Application of a Geometrically-Based Uniformity Criterion for Film Uniformity Optimization in a Planetary Gallium Nitride CVD System

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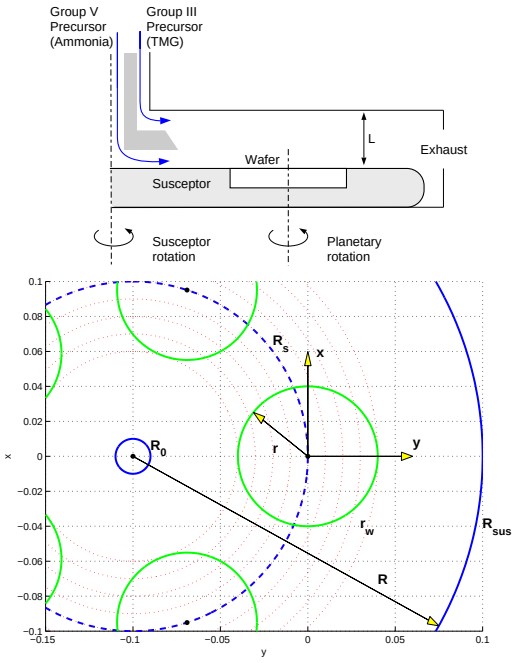
Abstract Gallium Nitride (GaN) growth chemistry can be visualized as consisting of two competing reaction routes. The upper route is more commonly referred to as the adduct formation pathway, whereas, the lower route refers to the thermal decomposition pathway of TMG. Each pathway is responsible for producing an array of chemical species that may eventually participate in GaN deposition. The primary gas phase reaction is the spontaneous interaction between commonly used precursors, trimethylgallium and ammonia, to form stable Lewis acid-Lewis base adducts. Adduct formation is a ubiquitous problem during MOVPE of GaN and has been widely studied. Upon formation, these adducts may condense on cold surfaces inside the reactor system. For this reason, the formation of these adducts is believed to degrade film quality, uniformity, and consume the feed stream of organometallic sources.

Consequently, numerous research groups have designed reactor systems, in particular gas delivery systems, with the intent to minimize precursor interactions. The most common approach is to use separate injectors to reduce any premature mixing of the precursors. Reactor systems of this type have been developed by SUNY/Sandia/Thomas Swann researchers to illustrate a connection between gas phase reactions and film-thickness uniformity. It should be noted that while these designs can suppress reactions in the gas delivery system, complete mixing of the precursors must take place close to the wafer surface to achieve uniform film thickness. Hence, these studies and others reinforce the critical role chemistry holds in designing efficient MOVPE reactors.

In conjunction with reactor design, numerous studies have focused on developing simulation tools aimed towards optimizing film-thickness uniformity. Fluid flow models that take into account heat, momentum, and mass transfer effects within both horizontal and vertical MOVPE reactors have been detailed in several papers. Many of these models incorporate large sets of chemical reactions and the model predictions ultimately are tied to the specific reactions chosen by the research group. Such models are routinely used to optimize the design and operating parameters to produce thin films of GaN with a spatially uniform thickness. A novel approach to film uniformity control is developed for planetary CVD based purely on the geometry of radial flow reactors with planetary wafer rotation. In this approach, a sequence of stalled-wafer (non-rotating) deposition profiles are identified that, when rotated, produce perfectly uniform films. Then, a deposition profile, produced either by simulation or by an actual CVD process is projected onto this sequence of uniformity-producing profiles to compute the Nearest Uniformity Producing Profile (NUPP), which under rotation would produce a uniform film. Thus, it becomes clear that one would want to drive the current profile to thenearest profile, NUPP, giving an unambiguous optimization criterion. Most importantly, the NUPP provides the process engineer with physical insight on how reactor operating conditions should be modified to drive the current profile towards the NUPP to improve uniformity. This technique is extremely powerful because it can be applied not only to film thickness but any distributed film quality for either process development or in a run-to-run control system.

In this paper, the NUPP approach is applied to a gallium nitride radial-flow chemical vapor deposition system with planetary wafer rotation. The results reveal three key points: (1) the influence of reactor geometry on gallium nitride deposition chemistry; (2) controllability of the competing nature (upper vs. lower pathways) of gallium nitride chemistry, and (3) utilization of the NUPP uniformity criterion to optimize deposition uniformity by adjusting reactor operating conditions, in particular, susceptor temperature.

Figure 1: A vertical cross-sectional view of radial-flow planetary reactor with a 2-flow gas inlet design (top); and the physical domain (bottom).



1 Uniformity Control Criterion

A vertical cross-sectional view of a radial-flow planetary reactor system along with its physical domain, $R_0 \leq R \leq R_{sus}$, is shown in Figure 1. The precursors and carrier gas species are injected into the center of the reactor through a 2-flow gas inlet design and flow outwards over wafers arranged in circular patterns over the susceptor. The 2-flow gas inlet design allows group III compounds to be introduced separately from group V compounds. In these reactors, the wafers are placed on rotating satellites which in turn rotate around the central axis of the susceptor plate. The radial flow geometry combined with the substrate planetary motion mechanism is commonly employed to produce uniform deposition profiles on the wafers [1]. It should be noted that reactors of this type can be run with both rotating and stalled (non-rotating) wafers.

1.1 Uniformity modes

Using the notation of [2], we summarize the derivation of the uniformity producing modes and the uniformity optimization criterion; the reader is directed to the cited work for additional details regarding this derivation. For this analysis, $\Delta(R)$ is defined as the 1-dimensional deposition profile over the susceptor radial coordinate and Ω is the interval of R corresponding to the location of the wafer; $\omega: \ 0 \leq r \leq r_w$ is the wafer radial coordinate. If $\delta(r,\theta)$ is the 2-dimensional profile that results when $\Delta(R)$ is projected onto the stalled (non-rotating) wafer physical domain, wafer rotation will eliminate the θ dependence by averaging the film quality over θ giving

$$\bar{\delta}(r) = \frac{1}{2\pi}\int_0^{2\pi} \Delta\left(\sqrt{r^2\cos^2\theta + (r\sin\theta + R_s)^2}\right)\, d\theta.$$

Any profile $\Delta(R)$ over the wafer segment domain $R \in \Omega$ can be represented by a shifted Legendre polynomial sequence expansion

$$\Delta(R) = \sum_{m=1}^{\infty} a_m P_m(R);$$

the reason why $P_0 = 1$ is not used is presented in [2]. The expansion approximation results in

$$\begin{aligned} \bar{\delta}(r) &= \sum_{m=1}^{\infty} \frac{a_m}{2\pi}\int_0^{2\pi} P_m\left(\sqrt{r^2\cos^2\theta + (r\sin\theta + R_s)^2}\right)\, d\theta \\ &= \sum_{m=1}^{\infty} a_m \alpha_m(r) \qquad \text{in } \omega. \end{aligned}$$

The goal is to find non-uniform $\Delta(R)$ profiles that produce uniform $\bar{\delta}(r)$ profiles under rotation, a criterion that can be written in terms of the minimization problem

$$\min_{a_m} || \sum_{m=1}^{M} a_m \alpha_m(r) - c|| \tag{1}$$

where c is a constant with respect to r and can be set $c = 1$ in (1) without loss of generality.

Defining the array $\mathbf{Q}$ of inner products over ω,

$$Q_{i,j} = \int_0^{r_w} \alpha_j \alpha_i \, r dr \qquad i = 1, \cdots, M,\ j = 1, \cdots, M$$

$$\mathbf{Q} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T \tag{2}$$

where the singular value decomposition (SVD) (2) produces $\mathbf{U}^{M\times M}$ containing the (orthogonal) left singular vectors and $\mathbf{\Sigma}$ the singular values. From these products of the SVD, we define an orthogonal set of basis functions $\{\alpha_n^v\}_{n=1}^N$ using

$$\alpha_n^v = \sum_{m=1}^{M} U_{m,n}\alpha_m(r)$$

for the space spanned by the $\{\alpha_m\}_{m=1}^M$. Observing the singular values of $\mathbf{Q}$ used to define the α_n^v, the set of relatively small magnitude σ_m indicate there are fewer than M α_n^v necessary to span the space of the sequence $\{\alpha_m\}_{m=1}^M$.

These calculations lead to the definition of the first non-flat deposition mode that generates perfectly uniform films when rotated:

$$\beta_1(R) = \sum_{m=1}^{M} b_m P_m(R)$$

where $\beta_0 =$ constant and

$$b_m = \sum_{n=1}^{N} U_{m,n}a_n^v$$

where the a_n^v are computed using (1) and the reduced basis $\{\alpha_m^v\}_{m=1}^N$.

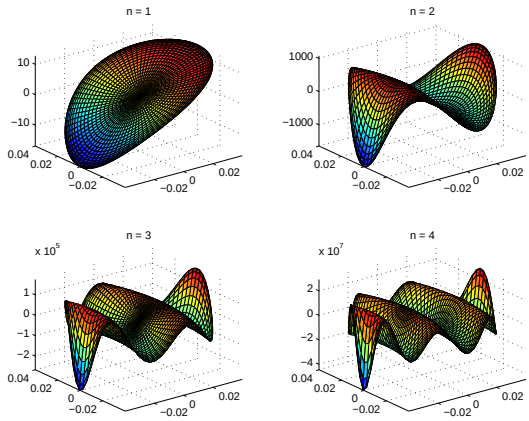
The procedure described above produces a single β_n profile; sequentially removing the lower-frequency α_j^v from the problem of finding the a_j^v that minimizes ϵ_N (refer to (3)) will force the minimization procedure to find a progression of modes correspondingly increasing in frequency. Therefore, we can produce additional β_n modes by minimizing the sequence of problems

$$\epsilon_N = \min_{a_j^v} || \sum_{j=n}^{N} a_j^v\alpha_j^v - 1|| \tag{3}$$

for $n = 2, 3, \ldots$ to obtain the corresponding β_n.

Projecting the β_n onto the stalled wafer domain, we observe illustrated in Figure 2 the first four non-flat deposition profiles that produce perfectly uniform profiles when rotated. Because these modes define at least part of a basis for the uniformity producing subspace of all possible deposition profiles, any linear combination of the β_n modes is guaranteed to produce a uniform deposition profile under rotation.

Figure 2: The first four β_n modes projected onto the stalled wafer.



These modes depend only on the wafer and susceptor geometry, therefore are truly universal in their nature.

1.2 Planetary Radial-Flow CVD Reactor Model Development

A one-dimensional model describing gas temperature and composition is developed for this reactor system. The equation of continuity for the total gas molar flow rate is used to obtain the gas velocity

$$\frac{d}{dR}(v\rho R) = 0 \qquad or \qquad v = \frac{v_0 R_0 T}{T_0 R} \tag{4}$$

where the assumption of the ideal gas law is used to determine an explicit relationship between temperature (T), radial position (R) and gas velocity (v); R_0 denotes the radius of the central feed tube and v_0 is the inlet gas velocity. The energy balance equation in cylindrical coordinates is obtained by assuming the heat capacity (C_p) and thermal conductivity (k) of the carrier gas are independent of temperature; the parameter values are evaluated using the average of the inlet temperature (T_{inlet}) and susceptor temperature (T_S):

$$\frac{C_p}{R}\frac{d}{dR}(R\rho v T) = \frac{k}{R}\frac{d}{dR}(R\frac{dT}{dR}) + \frac{2k}{L^2}(T_S - T) \tag{5}$$

with boundary conditions

$$T = T_{inlet} \text{ at } R = R_0, \quad \frac{dT}{dR} = 0 \text{ at } R = R_{sus} \tag{6}$$

Here, T_S represents the constant susceptor temperature and L is the spacing between the wafer top surface and the reactor roof which is assumed to be perfectly insulating. A material balance is written for each chemical species

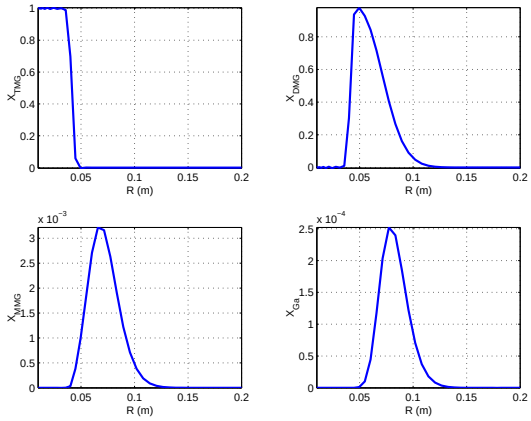
$$\frac{1}{R}\frac{d}{dR}(cx_i v) = R_i^G + \frac{R_i^S}{L/2} \tag{7}$$

where c is the total concentration of the gas ($c = P/R_{gas}/T$ for an ideal gas, P is the total reactor pressure, and R_{gas} corresponds to the ideal gas constant), x_i is the mole fraction of the ith species, R_i^G the rate of generation of species i per unit volume due to gas phase reactions and R_i^S the rate of generation of species i per unit area due to surface phase reactions; the model assumes that deposition occurs only on the susceptor surface. The quantity $L/2$ represents the distance that Ga-containing precursors must travel in order to adsorb onto the wafer surface after the divider (refer to Figure 1). Inlet boundary conditions for each chemical species material balance equation are the known mole fractions at the inlet, $x_i(R = R_0) = x_{i0}$.

The modeling equations thus are defined by a coupled set of one- and two-point boundary-value problems. To obtain steady-state temperature and deposition rate profiles, the modeling equations are discretized on a Gaussian quadrature grid, and a Newton-Raphson technique is used to drive the residual corresponding to each discretized differential equation, at their boundary conditions, to zero. An object-oriented MATLAB-based weighted residual tool-box [3] is used to carry out these computations. The same quadrature-based MWR tools are used to compute the β_n modes and to project deposition profiles onto these modes to compute the NUPP, described in the next section.

A representative set of operating parameters used to deposit gallium nitride for this reactor geometry is taken from [4]. In their planetary reactor system, they reported the following operating conditions: pressure 37.5 torr, susceptor temperature (T_S) 1373 K, and a total flow 6.5 slm. Based on these parameters and assuming that the total flowrate of 6.5 slm is split equally between the top and bottom inlets, $T_{inlet} = 300K$ and $L = 1.5cm$ [1], an initial value for $v_0 = 3.85m/s$ is computed. $R_0 = 0.01m$, susceptor radius $R_{sus} = 0.2m$, satellite wafer centerline radius $R_s = 0.1m$ and wafer radius $r_w = 0.04m$.

Figure 3: Simulation results illustrating normalized chemical species profiles.



The sum of the fluxes of monomethylgallium (MMG) and elemental gallium (Ga) are assumed to govern the growth rate and, accordingly, their surface reaction chemistry is also included in the computation. Simulation results describing mole fraction profiles of each chemical species for the representative operating conditions are shown in Figure 3. The composition profiles are normalized with respect to the inlet TMG mole fraction. It is evident from the results that TMG is rapidly consumed well before the wafer location and that the only species present over the wafer are DMG, MMG, and Ga. This is directly related to the rapid gas heating inside the reactor which encourages the dissociation of the first methyl group from TMG. Because no TMG is present over the wafer, the adduct pathway (upper route) is suppressed as NH_3 begins mixing with the organometallic stream shortly before the wafer location, illustrating how reactor geometry influences deposition kinetics.

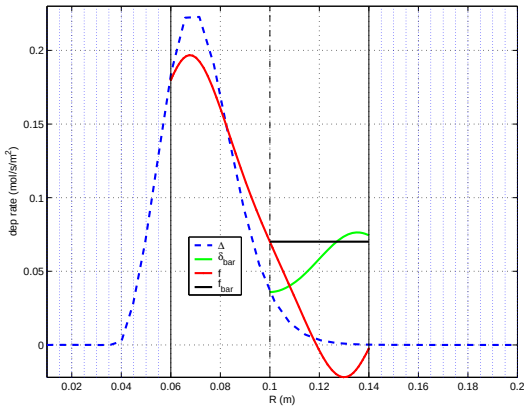
1.3 Uniformity Optimization

The deposition rate profile is a function of the gas phase mole fraction of MMG and Ga and is given by

$$\Delta(R) = R^S_{MMG} \cdot x_{MMG} + R^S_{Ga} \cdot x_{Ga} \tag{8}$$

For the planetary reactor deposition system simulation under consideration, the "nearest" deposition rate profile f that generates a uniform film upon rotation is shown in Figure 4. This optimal profile f, henceforth referred to as the NUPP (Nearest Uniformity Producing Profile), is computed as the

Figure 4: Wafer deposition profile Δ, the resulting profile upon rotation $\bar{\delta}$ and the nearest uniformity generating profile f and its profile upon rotation $\bar{f}$.



projection of the deposition profile $\Delta(R)$ onto the β_n:

$$f = \sum_{n=1}^{N} \beta_n \int_0^{r_w} \Delta(R)\beta_n \, r dr$$

When f and Δ intersect at the wafer center $R = R_s$ ($R_s = 0.1$ in this diagram), $C_d = 0$ and we are guaranteed of uniformity in the center region of the wafer. These observations lead to an unambiguous design criterion of $C_d = 0$ for improved wafer uniformity in the central region of the wafer - in many cases, the region where uniformity is most desired.

From Figure 4, it is obvious that this criterion is not met, seeing as, δ_{bar}, which is the profile that results from rotation of the current $\Delta(R)$, is not uniform. However, the results immediately indicate that uniformity can be achieved if current deposition rate profile were shifted upward and to the right (northeast direction), so that the C_d value is minimized. Physical intuition based on knowledge of gallium nitride growth chemistry suggests decreasing the susceptor temperature as a potential means to improving uniformity relative to the original set of operating conditions.

A decrease in susceptor temperature will reduce the rates of the decomposition reactions, which in turn, will spread the peak of $\Delta(R)$ and push it toward the northeast direction. At the same time, lowering the susceptor temperature also will decrease the deposition rate. A minimization procedure was implemented to find the optimal susceptor temperature that minimizes C_d, guaranteeing a uniform deposition rate profile in the neighborhood of the wafer center. For this reactor system, we find the optimal susceptor

Figure 5: Results for optimal susceptor temperature of $T_{sus} = 1312.60$ K (total flowrate=6.5 slm).

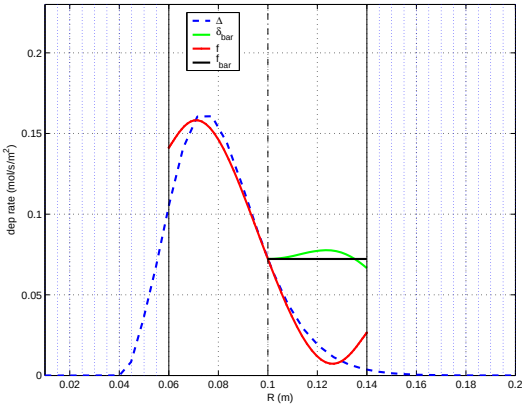
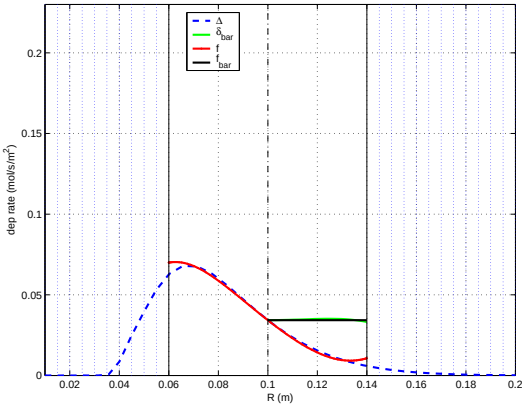


Figure 6: Results for optimal susceptor temperature of $T_{sus} = 1200$ K (total flowrate=3.5 slm).



temperature to be $T_S = 1312.60$ K. This analysis also reveals that the C_d value approaches zero at very low susceptor temperatures. This is expected because minimal decomposition of the precursor occurs in this regime causing $\Delta(R)$ to be nearly zero. Figure 5 clearly shows the improvement is uniformity in the center region of the wafer using the optimal susceptor temperature.

However, it is also obvious from Figure 5 that some degree of nonuniformity still exists towards the outer portion of the wafer. This occurs because $\Delta(R)$ and f do not completely overlap at the two ends of the wafer location. These results imply that modifying the susceptor temperature alone cannot be used to achieve uniform films over the entire wafer surface for this reactor system for a fixed set of other operating conditions. As a result, an analysis of the combined effect of susceptor temperature and total

feed flowrate is performed. A measure of the nonuniformity is defined as

$$\chi = \sqrt{\int_0^{r_w} (\delta_{bar} - f_{bar})^2 \, r dr}. \tag{9}$$

The total flowrate is decreased from 6.5 slm to 3.5 slm by increments of 1 slm and the computation of C_d with respect to susceptor temperature is performed in each case to find the optimal values of the parameters. The results indicate that low flowrates lead to a reduction in nonuniformity. Under these conditions, the optimal susceptor temperature occurs at $T_S = 1200$ K and the results for the rotated profiles are shown in Figure 6. These results immediately convey the improvement in uniformity towards the outer portion of the wafer. The reason for this improvement is attributable to the lower total flowrate's effect of increasing reactor residence times, pushing the peak of the deposition rate profile ($\Delta(R)$) closer to the nearest uniformity producing profile (f).

2 Concluding Remarks

A new approach to uniformity control was applied to a gallium nitride radial-flow chemical vapor deposition system with planetary wafer rotation. This approach provides a process engineer with physical insight on what design parameter(s) should be adjusted to improve uniformity. The results showed that by modifying the susceptor temperature, uniform films of gallium nitride can be produced upon rotation in the planetary radial-flow reactor system.

Acknowledgments

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