# Mass transport analysis of a showerhead MOCVD reactor

Li Hui(李晖)[1, 2, †]

[1] School of Energy and Power Engineering, Jiangsu University, Zhenjiang 212013, China
[2] School of Mechanical Engineering, Jimei University, Xiamen 361021, China

**Abstract:** The mass transport process in a showerhead MOCVD reactor is mathematically analyzed. The mathematical analysis shows that the vertical component velocity of a point over the substrate is only dependent on vertical distance and is independent of radial distance. The boundary layer thickness in stagnation flow is independent of the radial position too. Due to the above features, the flow field suitable for film growth can be obtained. The ceiling height of the reactor has important effects on residence time and the mass transport process. The showerhead MOCVD reactor has a short residence time and diffusion plays an important role in axial transport, while both diffusion and convection are important in radial transport.

## 1. Introduction

Metalorganic chemical vapor deposition (MOCVD) is a key process in manufacturing compound semiconductor devices, such as blue-light-emitting and high-power laser diodes[1, 2]. In the MOCVD process, reactant gases are introduced to a reactor chamber where chemical reactions occur under the activation of heat, light etc., followed by the formation of a single-crystal or poly-crystal film on the substrate. Every MOCVD process requires that precursors are transported from the location where the gases are supplied (inlet manifold, showerhead, injector) to the surface on which deposition must occur (substrate, wafer): that is, mass transport must occur. It is known that the rate of deposition can be controlled by the surface reaction rate (surface limited) or the mass transport rate (mass transport limited). The latter is frequently the case in commercial MOCVD reactors, where a high rate is desirable to reduce costs. In the case where mass transport is important, it often determines not merely the rate but also the uniformity of deposition, which is frequently critical in practical applications.

Showerhead MOCVD reactors have been widely applied in recent years. They employ a perforated or porous planar surface to dispense reactant gases more-or-less uniformly over a second parallel planar surface. Such a configuration can be used for batch processing multiple substrates, but also lends itself to processing single round wafers. In view of the fact that little theoretical research on showerhead MOCVD reactors has been carried out in China[3, 4], this paper presents a mathematical analysis of the mass transport process of the reactor type based on the basic theory of fluid mechanics. The results will help an understanding of the process of MOCVD film growth, and provide a reference for the structural design of reactors.

## 2. The showerhead MOCVD reactor

The showerhead MOCVD reactor is characterized by a showerhead flange and inlets very close to substrate. The reac-

tant gases are injected vertically from the showerhead flange with many small holes (in the order of 0.5 mm) toward the substrate. The showerhead distributes the reactant gases uniformly over the substrate and yields a uniform concentration field. Then reactant gases travel across the boundary layer onto the substrate surface by concentration diffusion. By adopting a close space (in the order of 1 cm) between the showerhead and the substrate, the convection rolls can be suppressed, the gas residence time can be reduced and the reactant gases can be used efficiently[5]. A typical showerhead reactor looks something like Fig. 1, where $H_C$ is called the ceiling height or electrode gap and $R$ refers to the radius of the reaction chamber.

## 3. Mathematical analysis of mass transport

### 3.1. Related definitions

It is well known that convection and diffusion are the two methods of mass transport. Convective transport occurs when mass is carried along with the fluid due to macro movement; while diffusive transport is the average of the random motions of the huge number of individual molecules that make up the fluid or gas. For convenience of discussion in the MOCVD process, we introduce the following physical quantities[6]:

(1) Residence time $t_{res}$: $t_{res} = \frac{V}{F_{in}}$, where $V$ is the chamber volume and $F_{in}$ is the inlet volume flow. Residence time is the time to remove mass by gas flow.

(2) Consumption time $t_{con}$: $t_{con} = \frac{V}{K_S S}$, where $V$ is the chamber volume, $K_S$ is surface reaction rate constant, and $S$ is the area of the growth surface. Consumption time is the time to consume available reactant at the growth surface.

When the residence time is short compared to the consumption time, the condition is often referred to as "surface limited", in which film uniformity is likely to be good but efficiency of utilization is low. When the consumption time is shorter, the condition is often known as "mass transport limited" and the uniformity of deposition is likely to be poor ow-
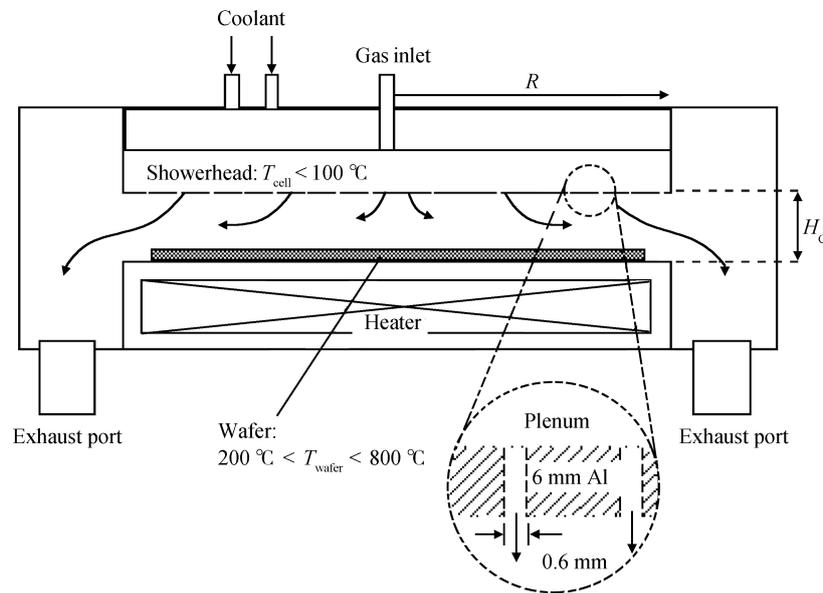
Fig. 1. Schematic of the showerhead MOCVD reactor.

ing to large gradients in concentration. Since a MOCVD reaction chamber usually works at high temperature and the surface reaction rates are much faster than the transport rate, "mass transport limited" deposition is the usual case for MOCVD processes. And residence time is the most important parameter to evaluate mass transport. On the one hand, the gas residence time can reflect the transport rate, the longer the residence time, the lower the mass transport rate and the lower the film growth rate; on the other hand, a long residence time may cause harmful parasitic reactions.

(3) Diffusion length $L_d$: $L_d = \sqrt{4Dt}$, where $D$ is the mass diffusivity and $t$ is the diffusion time. The diffusion length is the characteristic length scale for diffusion problems. It increases as the square root of the time. If the diffusion length is much longer than the system size, the profiles of concentration must be essentially linear, and are independent of time (if diffusion is the only thing happening). A change in one part of the reactor is reflected throughout the reactor in a diffusion time ($t = \frac{L_d^2}{4D}$). The relevant time used to find the diffusion length will often be the residence time of gases in the reactor. As we'll discuss below, in this case fluid velocity is generally not important: diffusion dominates transport. If the diffusion length is much shorter than the system size, concentrations can differ drastically from one part of the reactor to another. Gradients can be very large, and concentrations are highly time-dependent. Large changes in concentration in one region in the reactor will have no effect on other regions if the time involved is short enough that the diffusion length is small.

In order to determine that the mass transport is dominated by convection or by diffusion in a showerhead MOCVD reactor, it is usually preferable to use a dimensionless number which is the diffusion length divided by a characteristic size of the reactor. For example, the ratio of the diffusion length and the chamber radius ($\frac{L_d}{R}$) is used for radial mass transport, while the ratio of the diffusion length and the ceiling height ($\frac{L_d}{H_C}$) is for axial (vertical) mass transport of the reactor. Thus, if the relevant dimensionless number ($\frac{L_d}{R}$ or $\frac{L_d}{H_C}$) is much larger than 1,

then diffusion dominates transport; if the dimensionless number is much smaller than 1, then convection dominates; if the number is comparable to 1, both diffusion and convection are important.

### 3.2. Mathematical analysis

#### 3.2.1. Stagnation flow

In a showerhead reactor, if we approximate the showerhead itself as an ideal porous material and treat the flow as incompressible, gases are dispensed uniformly from the showerhead but must move radially to exit at the perimeter (shown in Fig. 2(a)). This flow pattern is called "stagnation flow" (shown in Fig. 2(b)) because the velocity of flow goes to zero in the middle of the flow. Thus, at any radius, all of the gas dispensed from inside must flow outward (ignoring changes due to reactions in the gas or at the surface). Since the area dispensing increases as the square of the radius and the perimeter area is linear, the radial velocity of the gases must increase linearly with radial distance: the radial velocity should be $\frac{r}{2H_C}$.

#### 3.2.2. Flow field in the reactor

It turns out to be pretty simple to derive an analytic expression for the gas velocity in a showerhead-like configuration in the inviscid incompressible flow approximation: that is, we assume that the gas is incompressible (also ignoring thermal expansion) so that the volume in is the same as the volume out, and we ignore the fluid viscosity. However, in this case we must account for the presence of an impermeable bottom boundary (the wafer and substrate holder): the vertical velocity must equal 0 at $z = 0$.

We treat the showerhead as a continuous source of gas, ignoring the individual dispensing holes: thus the vertical velocity is fixed at $z =$ ceiling height. Incompressibility means that the divergence of the velocity field must be zero everywhere: this is a potential flow. So we can list the analytic expressions as follows,
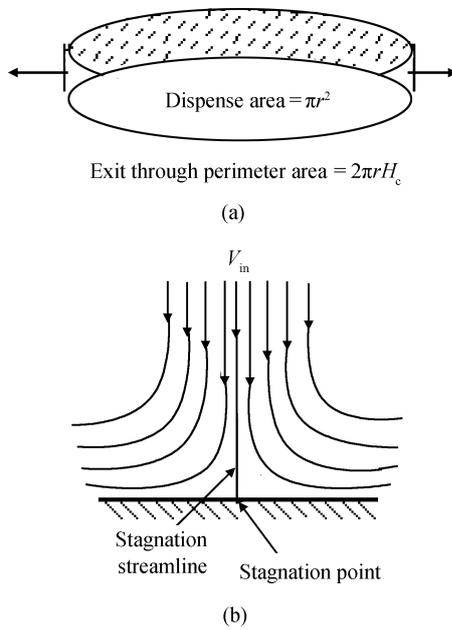
(a)

(b)

Fig. 2. Schematic diagram of (a) the dispense area and (b) the stagnation flow.

cylindrical symmetry: $v = (v_r, v_z)$,
constant entry velocity: $v_z = -v_{in}$ at ceiling $z = H_C$,
impermeable bottom wall: $v_z = 0$ at $z = 0$,
incompressible flow: $\nabla \cdot V = 0$.

Here, $v$ is the velocity vector; $v_r$ the radial velocity; $v_z$ the vertical velocity; $v_{in}$ the inlet velocity; $H_C$ the ceiling height; and $\nabla \cdot V$ the divergence of the velocity field.

In order to get the expressions of $v_r$ and $v_z$, the divergence equation must be written out in cylindrical coordinates (assuming no azimuthal flow),

$$\nabla \cdot V = \frac{1}{r}\frac{\partial}{\partial r}(rv_r) + \frac{\partial}{\partial z}v_z = 0. \qquad (1)$$

Equation (1) is solved and the solutions for the vertical and radial velocity are

$$v_z = v_{in}\left(-\frac{z}{H_C}\right), \qquad (2)$$

$$v_r = v_{in}\frac{r}{2H_C}. \qquad (3)$$

Obviously, Equations (2) and (3) satisfy the boundary conditions: $v_z = -v_{in}$ at $z = H_C$, and is 0 at $z = 0$. The radial velocity is just what we derived in Section 3.2.1, by conserving the total gas volume.

Let us examine the behavior of the solution. The vertical velocity is linear in height and the radial velocity similarly linear in radius. The total fluid velocity at any point is

$$|v| = \frac{v_{in}}{2H_C}\sqrt{r^2 + 4z^2}. \qquad (4)$$

For $r \gg H_C$, the velocity is dominated by the radial component.

To get a picture of what this flow looks like, we can derive an equation for the streamlines (paths of test particles trapped in the flow),

$$\frac{\partial}{\partial z}r = \frac{v_r}{v_z}, \qquad (5)$$

with a solution $r = r_0\sqrt{\frac{H_C}{z}}$ that is independent of the actual velocity $v_{in}$.

According to the solution of the streamline equation, we can draw the flow pattern, which looks like Fig. 3, for a ceiling height of 1.5 cm and a radius of 10 cm. It turns out to be a stagnation flow pattern with uniform velocity distribution above the substrate suitable for film growth.

### 3.2.3. Residence time

As mentioned in Section 3.1, since in MOCVD process the surface reaction rates are much faster than the transport rate, it is usually "mass transport limited" deposition. Therefore, both the rate and the uniformity of the film growth are determined by the rate of transporting precursor to the growth surface, which can be reflected by the residence time.

Based on the above analysis and according to the definition of residence time, we can calculate the time that a particle or a precursor gas molecule has spent in the stream since it entered the chamber, for any given position. The answer is

$$t_{st} = -\frac{H_C}{v_{in}}\ln\frac{z}{H_C}. \qquad (6)$$

From Eq. (6), we can find a necessary and interesting feature that the time in the stream goes to infinite as the height goes to zero, which means that gas molecules can never actually get to the wafer by pure convection. Diffusion is always necessary for deposition. In addition, since the time in the stream is only dependent on the height, the time for gas phase reactions is independent of the radial position. One may be tempted to think that the gases have been around for longer as we move towards the outside of the showerhead, but in fact the compression of the streamlines towards the bottom of the chamber (see Fig. 3) compensates.

Note that Equation (6) is based on the ideal gas assumption ignoring the viscosity of the fluid. In fact, all actual fluid has viscosity and there is a velocity boundary layer close to the substrate surface. Thus the diffusion time which particles spend travelling across the boundary layer should be taken into account. In reactors with large separations between the showerhead and the substrate-holder (i.e. large $H_C$), stagnation flow becomes relevant. Precursors are convected from the showerhead down and outward: when they reach the boundary layer height, they then proceed by diffusion to the wafer surface. The effective residence time for gases in the stream can be approximated by adding the time in the stream to reach the boundary layer to the time taken to diffuse across it,

$$t'_{st} = -\frac{H_C}{v_{in}}\ln\frac{\delta}{H_C} + \frac{\delta^2}{4D}, \qquad (7)$$

where $\delta$ is the boundary layer thickness in stagnation flow and $D$ is the mass diffusivity. Expression (7) is the correction form of Eq. (6). The second term $\frac{\delta^2}{4D}$ is the diffusion time calculated by the definition of the diffusion length. The time $t_{st}'$ scales as $(H_C/v_{in})$, with the multiplier being a slowly-varying logarithmic term, and thus in practical cases it doesn't differ very much
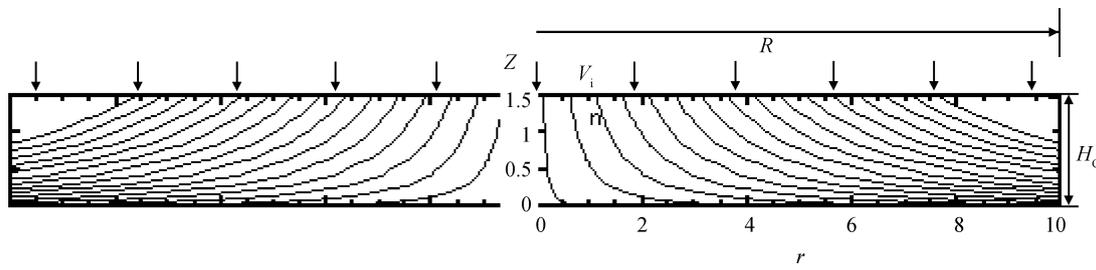
Fig. 3. Flow pattern in the chamber for a ceiling height of 1.5 cm and a radius of 10 cm.

from the simple residence time $t_{st}$ in Eq. (6). The discussion in Section 3.2.4 will reveal that the boundary layer thickness $\delta$ is independent of the radial position, so the effective residence time $t_{st}'$ is also only dependent on the height and is independent of the radial position.

From the above analysis, we can see that the residence time is roughly linear in the ceiling height $H_C$ for the slowly-varying logarithmic term and variation in $H_C$ is a simple way to influence the operation of showerhead reactors. That is why $H_C$ is always considered to be the most important size parameter for showerhead reactor design.

### 3.2.4. Boundary layer thickness

Since viscosity is the diffusion of momentum, and the above analysis showed that diffusion dominates convection in the vertical direction, we can't really ignore gas viscosity. Here, we give the boundary layer thickness in stagnation flow.

The boundary layer thickness in stagnation flow is independent of the radial position: we have approximately[7]

$$\delta \approx 3\sqrt{\nu \frac{H_C}{v_{in}}}. \tag{8}$$

Recalling that the kinematic viscosity increases as the reciprocal of the pressure $(1/P)$ and the inlet velocity has the same dependence, we can easily see that the boundary layer thickness is independent of the pressure, if the molar inlet flow is fixed. Thus we can re-express the boundary layer thickness in terms of the molar flow and molar volume at standard temperature and pressure (STP),

$$\frac{\delta}{H_C} = 3\sqrt{\frac{\pi R^2 \nu_{STP}}{V_m F_{in} H_C}}. \tag{9}$$

Here, $\nu$ is kinematic viscosity, $F_{in}$ is the molar flow, and $V_m$ is the molar volume at STP.

If $\frac{\delta}{H_C} \geqslant 1$, then the whole chamber is in the boundary layer and convection plays little role in vertical transport of mass and momentum. The stagnation flow solution is not relevant to the chamber. If $\frac{\delta}{H_C} \ll 1$, then the boundary layers would be thin compared to the chamber height and stagnation flow is relevant. From Eq. (9), we can see that if the flow and the ceiling height are increased, the convection will play a more important role in vertical transport.

It should be noted that the boundary layer mentioned above is actually called the velocity boundary layer. In addition to the velocity boundary layer, there exists the concentration boundary layer (the thickness is described as $\delta_C$) and the temperature boundary layer (the thickness is $\delta_T$) close to the substrate. According to the basic principles of fluid mechanics, the relation between $\delta$, $\delta_C$ and $\delta_T$ can be expressed as follows,

$$\delta/\delta_C \approx Sc^{1/2}, \tag{10}$$

$$\delta/\delta_T \approx Pr^{1/3}. \tag{11}$$

Here, Sc and Pr are both dimensionless numbers, the former is a Schmidt number and the latter is a Prandtl number. For most gases, Sc $\approx 0.1$–1 and Pr $\approx 1$ (Sc can be calculated by Sc $= \nu/D$, where $D$ is the mass diffusivity; Pr can be calculated by Pr $= \nu/\alpha$, where $\nu$ is also the kinematic viscosity and $\alpha$ is the thermal diffusivity.), so $\delta$, $\delta_C$ and $\delta_T$ are in the same order of magnitude.

From the relations between the thicknesses of the three boundary layers, it can be concluded that, similar to the velocity boundary layer, the thicknesses of the concentration and temperature boundary layers are also independent of the radial position, which means uniform velocity, concentration and temperature distribution above the substrate, thereby improving the uniformity of thin film growth.

### 3.3. Data example

With the above analysis in mind, let's see what can be learned from an overall examination of mass transport in a typical showerhead MOCVD reactor, without taking into account the detailed nature of the gas flow. We assume the transport properties for nitrogen as a representative gas. The results are shown in Table 1.

From the results shown in Table 1, we can see the following. (1) The diffusion length is much larger than the ceiling height, so we know that convection plays a weak role in transport in the axial (vertical) direction. The concentrations of precursors and products will be constant or linear in height. (2) On the other hand, the diffusion length is comparable to the chamber radius: both diffusion and convection are important in radial transport. (3) The residence time is very short (about 10 times less than in the comparable case for a horizontal tube reactor). The combination of a short residence time and confinement of high temperatures to the region near the wafer makes showerhead reactors appropriate for use in systems where high rate gas phase reactions are important. (4) $\delta/H_C > 1$ means that the whole chamber is in the boundary layer and convection plays little part in the vertical transport of mass, which is consistent with Eq. (1).

Table 1. Mass transport example in a typical showerhead MOCVD reactor.

| Parameter | Value |
| --- | --- |
| Ceiling height, $H_C$ | 2 cm |
| Chamber radius, $R$ | 15 cm |
| Chamber volume, $V$ | 1.4 L |
| Ceiling temperature, $T_{ceil}$ | 100 ℃ |
| Wafer temperature, $T_{wafer}$ | 400 ℃ |
| Pressure, $P$ | 0.5 Torr |
| Inlet volume flow, $F_{in}$ | 14 000 cm$^3$/s |
| Velocity at $r = R$, $v_{r=R}$ | 77 cm/s |
| Residence time, $t_{st}$ | 0.1 s |
| Mass diffusivity, $D$ (N$_2$) | 805 cm$^2$/s |
| Diffusion length, $L_d$ | 18 cm |
| Boundary layer thickness, $\delta$ | 9.2 cm |
| $\delta/H_C$ | 4.6 |
| $L_d/R$ | 1.2 |
| $L_d/H_C$ | 8.9 |

## 4. Conclusion

Showerhead MOCVD reactors have been widely used for their advantages, such as uniform deposition and high productivity. This paper focuses on the mass transport process in the reactor and provides an overall mathematical analysis. The main conclusions are as follows:

(1) The flow pattern in the showerhead MOCVD reactor is like "stagnation flow" and the vertical component velocity of a point above the substrate is only dependent on vertical distance and is independent of radial position. The boundary layer thickness in stagnation flow is independent of radial distance too. Thus uniform velocity, concentration and temperature boundary layer can be constructed above the substrate.

(2) The ceiling height of the reactor has important effects on the residence time and mass transport process. Due to the very small ceiling height, the showerhead MOCVD reactor has a short residence time and diffusion plays an important role in axial transport, while both diffusion and convection are important in radial transport.

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