Re \leqslant 35$ if $u_0 \geqslant 0{,}182$ m/sec.

At reduced pressures, the criterion Ga/Re is also small when the reactor is small and the value of T_0 is low. For example, at P = 1 kPa, h_0 = 0.05 m, T_0 = 293 K, and u_0 = 0.2 m/sec (under normal conditions), Ga/Re = 12.

Figure 4 shows data obtained without allowance for free convection. In a nonsymmetrically heated channel, the effect of thermodiffusion is not limited to the initial section (as it is in a symmetrically heated channel [1]) but instead extends over the entire length of the reactor (Fig. 4, a, b). However, its character depends on the relationship between the temperatures T_s, T_w, and T_0. If $T_0 \approx T_w$, then the curves $Nu_{0D} = f(\tilde{x}_T)$ obtained with and without allowance for thermodiffusion are approximately parallel. At $T_w > T_0$, thermodiffusion has a greater effect on the initial thermal section, so that the curves approach one another beyond this section (curves 5 and 7 in Fig. 4b). The result is stratification of the curves in Fig. 4c and curves 12-15 in Fig. 4d. Meanwhile, the curve is higher, the greater the temperature of the reactor wall.

The effect of thermodiffusion on deposition rate can be evaluated approximately in the same manner as in [1], i.e.

$$j/j' = 1 + K_{TD}, \tag{2}$$

where

$$K_{TD} = \left(\frac{\alpha_T X_1 (1 - X_1)}{T} \frac{\partial T}{\partial y}\right) \Big/ \frac{\partial X_1}{\partial y}. \tag{3}$$

After simplifications, we obtained the following expression [1] from (3)

$$K_{TD} = \frac{\alpha_T (1 - \tilde{T}_s) \mathrm{Pr}}{(1 + \tilde{T}_s) \mathrm{Pr}_D}. \tag{4}$$

Equation (4) can be used at small $\tilde{x}_T$, when wall temperature does not have an effect. It can be seen from Fig. 4 that these values are approximately $\tilde{x}_T \leqslant 0{,}03$. For these values of $\tilde{x}_T$, the difference between the results calculated from Eqs. (2) and (4) and the results of numerical solutions is no greater than 2.5%.

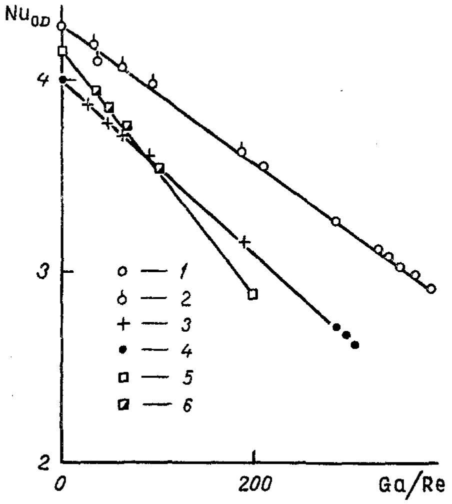

Fig. 3

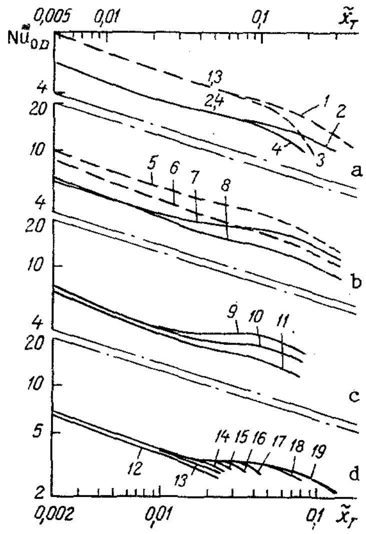

Fig. 4

Fig. 3. Effect of free convection on Nu_{0D} ($P = 101$ kPa, $X_{01} = 0.002$, $T_s = 1323$ K): $T_0 = 293$ (1-4) and 573 K (5, 6); $T_w = 323$ (3, 4) and 573 K (1, 2, 5, 6); $h_0 = 0.02$ (2, 3), 0.03 (1, 4, 5) and 0.05 m (6).

Fig. 4. Change in Nu_{0D} with $\tilde{x}_{D,T}$ in relation to different factors ($P = 101$ kPa, $X_{01} = 0.002$, $Ga = 0$): $T_0 = 293$ (1-5, 7, 9-19) and 573 K (6, 8); $T_s = 1323$ (1-8, 12-19) and 1423 K (9-11); $T_w = 293$ (11, 12), 323 (1-4), 393 (13), 493 (14), 573 (5-8, 10, 15-19) and 773 K (9); $\alpha = 0$ (1, 2, 5-11, 19), 2 (18), 3 (3, 4) and 5° (12-17); Re tg $\alpha = 2.04$ (18), 5.11 (3, 4), 12.9 (17), 17.2 (16) and 21.5 (12-15); the dashed lines show the results obtained without thermodiffusion.

At large $\tilde{x}_T$ and $\tilde{x}_D$, when we can assume that

$$\frac{\partial T}{\partial y} = \frac{T_w - T_s}{h}, \quad \frac{\partial X_1}{\partial y} = \frac{X_{01}}{h}, \quad T = \frac{T_s + T_w}{2},$$

and we can use the simplifications employed in [1], we find from Eq. (3) that

$$K_{TD} = \frac{\alpha_T (\tilde{T}_w - \tilde{T}_s)}{\tilde{T}_w + \tilde{T}_s}. \tag{5}$$

At $T_w < T_s$, an increase in T_w is accompanied by a decrease in the absolute value of K_{TD}. This explains the above-mentioned change in the effect of thermodiffusion along the channel.

Figure 4d shows the effect of the angle of convergence of the channel α. The number Nu_{0D} was determined not from h_0 but from the running value $h = h_0 - x \tan \alpha$. At small values of αRe, the curve $Nu_{0D}(\tilde{x}_D)$ coincides with this curve when $\alpha = 0°$ if $\tilde{x}_D$ does not exceed a certain value of $\tilde{x}_D$ which decreases with an increase in αRe. A further increase in $\tilde{x}_D$ leads to a decrease in Nu_{0D} compared to Nu_{0D} at $\alpha = 0°$.

The decrease in Nu_{0D} with an increase in αRe at small $\tilde{x}_D$ is due to the decrease in the quantity h, which goes into Nu_{0D}. The dimensional mass flux j_1 and, thus, the rate of deposition of the epitaxial layer decrease with an increase in αRe as does the value of Nu'_{0D} calculated from h_0 (see Fig. 2).

It makes sense to use h instead of h_0 when determining the diffusional Nusselt number because Nu_{0D} is independent of αRe within a larger range of $\tilde{x}_D$ than is Nu'_{0D}.

As in [1], in the absence of thermodiffusion and free convection, the dependence of Nu_{0D} on $\tilde{x}_D$ can be approximated by the formulas

$$Nu_{0D} = A\tilde{x}^{-n} \tag{6}$$

at $\tilde{x}_D \leqslant 0.1$ and

$$\mathrm{Nu}_{0D} = B\exp(-m\tilde{x}_D) \tag{7}$$

at $\tilde{x}_D \geqslant 0.1$.

In contrast to the case of a symmetrically heated channel, the quantities A, B, m, and n depend on two temperature factors: $\psi_S = T_S/T_0$ and $\psi_W = T_W/T_0$. However, since the temperature factor ψ_W is usually small in reactors with cooled walls, its effect can be ignored. In fact, at T_0 = 293 K, a change in T_W from 323 to 573 K causes Nu_{0D} to change by 4-6% (curves 1 and 5 in Fig. 4).

We therefore determine these quantities as a function only of ψ_S:

$$A = 0.66\exp(0.17\psi_s),\ n = 0.39\exp(-0{,}053\psi_s),\ B = 1{,}3\cdot 0.1^{-12}A,$$
$$m = 0.45\psi_s + 1.46. \tag{8}$$

In the range $1 \leqslant \psi_s \leqslant 4.5$ the results of the numerical solution and results calculated from approximate formulas (6-8) differ by no more than 5% throughout the range $0{,}002 \leqslant \tilde{x}_D \leqslant 0{,}2$ except for the neighborhood of the point $\tilde{x}_D \approx 0{,}1$. Here, this difference increases to about 8%.

The effect of thermodiffusion and free convection can be evaluated from the relations shown in Figs. 2-4 and from Eqs. (2-5).

A similar calculation of heat fluxes in a reactor was performed in [4], while temperature and concentration profiles described by polynomials were presented in [3, 4].

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EFFECT OF THE FORM OF THE TEMPERATURE DEPENDENCE OF SURFACE TENSION ON MOTION AND HEAT TRANSFER IN A LAYER OF LIQUID DURING LOCAL HEATING

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The nonsteady distribution of velocity and temperature in a layer of liquid during thermoconvective motion caused by local heating is calculated. The cases of an increasing and decreasing temperature dependence of surface tension are examined.

A large number of studies has been devoted to explaining the relative role of thermocapillary (TC) and thermogravitational (TG) convection in the motion of a liquid in a system with temperature gradients. These studies have become particularly important in connection with investigation of the behavior of liquids under conditions of reduced gravitation [1, 2].

Until recently, it was usually assumed when theoretically describing thermocapillary motion that surface tension decreased linearly with an increase in temperature (positive

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