Effect of embedding a porous medium on the deposition rate in a vertical rotating MOCVD reactor based on CFD modeling ☆

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ARTICLE INFO

ABSTRACT

This paper investigates numerically the effect of embedding a porous medium on the deposition rate in a two-dimensional (2-D) axi-symmetric vertical rotating metalorganic chemical vapor deposition (MOCVD) reactor. The 2-D Navier–Stokes, thermal-energy, and mass transfer equations as well as the wall surface reaction for growth rate in this model are solved by using commercial computational fluid dynamics (CFD) package, FLUENT (version 6.2), with a segregated method. As shown in the results, the recirculation cell caused by a buoyancy effect above the susceptor may be eliminated due to a large pressure drop during CVD process. Under a condition of the appropriate porosity and the appropriate distance between a porous medium and the susceptor, the film uniformity may be increased about 53.3% owing to a thin boundary layer near the susceptor. In addition, the case of a porous medium embedded in a modified MOCVD reactor is considered in this study to increase the film uniformity further. The numerical results show that the uniformity of the film may be enhanced about 77.9%.

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1. Introduction

Metalorganic chemical vapor deposition (MOCVD) processes have been widely used for depositing thin films on wafer, optical components, and electronic materials [1]. It offers good control of the deposition rate and the film uniformity. In a reactor, the transport processes are affected by a natural convection driven recirculation above the susceptor due to a large thermal gradient, which results in poor film uniformity. Over the past few decades, computational fluid dynamics (CFD) has become one of the most important tools used for designing CVD reactors. Many studies have been proposed to enhance the uniformity of the deposited film in vertical or horizontal CVD reactors through CFD by studying lots of parameters such as pressure, total flow rate, carrier gas flow rate, temperature, susceptor rotation speed, reactor geometry, and different carrier gas [2–11]. In addition, Cheng et al. [12] integrated the thermal CVD with the Taguchi method to optimize the CVD process.

In addition, the addition of a porous medium that was employed at the inlet of a CVD reactor to eliminate the rotational component of the gas velocity [13,14]. Nevertheless, the effect of a porous medium embedded in a vertical CVD reactor to eliminate the re-

circulation cell and enhance the growth rate as well as the film uniformity has not been investigated. Therefore, a numerical prediction is carried out by taking the growth of GaAs as an example in the present study to investigate the effect of embedding a porous medium on the deposition rate and the film uniformity in a 2-D axi-symmetric vertical rotating MOCVD reactor. Furthermore, the condition of a porous medium embedded in a modified MOCVD reactor is considered in this work to predict the variation of the film uniformity.

2. Problem formulation

2.1. Physical model and mathematical formulation

Consider a two-dimensional steady laminar flow coupled with heat and mass transfer as well as the wall surface reaction in a vertical rotating MOCVD reactor. Fig. 1(a) displays the physical configuration of the vertical rotating MOCVD reactor in this work [15]. Only one half of the r–z plane is simulated due to axi-symmetry. The height of the reactor is 0.2 m. The susceptor with a diameter $2R_s = 0.3$ m is placed at the distance of 0.1 m below the inlet, and the width of the exhaust is 0.05 m. In addition, we suppose a porous medium embedded in the reactor. The gravity direction is opposite to that of the z-axis. The gas mixture in the reactor is used as an ideal compressible gas. Effects of radiation, pressure diffusion, and forced diffusion are negligible. According to the above assumptions, the continuity equation, the Navier–Stokes, energy, and mass

Nomenclature

$C_{j,k}$	molar concentration of each reactant and product species j in reaction k
C_p	heat capacity
d	The particle diameter of a porous medium
D_i	diffusion coefficient of ith component
D_i^T	thermal diffusion coefficient of ith component
F	source term
$\vec{g}$	gravity
h_i	enthalpy of species i
I	unit tensor
$\vec{J}_i$	mass flux of species i
$\vec{J}_i^C$	concentration diffusion flux
$\vec{J}_i^T$	thermal diffusion flux
$\vec{J}_m$	Gas-phase mass flux of each gas species at the surface
k_{eff}	effective thermal conductivity
k_f	thermal conductivity of the gas mixture
$k_{f,k}$	the forward rate constant for reaction k
k_s	thermal conductivity of a porous medium
M_i	molecular weight of species i
m_{dep}	deposition rate on the reacting surface
$m_{dep,max}$	the maximum deposition rates
$m_{dep,min}$	and minimum deposition rates
N_k	number of reactions
N_r	number of chemical species in reaction k
$\vec{n}$	normal vector at the reacting surface
p	pressure
R	gas constant
$R_{i,k}$	molar reaction rates of species i in reaction k
R_{gas}	the rate of production of each gas-phase species
T	temperature
$\vec{u}$	velocity vector
w_i	mass fraction of species i
$w_{i,wall}$	mass fraction of species i on the reacting surface
r	radial direction
z	axial direction

Greek symbols

ε	porosity
τ	shear stress
Ω	rotation speed of the susceptor
μ	viscosity
ρ	density
$\eta_{j,k}^f$	forward rate exponent for each reactant and product

transfer equations, respectively, are written in vector form and given as

$$\nabla \cdot (\rho \vec{u}) = 0, \qquad (1)$$

$$\nabla \cdot (\rho \vec{u}\,\vec{u}) = -\nabla p + \nabla \cdot \tau + \rho \vec{g} + F, \qquad (2)$$

$$\nabla \cdot (\rho C_p \vec{u}\,T) = \nabla \cdot (k_{eff} \nabla T) + \nabla \cdot \left(\sum_{i=1}^{n} h_i \vec{J}_i \right), \text{ and} \qquad (3)$$

$$\nabla \cdot (\rho \vec{u} w_i) = -\nabla \cdot \vec{J}_i + M_i \sum_{k=1}^{N_k} R_{i,k}, \qquad (4)$$

where $\vec{u}$, p, and g are the velocity vector, pressure, and gravity, respectively; τ is shear stress expressed by

$$\tau = \mu \left[\left(\nabla \vec{u} + \nabla \vec{u}^T \right) - \frac{2}{3} \nabla \cdot \vec{u} I \right]. \qquad (5)$$

In Eq. (5), μ is the viscosity of the gas mixture that is calculated from ideal mixing law [16]; I is the unit tensor, and the second term of the right hand side is the effect of volume dilation, respectively; C_p is the specific heat capacity at constant pressure which is calculated from mixing law [16], and T is the temperature; w_i, M_i, and N_k are the mass fraction of species i, the molecular weight of species i, and the number of reactions, respectively; k_{eff} is the effective thermal conductivity of a porous medium given by $k_{eff} = (1-\varepsilon)k_s + \varepsilon k_f$, where k_s and k_f are the thermal conductivities of a porous medium and the gas mixture, respectively; $R_{i,k}$ is the Arrhenius molar rate of destruction of species i in the reaction k. Source term F in Eq. (2) means the resistance to the flow through a porous medium that is calculated by means of the Ergun equation [17]

$$F = -150\mu \frac{(1-\varepsilon)^2}{\varepsilon^2 d^2} \vec{u} - 1.75\rho \frac{1-\varepsilon}{\varepsilon d} |\vec{u}| \vec{u}, \qquad (6)$$

where ε and d are the porosity and the particle diameter of a porous medium. The second term of the right hand side in the Eq. (3), $\sum_{i=1}^{n} h_i \vec{J}_i$, means interdiffusion effect due to species diffusion, and h_i represents the enthalpy of species i. ρ is the density that can be computed by

$$\rho = \frac{p}{RT \sum_i \frac{w_i}{M_i}} \quad [16], \qquad (7)$$

where R is the gas constant. In the mass transfer equation, $\vec{J}_i$ is the mass flux of ith component which can be shown as

$$\vec{J}_i = \vec{J}_i^C + \vec{J}_i^T = -\rho D_i \nabla w_i, -D_i^T \nabla \ln T \qquad (8)$$

where D_i and D_i^T are the ith component diffusion coefficient and the thermal diffusion coefficient computed from kinetic theory [16]. Eq. (8) means the mass flux $\vec{J}_i$ can be separated into concentration diffusion ($\vec{J}_i^C$) given by concentration gradients, and thermal diffusion ($\vec{J}_i^T$) given by temperature gradients [18]. The second term, $R_{i,k}$, in the right hand side of the Eq. (4) can be expressed as

$$R_{i,k} = k_{f,k} \prod_{j=1}^{N_r} \left[C_{j,k} \right]^{\eta_{j,k}^f}, \qquad (9)$$

where $k_{f,k}$, $C_{j,k}$, and $\eta_{j,k}^f$ are the forward rate constant for reaction k, the molar concentration, and the forward rate exponent for each reactant and product species j in reaction k, respectively. N_r is the number of chemical species in reaction k.

The gas-phase mass flux of each gas species is balanced with its production or consumption rate on the reacting surface [19,20], the balance equation can be written

$$\vec{J}_m \cdot \vec{n} - m_{dep} w_{i,wall} = M_i R_{gas} \qquad (10)$$

where $\vec{J}_m$ is the gas-phase mass flux of each gas species at the surface, which is a combination of diffusive and convective processes. $\vec{n}$, m_{dep}, and $w_{i,wall}$ are the normal vector, the deposition rate, and the mass fraction on the reacting surface, respectively. R_{gas} is the rate of production of each gas-phase species.

2.2. Boundary conditions

The following boundary conditions are imposed:

(1) The carrier gas is assumed to be hydrogen (H_2);
(2) The gas mixture, which the mass fraction of trimethyl gallium ($Ga(CH_3)_3$) is 0.15 and Arsine (AsH_3) is 0.4, respectively, enters the reactor with a uniform temperature $T_{in} = 300$ K and a uniform velocity $U_{in} = 0.0964$ m/s;