Surface Review and Letters, Vol. 15, Nos. 1 & 2 (2008) 111–116

World Scientific
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EFFECTS OF OPERATING CONDITIONS ON THE DEPOSITION OF GaAs IN A VERTICAL CVD REACTOR

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Received 31 March 2007
Revised 23 July 2007

A numerical study is needed to gain insight into the growth mechanism and improve the reactor design or optimize the deposition condition in chemical vapor deposition (CVD). In this study, we have performed a numerical analysis of the deposition of gallium arsenide (GaAs) from trimethyl gallium (TMG) and arsine in a vertical CVD reactor. The effects of operating parameters, such as the rotation velocity of susceptor, inlet velocity, and inlet TMG fraction, are investigated and presented. The three-dimensional model which is used in this investigation includes complete coupling between the thermal-fluid transport and species transport with chemical reaction.

Keywords: CVD; gallium arsenide; reactor design; Arrhenius model; deposition rate.

1. Introduction

The chemical vapor deposition (CVD) to produce thin films represents an important and widely used manufacturing process in high technology applications. The understanding of macroscopic transport phenomena in a reactor chamber, especially in the region from the gas inlet to the wafer surface is a crucial factor for successful thin-film deposition with the chemical reaction and the surface phenomena on the wafer. The gaseous flow behavior and, in turn, the deposition rate can be influenced by the thermo-flow conditions, operation procedure, and sequential control. Therefore, an improved understanding of the transport phenomena is necessary for reactor design as well as process optimization.

The rotating susceptor CVD reactor was first studied in the early 1970s, in which incompressible stream function vorticity formulation with consideration of natural convection and chemical reaction was employed to simulate the transport process. Kusumoto *et al.*[1] studied the effects of working conditions and reactor geometry using a transport model without consideration of the chemical reaction. In the past two decades, a number of investigations concerned with rotating-disk CVD reactors have been appeared. The most simplified analysis may be the similarity models used widely in a variety of thermal-fluid flow problem.[2] Since the flow over a rotating-disk is of one-dimensional nature in some situations, similarity analysis becomes a useful

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tool for obtaining approximate solution. Evans and Grief[3] concluded that, for weak buoyancy effects, the one-dimensional similarity solutions agree well with two-dimensional computations. Biber *et al.*[4] classified the buoyancy-induced plug flow and the rotation-induced flow patterns, using thermal and rotational flow parameters. Moffat and Jensen[5] used a parabolized approximation to the flow and transport equations to show that buoyancy forces can cause three-dimensional roll cells to develop, which seriously degrade the uniformity of the deposition in the reactor.

Previous modeling efforts have made significant contributions toward an understanding of the phenomena involved in a vertical CVD reactor. And the process is usually controlled by kinetics instead of equilibrium chemistry. So, in this study, the effects of various operating conditions in CVD reactor are concerned to elucidate the velocity fields and the value of deposition rate. The noticeable feature of model used is variability that we can control the susceptor temperature, the rotational speed of susceptor, and the inlet velocity. These effects have played an important role on the uniformity of gallium arsenide (GaAs) deposition which is a common material used in electronic and optical devices.[6,7]

2. Methodology

2.1. *Governing equations*

The following governing equations, which can be described by Navier–Stokes equation, are adopted to investigate the characteristics of flow fields in CVD reactor[8]:

$$\nabla \cdot \rho \vec{u} = 0, \tag{1}$$

$$\nabla \cdot \rho \vec{u}\vec{u} = -\nabla p + \nabla \cdot \vec{\tau} + \rho \vec{g}, \tag{2}$$

$$cp \nabla \cdot \rho \vec{u} h = \nabla \cdot (k \nabla T) + \vec{u} \nabla p. \tag{3}$$

Equations for chemical species are applied to predict the local mass fraction of each species through the solution of convection–diffusion equation for the ith species.[9]

$$\nabla \cdot (\rho \vec{u} Y_i) = -\nabla \vec{J_i} + R_i, \tag{4}$$

where $\vec{J_i}$ is the diffusion flux of species i, which arises due to concentration gradients and Y_i is the local mass fraction of each species.

$$\vec{J_i} = -\rho D_{i,m} \nabla Y_i. \tag{5}$$

Here, $D_{i,m}$ is the diffusion coefficient of chemical species i and R_i is the reaction rate of the formation or extinction through the Arrhenius model.

$$R_i = A \exp(-E/RT), \tag{6}$$

where A, E, and R are denoted as the frequency factor, the activation energy, and the gas constant, respectively.

2.2. *Numerical model and method*

A numerical model of CVD reactor was made by 3D CAD tool, Inventor. It is divided into two portions; the rotating susceptor and the CVD chamber. When the parameters of susceptor were fixed, the investigations are carried out with the geometry of CVD chamber; distance from the inlet to the surface of susceptor with 150 mm, the outer radius of the CVD chamber with 120 mm and the radius of susceptor with 90 mm. The CVD reactor used in this study and the main geometrical parameters are given in Fig. 1.

The flow was assumed to be laminar because the calculated Re is low and the analysis is performed to assume steady-state. In previous studies,[10] different

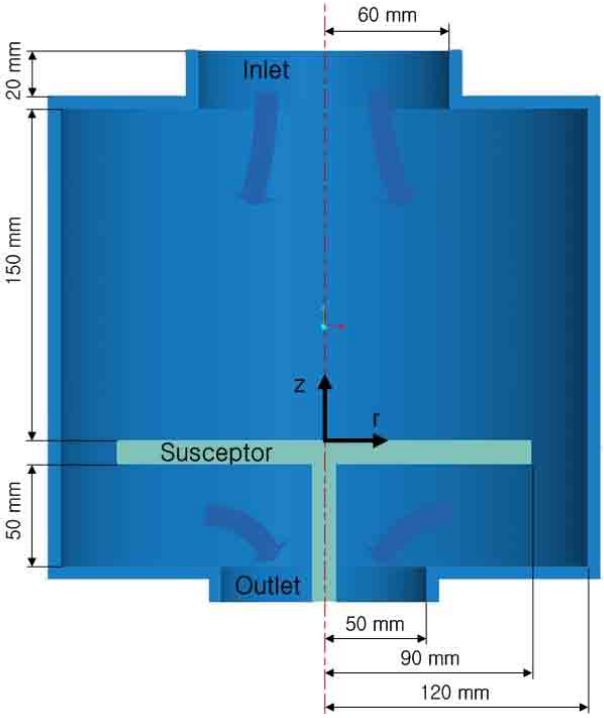

Fig. 1. Schematic of the modeled CVD reactor [unit: mm].

assumptions were made regarding the chemical reaction rate, including (i) infinitely fast reaction rate; (ii) finite reaction rate limited by turbulent mixing; (iii) finite reaction rate in Arrhenius form. In this work, we use the Arrhenius form which is exact for laminar flames and represents a relationship between the rate of a reaction and temperature on the surface of susceptor. The mass fraction rate was assumed that there is no change along the vertical direction. Also the influence of radiation is ignored because the medium does not take part in the radiation. The flow velocity entering the reactor was prescribed as the uniform velocity calculated from the volume flow rate. The hydrogen was used as the carrier gas.

For gas-phase reactions, the reaction rate is defined on a volumetric basis and the rate of creation or destruction of chemical species becomes a source term in the species conservation equation. The rate of deposition is governed by both chemical kinetics and the diffusion rate from the fluid to the surface. Wall surface reactions thus create sources of chemical species in the bulk phase and determine the rate of deposition of surface species.

Ga and As are deposited on the heated susceptor governed by the following surface reaction:

$$\mathrm{AsH_3 + Ga\_s \rightarrow Ga + As\_s + 1.5H_2} \qquad (7)$$

$$\mathrm{GaCH_3 + As\_s \rightarrow As + Ga\_s + 3CH_3} \qquad (8)$$

The trimethyl gallium ($GaCH_3$) and arsine (AsH_3) were the sources of Ga and As, respectively. $GaCH_3$ and AsH_3 in hydrogen flow down from the top of the wall and move to the high-temperature susceptor. In the inlet mixture, the mass fraction of $GaCH_3$ is 0.15 and AsH_3 is 0.4. The mixture properties and the mass diffusivity are determined based on kinetic theory. Using these assumptions, the foundation for the simulations is being developed with a commercial code, FLUENT, which solves for the conservation equations of mass, momentum, energy, and species using a finite-volume approach and SIMPLE (Semi-Implicit Method for Pressure-Linked Equations) algorithm.[11]

3. Results and Discussion

3.1. *Effect of the rotation of the susceptor*

The effect of the disk rotation on the deposition rate and uniformity is investigated in this section. We examined the deposition rates and analyzed the flow patterns using the results of velocity distribution, Nusselt number, and static pressure on the susceptor. When the inlet velocity ($u_{\mathrm{in}} = 0.38\,\mathrm{m/s}$) and the temperature of the susceptor ($T_{\mathrm{sus}} = 1023\,\mathrm{K}$) are kept constant value, the rotating speed of the susceptor is varied from $\Omega = 0$ to $80\,\mathrm{rad/s}$ in the increment of 40.

The result of the parametric study on the disk spin Ω is depicted in Figs. 2 and 3. For the case with no susceptor rotation, $\Omega = 0\,\mathrm{rad/s}$, the velocity layer ($\mathrm{v_z} = 5 \times 10^{-2}\,\mathrm{m/s}$) which has opposite direction to inlet flow is found above the susceptor. It is known as a buoyancy-dominated flow which is generated by high susceptor temperature. It disturbed to allow reactant gases to contact with a solid susceptor. At higher rotation rates (see Fig. 2), the thickness of the boundary layer at the susceptor decreases as the rotation rate is increased. It is noted that the susceptor rotation causes centrifugal pumping that pulls inlet gas down along the centerline and pushes it out radially along the susceptor top. The pumping action is evident in Fig. 3(a) which is depicted as pressure distribution. The static pressure above the susceptor decreases as the rotation rate is increased. And we can also observe that a gradient of pressure at the end of disk is dropped rapidly. On the contrary, the deposition rate is increased at the end of disk as shown in Fig. 3(c). The mechanism for this is that faster flow causes a thinner boundary layer at

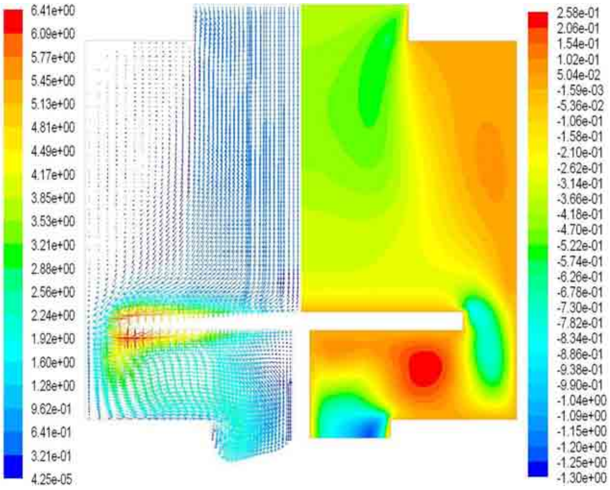

Fig. 2. Effect of susceptor rotation ($\Omega = 80\,\mathrm{rad/s}$) on the velocity vector and z-direction velocity distribution for $u_{\mathrm{in}} = 0.38\,\mathrm{m/s}$, $T_{\mathrm{sus}} = 1023\,\mathrm{K}$ [unit: m/s].
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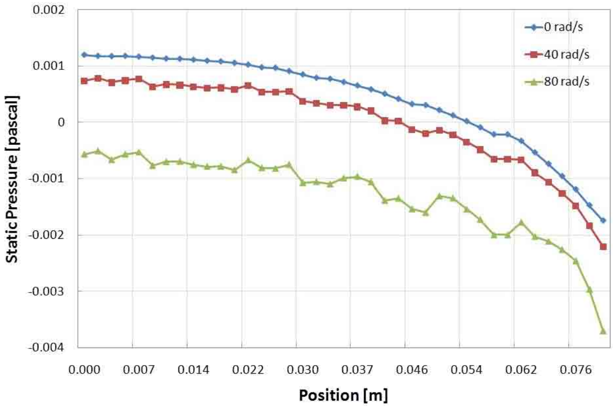
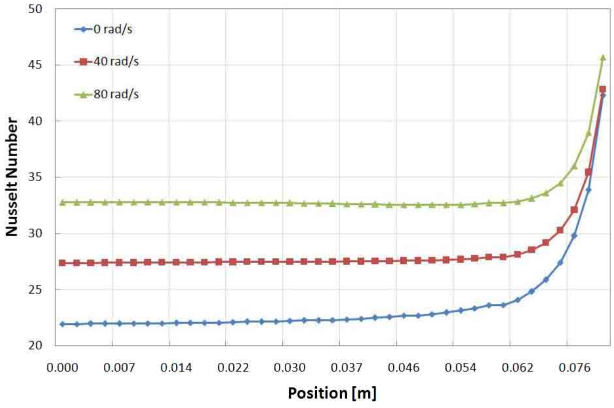
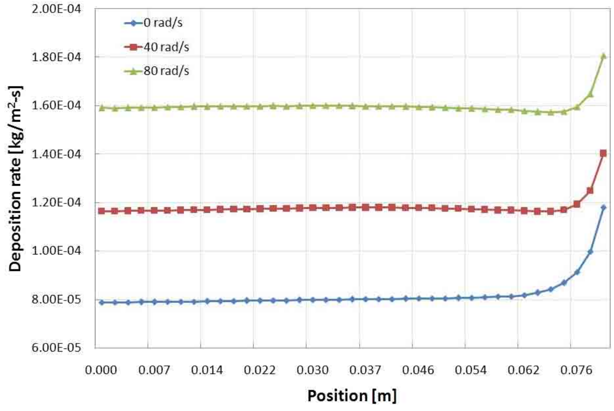


(a) Static pressure above the susceptor



(b) Nusselt number



(c) Deposition rates

Fig. 3. Effect of susceptor rotation on the static pressure, Nusselt number, and deposition rates above the surface of susceptor for $u_{\text{in}} = 0.38\,\text{m/s}$, $T_{\text{sus}} = 1023\,\text{K}$.

the susceptor, and therefore less resistance to mass transfer to the surface. In other words, the nonuniformity of the deposition rate at the surface is due to different of velocity. As shown in Fig. 2, the value of velocity passing between the susceptor and wall is represented a high value compared with the whole region in the CVD reactor. And the rotation rate is increased further, the vortex becomes stronger and modifies the concentration fields at the edge of the disk surface. It is the reason for the increment of deposition rate and pressure drop at the end of the susceptor.

3.2. *Effect of temperature of the susceptor*

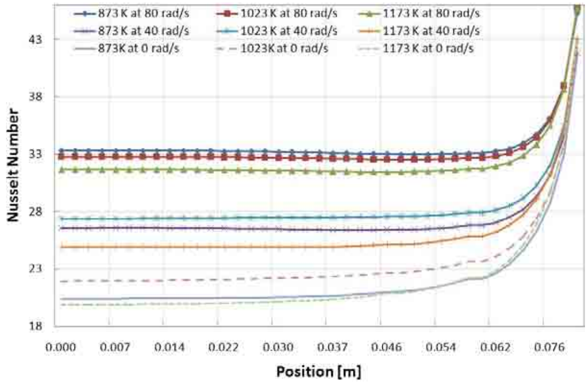
The effect of thermal boundary condition on the heat transfer has been considered for the parameter range of importance in CVD application. The temperature boundary condition at the susceptor has an important effect on the chemical reaction. Accordingly, in order to analyze the influence of temperature, we use the Nusselt number, Nu which is a dimensionless number that measures the heat transfer above the susceptor.[12]

$$Nu = \frac{h_{\text{eff}} L_{\text{ref}}}{k}, \tag{9}$$

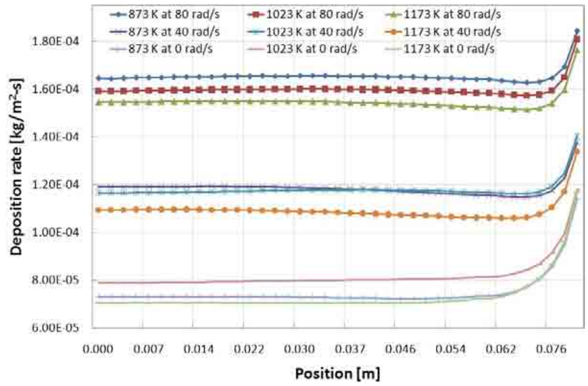
where h_{eff} is the convection heat transfer coefficient, L_{ref} is the reference length, and k is the molecular thermal conductivity, respectively.

The influence of deposition rate changes with various values of the susceptor temperature is studied when the susceptor has rotational speed of 0, 40, and 80 rad/s and with temperature 873, 1023, and 1173 K, respectively.

The high susceptor temperature provides the driving force for buoyant convection above the susceptor.[13] As a result of that the buoyancy-induced circulation blocks the flow of the inlet gas mixture, most of the $GaCH_3$ and AsH_3 cannot be reached to the susceptor surface, but moved along the chamber wall toward the outlet directly. Only a small amount of inlet gases can be transported to the surface via diffusion effect. In addition, some of injected gases are not reacted on the surface but reacted above the surface, so that the product is dropped to the susceptor. Accordingly, it is necessary to apply rotating disk to constrict the buoyancy effect on the susceptor surface. As the rotating speed increases, the buoyancy-driven recirculation cell disappears and the rotation induced flow becomes dominant. In this mode, the feed gases directly reach the hot susceptor, and the source gases spread almost uniformly and parallel to



(a) Nusselt number



(b) Deposition rate

Fig. 4. Effect of susceptor temperature and rotation on the Nusselt number and deposition rates above the surface of susceptor for $u_{\rm in} = 0.38\,{\rm m/s}$.

the susceptor over a large area. From the results of Fig. 4 which represents Nusselt number and deposition rate at various susceptor temperatures and rotational speed, the value of deposition rate is represented between 1.55×10^{-4} and $1.65 \times 10^{-4}\,{\rm kg/m^2\,s}$. As the susceptor temperature value is lower, it can obtain the highest deposition rate at the surface when the susceptor speed is 80 rad/s. Also, it shows that the Nusselt number at the susceptor surface increases as the rotation rate is increased and the pattern of deposition rate is similar to the Nusselt number distribution. In other words, we can control the deposition rate by adjusting the operating conditions and predict the deposition rate with calculated Nu above the susceptor.

3.3. *Effect of the inlet velocity*

The effect of the deposition rate with various values of inlet velocity is investigated when the rotational speed of the susceptor was fixed at 80 rad/s. Numerical result is depicted for deposition rate with each case. Figure 5 represents the results of deposition rate of Ga and As on the susceptor for various values of inlet velocity. It is seen from these results that the patterns of the deposition rate of Ga and As are almost the same nature. Also, the deposition rate of As is higher than that of Ga about $1.2 \times 10^{-5}\,{\rm kg/m^2\,s}$ because the mass fraction ratio of AsH_3 (= 0.4) was higher than that of $GaCH_3$ (= 0.15). It means that the deposition rate can be controlled by the mass fraction ratio of inlet gases.

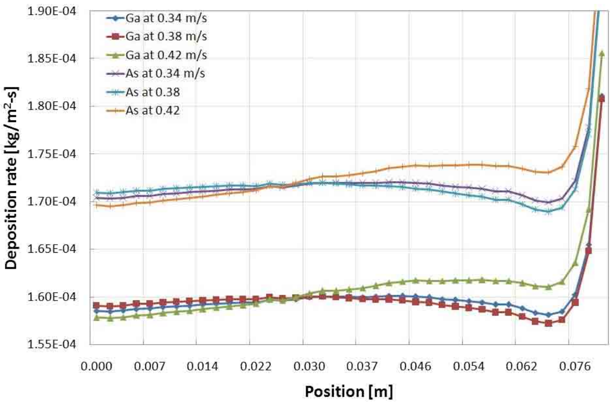


Fig. 5. Effect of various inlet velocities on the deposition rates of Ga and As on the surface of susceptor for $T_{\rm sus} = 1023\,{\rm K}$ and $\Omega = 80\,{\rm rad/s}$.

As shown in Fig. 5, the value of deposition rate is changed at the distance from the center ($r = 0\,{\rm m}$) to the end of the susceptor ($r = 0.09\,{\rm m}$) as the inlet velocities varied 0.34, 0.38, and 0.42 m/s. It is important to find the optimum operating condition which is obtained the uniform deposition rate because the aim of CVD is to coat the uniform thin film all over the susceptor. The value of deposition rate is almost the same at $r = 0.03\,{\rm m}$ but the deposition rate is continually increased at $u_{\rm in} = 0.42\,{\rm m/s}$. As a result of that, the value of deposition rate has a discrepancy about $5 \times 10^{-6}\,{\rm kg/m^2\,s}$ from center to $r = 0.076\,{\rm m}$. Also, it is depicted that the deposition rate is rapidly increased at the end of the susceptor. Therefore, it is hard to get the uniform deposition from $r = 0.076\,{\rm m}$ to $r = 0.09\,{\rm m}$. It is anticipated that the narrow distance from susceptor to CVD wall makes flow distribution fast near the edge of the susceptor, so the value of pressure becomes lower.

4. Conclusions

A three-dimensional model of GaAs deposition in a vertical CVD reactor has been numerically investigated, and the following conclusions can be drawn:

1. The temperature is one of the important parameters in the chemical reaction. The results are shown through the comparison with Nu and deposition rate. As the result, it can be found that the pattern of deposition rate is similar to Nusselt number. It is noted that we can predict the deposition rate with calculated Nu above the susceptor.
2. The buoyancy-induced flow fields are formed when the susceptor has lower rotating speed. As the rotating speed increases, however the buoyancy-driven recirculation cell disappears and the rotation induced flow becomes dominant. The reason is that high rotation speed is generated by pressure drop above the susceptor, it makes the feed gases directly reach the hot susceptor, and the source gases spread almost uniformly.
3. Comparison results of deposition rate between Ga and As show that the pattern of deposition is the same on the susceptor but the deposition value of As is higher than that of Ga. Because the mass fraction ratio of AsH_3 was higher than that of $GaCH_3$. In other words, one can control the deposition thickness through the change of mass fraction.

Acknowlegedments

This work was partly supported by the Center of Excellency Program of the KOSEF/MOST through the Center for Advanced Plasma Surface Technology (CAPST, Grant No. R11-2000-086-0000-0) at the Sungkyunkwan University. Financial aid also from the Korea Ministry of Education through the Brain Korea 21 Project is gratefully acknowledged.

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