Modeling Epitaxial Layer Growth from Gas Phase for Analysis of Influence of Changing Technological Process with Variation in Growth Zone Heating

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Abstract

In this paper, we analyze the nonstationary heat transfer during growth of epitaxial layers in epitaxy reactors from the gas phase. Based on this analysis, we formulate several recommendations on organization of heating of the growth zone for increasing homogeneity of epitaxial layers. We introduce an analytical approach for analysis of heat transfer during the growth of epitaxial layers from the gas phase. The approach gives a possibility to simultaneously take into account the nonlinearity of heat transfer, as well as changes of their parameters both in space and time.

Keywords

comparator, manufacturing, optimization, modeling

1. Introduction

In the present time, different heterostructures are widely used to form solid-state electronics devices. The most common methods for growing heterostructures are gas and liquid phase epitaxy, magnetron sputtering, and molecular beam epitaxy. A large number of experimental works have been described for manufacturing and using heterostructures because of their wide usage [1–11]. At the same time, essentially, a small number of works describe prognosis of epitaxy processes [12]. The main aim of the present paper is to study the change in properties of epitaxial layer growth, along with changes in technological process parameters and account native convection.

In this paper, we consider a vertical reactor for epitaxy from the gas phase (see Figure 1). The reactor consists of an external casing, a substrate holder with a substrate, and a spiral around the casing: this setup generates induction heating and activates chemical reactions, which decay reagents and allow growth of the epitaxial layer. A gaseous mixture of reagents together with a gas carrier enters into the inlet of the reactor, as shown in Figure 1. The main aim of the present paper is to analyze the change in properties of growing epitaxial layers and parameters of growth with account native convection.

2. Method of Solution

To solve this, we determine spatio-temporal distribution of temperature. We determined the spatio-temporal distribution as the solution using the second Fourier law [13]:

\[
c \frac{\partial T(r, \phi, z, t)}{\partial t} = p(r, \phi, z, t) + \text{div} \left\{ \lambda \cdot \text{grad} [T(r, \phi, z, t)] \right\} - \frac{1}{\lambda} \left( \bar{V}(r, \phi, z, t) \cdot \nabla \left( r, \phi, z, t \right) \cdot C(r, \phi, z, t) \right)(1)
\]

where \(\bar{V}\) is the speed of flow of mixture of gases, \(c\) is the heat capacity, \(T(r, \phi, z, t)\) is the spatio-temporal distribution of temperature, \(p(r, \phi, z, t)\) is the density of power in the system substrate – keeper of the substrate, \(r, \phi, z\) and \(t\) are the cylindrical coordinates and time, \(C(r, \phi, z, t)\) is the spatio-temporal distribution of concentration of mixture of gases, and \(\lambda\) is the heat conductivity. The value of heat conductivity is determined by using the following relation: \(\lambda = \frac{1}{3} \rho c \bar{V}^2\), where \(\bar{V}\) is the modulus of the mean squared speed of the gas molecules, which is expressed as \(\bar{V} = \sqrt{2kT/m}\), \(T\) is the average free path of gas molecules between collisions, \(c\) is the specific heat at a constant volume, and \(\rho\) is the density of gas.

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To solve this boundary problem, we take into account moving of mixture of gases and concentration of the mixture. We determine the required values by solving the equation of Navier–Stokes and the second Fourier law. We also assume the radius of the keeper of substrate \( R \) to be essentially larger than the thickness of diffusion and near-boundary layers. We further assume that the stream of gas is laminar. In this situation, the appropriate equations could be written as follows:

\[
\begin{align*}
\frac{\partial \nabla}{\partial t} + (\nabla \cdot \mathbf{v}) \mathbf{v} &= -\nabla p + \nabla \cdot \mathbf{S}, \\
\nabla \cdot \mathbf{v} &= 0,
\end{align*}
\]

where \( \mathbf{v} \) is the velocity of flow of the mixture of gases from this framework and \( \mathbf{S} \) is the stress tensor.

The equation for the components of velocity of flow with account cylindrical systems of coordinates could be written as follows:

\[
\begin{align*}
\frac{\partial v_r}{\partial t} + \frac{1}{r} \frac{\partial}{\partial r} \left( r v_r \right) &= -\frac{1}{\rho} \frac{\partial p}{\partial r} + \frac{\partial}{\partial r} \left( \mu \frac{\partial v_r}{\partial r} \right) + \frac{1}{r} \frac{\partial}{\partial \phi} \left( \mu \frac{\partial v_\phi}{\partial \phi} \right) - \frac{\mu}{\rho} \frac{\partial v_z}{\partial z}, \\
\frac{\partial v_\phi}{\partial t} + \frac{1}{r} \frac{\partial}{\partial r} \left( r v_\phi \right) &= -\frac{1}{\rho} \frac{\partial p}{\partial \phi} + \frac{\partial}{\partial r} \left( \mu \frac{\partial v_r}{\partial r} \right) + \frac{1}{r} \frac{\partial}{\partial \phi} \left( \mu \frac{\partial v_\phi}{\partial \phi} \right) + \frac{\mu}{\rho} \frac{\partial v_z}{\partial z}, \\
\frac{\partial v_z}{\partial t} &= -\frac{1}{\rho} \frac{\partial p}{\partial z} + \frac{\partial}{\partial r} \left( \mu \frac{\partial v_r}{\partial r} \right) + \frac{1}{r} \frac{\partial}{\partial \phi} \left( \mu \frac{\partial v_\phi}{\partial \phi} \right) + \frac{\mu}{\rho} \frac{\partial v_z}{\partial z}.
\end{align*}
\]

We determine the solution of this system of equations by using of the method of averaging functional corrections [14–19]. To determine the first-order approximation of components of speed of flow of the mixture of gases from this framework approach, we replace the required functions with their average values \( \langle v_r \rangle, \langle v_\phi \rangle, \text{ and } \langle v_z \rangle \) in right sides of the equations (5). After replacing these, we obtain equations for first-order approximations of the components:

\[
\begin{align*}
\frac{\partial v_r}{\partial t} - \frac{1}{\rho} \frac{\partial p}{\partial r} &= \frac{1}{r} \frac{\partial}{\partial r} \left( \mu \frac{\partial v_r}{\partial r} \right) + \frac{1}{r} \frac{\partial}{\partial \phi} \left( \mu \frac{\partial v_\phi}{\partial \phi} \right) - \frac{1}{\rho} \frac{\partial v_z}{\partial z}, \\
\frac{\partial v_\phi}{\partial t} - \frac{1}{\rho} \frac{\partial p}{\partial \phi} &= \frac{1}{r} \frac{\partial}{\partial r} \left( \mu \frac{\partial v_r}{\partial r} \right) + \frac{1}{r} \frac{\partial}{\partial \phi} \left( \mu \frac{\partial v_\phi}{\partial \phi} \right) + \frac{\mu}{\rho} \frac{\partial v_z}{\partial z}, \\
\frac{\partial v_z}{\partial t} - \frac{1}{\rho} \frac{\partial p}{\partial z} &= \frac{1}{r} \frac{\partial}{\partial r} \left( \mu \frac{\partial v_r}{\partial r} \right) + \frac{1}{r} \frac{\partial}{\partial \phi} \left( \mu \frac{\partial v_\phi}{\partial \phi} \right) + \frac{\mu}{\rho} \frac{\partial v_z}{\partial z}.
\end{align*}
\]
We determine the average values of \( a_{2x}, a_{2y} \) and \( a_{2z} \) by using the following relations:

\[
\begin{align*}
\alpha_{2x} &= \frac{1}{\pi \Theta R^2 L} \int_0^L \int_0^{2\pi} \int_0^t (v_{2x} - v_{1x}) dz d\phi dr dt, \\
\alpha_{2y} &= \frac{1}{\pi \Theta R^2 L} \int_0^L \int_0^{2\pi} \int_0^t (v_{2y} - v_{1y}) dz d\phi dr dt, \\
\alpha_{2z} &= \frac{1}{\pi \Theta R^2 L} \int_0^L \int_0^{2\pi} \int_0^t (v_{2z} - v_{1z}) dz d\phi dr dt,
\end{align*}
\]

where \( Q \) is the continuance of moving of the mixture of gases through the reactor. Substitution of the first- and second-order approximations of the required components of speed into the relation in Eq. (9) give us the possibility to obtain a system of equations to determine required average values:

\[
\begin{align*}
&\begin{cases}
A_{a_{2x}} + B_{a_{2y}} + C_{a_{2z}} = D_1 \\
A_{a_{2x}} + B_{a_{2y}} + C_{a_{2z}} = D_2 \\
A_{a_{2x}} + B_{a_{2y}} + C_{a_{2z}} = D_3
\end{cases} \\
&\begin{cases}
A = 1 + \int_0^t \int \left( \Theta - t \right) \int_0^L \int \frac{\partial v_{2x}}{\partial r} d\phi d\tau dtdr \\
B = \int_0^t \left( \Theta - t \right) \int_0^L \int \frac{\partial v_{2x}}{\partial r} d\phi d\tau dtdr
\end{cases}
\end{align*}
\]

\[
C_1 = C_2 = \frac{\pi \Theta R^2 L v_0}{2},
\]

Integration of the above equations leads to the following result:

\[
\begin{align*}
\frac{\partial v_{2x}}{\partial t} &= \frac{\partial}{\partial r} \left( \frac{\partial v_{2x}}{\partial r} \right) - \frac{\partial}{\partial z} \left( \frac{\partial v_{2x}}{\partial z} \right), \\
\frac{\partial v_{2y}}{\partial t} &= \frac{\partial}{\partial r} \left( \frac{\partial v_{2y}}{\partial r} \right) + \frac{2}{r} \frac{\partial v_{2y}}{\partial \phi} - \frac{1}{r} \frac{\partial v_{2y}}{\partial \phi} - \frac{1}{r} \frac{\partial v_{2y}}{\partial \phi} + \frac{\partial}{\partial z} \left( \frac{\partial v_{2y}}{\partial z} \right), \\
\frac{\partial v_{2z}}{\partial t} &= \frac{\partial}{\partial r} \left( \frac{\partial v_{2z}}{\partial r} \right) + \frac{1}{r} \frac{\partial v_{2z}}{\partial \phi} + \frac{\partial}{\partial z} \left( \frac{\partial v_{2z}}{\partial z} \right),
\end{align*}
\]
Let us re-write Eqs. (1) and (3) by using the cylindrical system of coordinates

\[ a_\tau = \left(1 - \frac{\partial}{\partial r} \right) \frac{1}{r^2} \left(1 - \frac{\partial}{\partial r} \right) - \frac{\partial}{\partial \phi} - \frac{\partial}{\partial z} \]

where \( \Delta = A(B_2C_3 - B_3C_2) - B_1(A_2C_1 - A_3C_2) + C_1(A_1B_2 - A_2B_1), \)

\[ a_{\phi \phi} = \Delta_{\phi} \]

\[ a_{\phi z} = \Delta_{\phi} \]

\[ a_{z z} = \Delta_{z} \]

Solution of the above system of equations could be determined by standard approaches [19] and could be written as follows:

\[ \alpha_{\phi \phi} = \Delta_{\phi} \]

where \( \Delta = A(B_2C_3 - B_3C_2) - B_1(A_2C_1 - A_3C_2) + C_1(A_1B_2 - A_2B_1), \)

\[ a_{\phi \phi} = \Delta_{\phi} \]

\[ a_{\phi z} = \Delta_{\phi} \]

\[ a_{z z} = \Delta_{z} \]

In this section, we obtained velocity components of the mixture in the gas phase, which are used for the growth of heterogeneous structures, and the gas carrier in the second-order approximation framework method, by averaging functional corrections. Usually, the second-order approximation is good enough for qualitative analysis of the obtained solution and to obtain some quantitative results.

Let us re-write Eqs. (1) and (3) by using the cylindrical system of coordinates

\[ \frac{\partial T}{\partial t} = \frac{1}{r^2} \left(1 - \frac{\partial}{\partial r} \right) \frac{1}{r^2} \left(1 - \frac{\partial}{\partial r} \right) - \frac{\partial}{\partial \phi} - \frac{\partial}{\partial z} \]

To determine spatio-temporal distribution of temperature and concentration of the gas mixture, we used the method of averaging functional corrections. To determine the first-order approximations of the required functions, we replace them with their not yet known average values \( a_{\tau \tau} \) and \( a_{\phi \phi} \) in right sides of the above equations. Further, we used the recently considered algorithm to obtain the first-order approximations of temperature and concentration of the gas mixture:

\[ T_t(r, \phi, z, t) = T + \int \frac{p(r, \phi, z, t)}{c} d\tau - a_{\tau \tau} \int \frac{\phi (r, \phi, z, t) - \phi (r, \phi, z, t)}{c} d\tau \]

\[ a_{\phi \phi} \int \frac{\phi (r, \phi, z, t) - \phi (r, \phi, z, t)}{c} d\tau \]

The above not yet known average values could be determined by the standard relations:

\[ a_{\tau \tau} = \frac{1}{\pi \Theta RL} \int_0^\pi \int_0^\pi \int_0^\pi T_t(r, \phi, z, t) d\phi d\tau d\phi \]

\[ a_{\phi \phi} = \frac{1}{\pi \Theta RL} \int_0^\pi \int_0^\pi \int_0^\pi \phi (r, \phi, z, t) d\phi d\tau d\phi \]

Substitution of the first-order approximations of temperature and concentration of the gas mixture into relations (16) gives us the following results [20]:

\[ a_{\phi \phi} = C_1 \frac{1}{\pi \Theta RL} \int_0^\pi \int_0^\pi \int_0^\pi \phi (r, \phi, z, t) d\phi d\tau d\phi \]

\[ a_{\phi \phi} = C_2 \frac{1}{\pi \Theta RL} \int_0^\pi \int_0^\pi \int_0^\pi \phi (r, \phi, z, t) d\phi d\tau d\phi \]
For the second-order approximations of temperature and concentration of the gas mixture, we used the method of averaging the functional corrections [14–19], i.e., by replacing the required functions in the right sides of Eqs. (12) and (13) on the following sums $T\rightarrow a_{2T}+ T_1$ and $C\rightarrow a_{2C}+ C_1$. In this case, the second-order approximations of the above required functions could be written as follows:

$$c\cdot T_1(r, \phi, z, t) = \lambda_2 \int \frac{\partial^2 T(r, \phi, z, t)}{\partial r^2} dr + \frac{\lambda_1}{r} \int \frac{\partial^2 T(r, \phi, z, t)}{\partial \phi^2} d\phi + \frac{\lambda_1}{r} \int \frac{\partial^2 T(r, \phi, z, t)}{\partial z^2} dz +$$

$$-c\frac{\partial}{\partial t} \left[ \left( v_T(r, \phi, z, t) - T(r, \phi, z, t) \right) \left[ a_{2T} + C_1(r, \phi, z, t) \right] \left[ a_{2T} + T_1(r, \phi, z, t) \right] - \frac{\partial}{\partial t} \right] -$$

$$-c\frac{\partial}{\partial \phi} \left[ \left( v_T(r, \phi, z, t) - T(r, \phi, z, t) \right) \left[ a_{2T} + C_1(r, \phi, z, t) \right] \left[ a_{2T} + T_1(r, \phi, z, t) \right] - \frac{\partial}{\partial t} \right] -$$

$$-c\frac{\partial}{\partial z} \left[ \left( v_T(r, \phi, z, t) - T(r, \phi, z, t) \right) \left[ a_{2T} + C_1(r, \phi, z, t) \right] \left[ a_{2T} + T_1(r, \phi, z, t) \right] - \frac{\partial}{\partial t} \right] +$$

$$+ \frac{1}{\delta} \int \rho(r, \phi, z, t) d\phi + T_1,$$

(16)

$$C_1(r, \phi, z, t) = \frac{1}{r} \int \frac{\partial C(r, \phi, z, t)}{\partial r} dr + \frac{1}{r^2} \frac{\partial}{\partial \phi} \int \frac{\partial C(r, \phi, z, t)}{\partial \phi} d\phi +$$

$$+ \frac{1}{r^2} \int \frac{\partial}{\partial z} \left[ \left( v_T(r, \phi, z, t) - T(r, \phi, z, t) \right) \left[ a_{2T} + C_1(r, \phi, z, t) \right] \left[ a_{2T} + T_1(r, \phi, z, t) \right] - \frac{\partial}{\partial t} \right] -$$

$$-\frac{1}{r^2} \frac{\partial}{\partial \phi} \left[ \left( v_T(r, \phi, z, t) - T(r, \phi, z, t) \right) \left[ a_{2T} + C_1(r, \phi, z, t) \right] \left[ a_{2T} + T_1(r, \phi, z, t) \right] - \frac{\partial}{\partial t} \right] -$$

$$-\frac{\partial}{\partial z} \left[ \left( v_T(r, \phi, z, t) - T(r, \phi, z, t) \right) \left[ a_{2T} + C_1(r, \phi, z, t) \right] \left[ a_{2T} + T_1(r, \phi, z, t) \right] - \frac{\partial}{\partial t} \right].$$

(17)

Averages values of the second-order approximations of temperature and concentration of the mixture $a_{2T}$ and $a_{2C}$ have been calculated by using the following standard relations:

$$a_{2T} = \frac{1}{\pi R L^2} \int \frac{V_0}{2} \frac{\partial}{\partial t} \left[ T(r, \phi, z, t) \right] d\phi d\phi d\phi d\phi dt,$$

$$a_{2C} = \frac{1}{\pi R L^2} \int \frac{V_0}{2} \frac{\partial}{\partial t} \left[ C(r, \phi, z, t) \right] d\phi d\phi d\phi d\phi dt.$$

(18)

Substitution of the first- and second-order approximations of temperature and concentration of the mixture into relations (18) gives us the possibility to obtain equations to determine required average values.

In this section, we analyze dynamics of mass and heat transfer during growth of epitaxial layers from the gas phase to formulate conditions to increase homogeneity of epitaxial layers. Figure 2 shows the dependence of temperature on time in the reactor under low-frequency (curve 1) and high-frequency (curve 2) induction heating conditions, respectively. From this figure, it follows that with high-frequency heating, the growth temperature reaches its stationary value more rapidly. In this case, a shorter growth time of the epitaxial layer is achieved, as well as a more stable composition if it is necessary to change the growth temperature before the finishing of the process due to the greater stability of the rate of interaction between the reactants. Figure 3 shows temperature dependence on the value of the axial coordinate in the reaction zone with various velocity values of the gas mixture at the inlet of the reactor. It follows from this figure that increasing the considered velocity leads to a decrease in temperature (probably due to convective heat transfer) in the growth zone of the epitaxial layer and its area, bringing it closer to the value that existed in the reactor before the start of the technological process. In this situation, it is interesting to choose the power of induction heating of the growth zone of the epitaxial layer to compensate heating losses caused by convective heating transfer [21]. In this case, the time of achievement of the stationary heating regime $T$ can be
estimated from the framework previously introduced [22] and has the value \( \vartheta \approx (6\pi-1)R^2/24\lambda_c \), where \( \lambda_c \) is the average value of the thermal conductivity. In this case, the power, which is required to compensate the cooling of the region of growth of the epitaxial layer, could be estimated from the relation:

\[
\int_0^R r \cdot p (r, \phi, z, t) dr \approx \sigma \cdot T \cdot \Theta (r, \phi, z, t)/4\pi R^2,
\]

4. Conclusion

In this work, we analyze the nonstationary heat transfer in reactors for epitaxy from the gas phase and dependence on the physical and technological parameters. We formulate several recommendations to improve properties of epitaxial layers. The growth temperature reaches its stationary value more rapidly with high-frequency heating. In this case, a shorter growth time of the epitaxial layer is achieved, as well as a more stable composition if it is necessary to change the growth temperature before the finishing of the process due to the greater stability of caused by convective heating transfer.

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