A TWO-DIMENSIONAL NUMERICAL MODEL OF GAS MIXING AND DEPOSITION IN A ROTATING DISK CVD REACTOR

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Gas phase transport with mixing and surface chemistry is studied in an axisymmetric, isothermal rotating disk chemical vapor deposition reactor. A simple one-step surface reaction is used to model deposition of gallium on the rotating surface. Partitioning of the inlet flow into separate gas streams of different species can lead to nonuniform deposition on the growth surface. The nonuniformity is caused by incomplete radial diffusion of gas species; depending on reactor temperature and pressure it can be worsened by large buoyant flow instabilities. The nonuniformity is relatively insensitive to the magnitude of the specified sticking coefficient.

INTRODUCTION

Deposition rates and uniformity are strongly influenced by gas phase transport in many chemical vapor deposition (CVD) processes. Typically, reacting gases enter the reactor through multiple openings; a carrier gas may also be present and is sometimes premixed with the reacting gases. Separation of the reacting gases prior to heating and decomposition in the thermal boundary layer adjacent to the deposition surface may be required if undesirable reactions occur between the unheated reactants. Hydrogen is a common carrier gas in MOCVD processes; its small mass and high diffusivity can have important implications for deposition. Reacting gases can have molecular weights exceeding 100 g/mole (e.g. TMG and SiF₄). The fluid mechanics and transport in CVD can encompass a broad range of flow phenomena; typically, the flows are laminar with convection and diffusion transport being comparable. It is noted that for large temperature differences and/or large molecular weight differences, the effects of buoyancy can be significant, resulting in unstable and recirculating flow.

One of the primary reactor design objectives in microelectronics materials fabrication by CVD is to achieve uniform growth of material on the substrate. The rotating disk reactor (RDR) is an attempt to take advantage of the uniform transport induced by an infinite rotating disk in an infinite medium. Deviations from the ideal flow behavior can occur due to variable properties, reactor geometry, and for some combinations of spin rates and gas flow rates. Previous studies by Evans and Greif (1,2), Patnaik (3), and Fotiadis (4) have examined these effects for a single component gas in a nonisothermal RDR. An experimental isothermal study of gas mixing in a stagnation flow reactor was made by
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Palmateer (5). In a recent isothermal study Winters et al. (6) showed that buoyant effects can be present in a RDR for some reactor configurations having separate inlet gas streams of different species.

The present study examines the effects of gas mixing on the deposition in a RDR. We restrict the study to isothermal flow of a multispecies gas flowing over a high speed rotating disk in a cylindrical reactor. In some cases complex flow fields are produced as a result of the interactions that occur between the solutal buoyant force, the forced flow, and the flow induced by the rotation of the disk. A simple one-step surface reaction utilizing a TMG sticking coefficient is used to model the deposition of Ga on the growth surface; the sticking coefficient is varied over a wide range (10^{-4} to 1.0). The results predicted for the deposition in the two-dimensional system are compared to the infinite rotating disk result.

THE MODEL

The physical model for this study is shown in Figure 1. A cylindrical reactor having a radius \( r \), and height \( H \) contains a spinning disk of radius \( r_d \) located a distance \( h \) from the top inlet. The incoming flow is divided into two sections, a circular “core” of radius \( r_c \) and an annular “shroud” bounded by radii \( r_c \) and \( r_o \). This study is restricted to the case where \( r_c = r_d \) and the dimensions listed in the figure. In all cases the core and shroud inlet velocities are uniform and equal. All surfaces are stationary except for the spinning disk surface which faces upward in Figure 1. The flow throughout the reactor is isothermal.

The core and shroud gas mixture enters through the top, mixes as it flows downward, impinges on the rotating disk where the surface reaction occurs and exits through the annular channel at the bottom. In all cases considered here, the inlet velocity for gases entering the core and shroud is equal to the natural drawing velocity of an infinite rotating disk being supplied by gas having the inlet core composition. For the case where the core and shroud gas compositions are identical, this situation reduces to the single species rotating disk problem (see e.g. 1-4). Here we emphasize the influence of nonuniform inlet composition on the reactor flow and the uniformity of deposited Ga.

The shroud gas composition is shown in Table 1; for all cases the core gas is 99% NH\(_3\) and 1% TMG. Gas phase chemistry is not considered; Ga is assumed to be deposited on the rotating disk according to the following surface reaction:

\[
Ga(CH_3)_3 \rightarrow Ga + 3CH_3
\]  

(1)

\[
r = \frac{\gamma C_{TMG}}{r} \left|_{r=0} \right. \sqrt{RT/(2\pi M_{TMG})}
\]

(2)

where \( \gamma \), \( C_{TMG} \) and \( M_{TMG} \) are the sticking coefficient, molar concentration and molecular weight of TMG, respectively.
The axisymmetric variable property Navier-Stokes and species transport equations were solved numerically using the SIMPLER algorithm. Details are provide in Winters et al. (6) and Patankar (7). The viscosity of the mixture of H₂, NH₃, TMG, and CH₃ was determined using mixture averaging rules; the mixture averaged approximation was used for the diffusion coefficients (Kee, et al. 8) Surface chemistry was implemented using Surface CHEMKIN (Coltrin et al., 9).

DISCUSSION OF RESULTS

Table 1 summarizes the values of the parameters used and the deposition results in a series of 6 RDR transport calculations. We refer to these as Cases A through F.

Case A is a uniform inlet mixture of 99% NH₃ and 1% TMG at 76 torr and 523 °K. Figure 2a shows shaded contours of TMG concentration with superimposed streamlines. Dark shades imply the highest concentrations. The flow resembles the infinite rotating disk flow deviating from the infinite disk result only near the edge of the disk and the reactor wall. Similarly, the deposition of Ga is uniform over most of the disk and equals the one-dimensional result as shown in Figure 3. The radius in Figure 3 is normalized by the disk radius (r_c = 9 cm) and the Ga deposition rate is normalized by the one-dimensional result (see Table 1) which was calculated using the SPIN code (Coltrin et al., 10).

Case B differs from case A in that the inlet composition is nonuniform; now the TMG is confined to the core. (The shroud is 100% NH₃.) Reasons for confining the TMG include more efficient utilization of reactant, reduced side wall reactions, etc. Note however, that the deposition rate is now nonuniform and decreases significantly over the outer half of the disk. (See Figure 3.) The nonuniform inlet composition results in radial diffusive and buoyant effects which are not present in case A. This is evident from the reactor cross-section shown in Figure 2b.

Case C contains 100% H₂ at the shroud inlet with 99% NH₃ and 1% TMG at the core inlet (i.e. the core inlet is the same in all cases). Now note the decrease in the deposition rate (Table 1) and the dramatic nonuniformity (Figure 3c). The presence of H₂ in the shroud greatly increases the radial diffusion described above in case B in addition to causing a buoyant flow instability (cf. Figure 2c).

To study the effects of process pressure and temperature additional calculations (cases D, E, and F) were made using the inlet composition of case C. In each case the inlet velocity was equal to the infinite rotating disk induced velocity (see Table 1). Case D demonstrates the effect of increasing the temperature from 523 to 800 °K. The increased diffusion at elevated temperature results in a decrease in deposition but an increase in uniformity. The streamlines shown in Figure 2d indicate smaller and weaker recirculation when compared to case C (Figure 2c).

Case E demonstrates the effect of decreasing the pressure from 76 to 50 torr while maintaining the temperature at 800 °K. The increased diffusion at lower pressure results in
only a very small recirculation (not shown in Figure 2e) and further decreased deposition. At an even lower pressure of 25 torr (case F) the recirculation is completely eliminated and a further reduction in deposition occurs.

In summary, cases A, B, C show the effects of inlet composition on the flow field and on the deposition magnitude and uniformity while cases D, E, and F show the effects of process conditions on these quantities.

The effects of surface chemistry on the deposition rate and uniformity have been studied by varying the sticking coefficient from $10^{-6}$ to 1.0 for the conditions of case C. Figure 4 shows the radial variation of Ga deposition rates normalized by the value at the center of the disk. Over the entire range of sticking coefficients the deposition rate remains highly nonuniform. Increasing the sticking coefficient increases the deposition rate (Table 1) and the nonuniformity since the radial composition distribution due to transport is relatively more important at higher sticking coefficients. For sticking coefficients greater than 0.1 the deposition is unchanged because it is limited by transport to the disk. An asymptote is also reached at low values of the sticking coefficient as shown in Figure 4. This because the convection transport to the disk is faster than the radial diffusion for the process conditions of case C ($\tau_{\text{conv}}/\tau_{\text{diff}}=0.1$).

CONCLUSION

RDR deposition rates are highly dependent on inlet mixture composition and distribution as well as process conditions. Diffusion, convection, and buoyancy are important factors for the deposition as was shown by substituting H₂ for NH₃ in the shroud; that is, cases B and C. Furthermore, the effects of diffusion result in decreased deposition rates and improved uniformity as the temperature is increased and pressure is decreased. The deposition profile was shown to be relatively insensitive to the value of the sticking coefficient due to the dominating influence of transport processes (convection and diffusion).

ACKNOWLEDGMENTS

Discussions with Rick Stall of Emcore and Mark Allendorf of Sandia are acknowledged.

REFERENCES


Table 1. Summary of run parameters for cases A-F

<table>
<thead>
<tr>
<th>Case</th>
<th>Press. (Torr)</th>
<th>Temp. (°K)</th>
<th>Inlet Shroud Composition</th>
<th>1-D Inlet Velocity (cm/s)*</th>
<th>1-D Ga Dep. Rate (gm/cm²-s)*</th>
<th>2-D Ga Dep. Rate (gm/cm²-s)**</th>
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</thead>
<tbody>
<tr>
<td>A</td>
<td>76</td>
<td>523</td>
<td>1% TMG+99% NH₃</td>
<td>13.5</td>
<td>7.21x10⁶</td>
<td>7.25x10⁶</td>
</tr>
<tr>
<td>B</td>
<td>76</td>
<td>523</td>
<td>100% NH₃</td>
<td>13.5</td>
<td>7.21x10⁶</td>
<td>7.29x10⁶</td>
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<tr>
<td>C</td>
<td>76</td>
<td>523</td>
<td>100% H₂</td>
<td>13.5</td>
<td>7.21x10⁶</td>
<td>6.55x10⁶</td>
</tr>
<tr>
<td>D</td>
<td>76</td>
<td>800</td>
<td>100% H₂</td>
<td>20.6</td>
<td>7.06x10⁶</td>
<td>5.32x10⁶</td>
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<td>E</td>
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<td>800</td>
<td>100% H₂</td>
<td>25.3</td>
<td>5.68x10⁶</td>
<td>4.04x10⁶</td>
</tr>
<tr>
<td>F</td>
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<td>800</td>
<td>100% H₂</td>
<td>35.6</td>
<td>3.96x10⁶</td>
<td>2.64x10⁶</td>
</tr>
</tbody>
</table>

* 1-D rotating disk values based on core composition (99% NH₃, 1% TMG in all cases) were calculated using SPIN code (10)
** 2-D values calculated at the centerline
  All runs: 500 RPM, shroud & core inlet velocities set to ideal values.

![Rotating disk reactor geometry](image)

Figure 1. Rotating disk reactor geometry.
Figure 2. Gray shaded contours of TMG mole fractions (dark=.01, light=0.0) with superimposed streamlines for cases A-F.

Figure 3. Radial Ga deposition rates.

Figure 4. Influence of sticking coefficient.
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