Analysis of Channel Confined Selective Area Growth in Evolutionary Growth of GaN on SiO₂

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Abstract

Here, we analyze the chemical vapor deposition of semiconductor crystals by selective area growth in a non-planar geometry. Specifically, the growth process in laterally and vertically confined masks forming single-crystal GaN on SiO₂ by metal-organic chemical vapor deposition is considered in detail. A textured AlN seed is used to initiate growth of oriented GaN selectively through the mask, allowing the reduction of degrees of freedom by the evolutionary grain selection process. As shown by measurements of growth rates within the mask, the sub micron length scale of the channel opening is comparable to the mean free path of precursors in the gas phase, resulting in transport characteristics that can be described by an intermediate flow regime between continuum and free-molecular. Mass transport is modeled through kinetic theory to explain the growth rate enhancements of more than a factor of two by changes in reactor pressure. The growth conditions that enable the modification of nucleation density within the channel are then discussed, and are measured by electron-back scatter diffraction of the nucleated grains on the AlN seed. Finally, the selectivity behavior using the low fill factor masks needed in these configurations has been optimized by control of precursor flow rates and the H₂ enhanced etching of the polycrystalline GaN nuclei.

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1. Introduction

Selective area growth (SAG) is a well documented process in chemical vapor deposition (CVD). In this process, the surface of a wafer is patterned with a dielectric mask by lithography, followed by selective epitaxy enabled by the
5 diffusive transport of reactants to the openings (windows) of the mask. The technique of SAG has been exploited for the reduction of crystalline defects such as dislocations, [1, 2] heterogeneous integration,[3, 4, 5] for the creation of novel nanostructures,[6] and achieving desired gradient effects not possible in conventional growth.[7, 8]

10 With the advance in both top-down and bottom-up fabrication techniques, there have been extensions of planar SAG into more sophisticated geometries such as multi-dimensional constrictions,[9, 10] anisotropy in aspect ratios,[11, 12, 13] and nanoscale deep trenches[14] which we collectively term as channel confined SAG. The constriction in the cross-section of material growth in
15 channel confined SAG is of particular importance in alleviating the problems of heavily-mismatched epitaxy, in molding the SAG crystals into designed configurations, and, most recently, in enabling a novel non-epitaxial preparation of single-crystalline semiconductor on amorphous templates through evolutionary selection (ES) growth.[15] While the growth processes in planar SAG have been
20 well investigated,[8, 16] imposing the physical boundaries of the scale used in channel confined SAG has not been analyzed in detail. In this work, we have used specially-fabricated, two-dimensionally confined growth tunnels, developed for ES growth of GaN on SiO₂,[15] as a platform to study the gas-phase transport phenomena within the construct of "micro-reactors on a chip", where the
25 mean free path of metal-organic chemical vapor deposition (MOCVD) is typically within the range of the feature sizes desired.[17] We note that most of the experimental work on channel confined SAG has been carried out empirically

to circumvent problems including the clogging of channels and insufficient mass transport through the channels.[11] In this paper, a general description is given
30 of the behavior of gas phase transport in channel confined structures during MOCVD growth. It is discovered that, in spite of the regular MOCVD process conditions employed, shrinking the cross-section in a channel confined geometry can effectively transform the gas transport from the continuum regime[18] into the free-molecular regime. The observed growth rates as functions of channel
35 depth and reactor pressure require a hybrid model invoking both continuum and free-molecular transport. With this understanding as a foundation, we explore the primary considerations in successfully designing channel confined SAG. First, by applying this model of gas dynamics within such structures, precursor transport is optimized to increase growth rates and reach deeper channel
40 depths. Secondly, we observe and manipulate the nucleation behavior on the crystalline seed within the channel. This stage of growth is of critical importance in determining the final microstructural quality of the material. Finally, the use of low fill-factor masks have become requisite in many of these advanced SAG techniques, as the one used here with fill factor of 0.1%. The conditions
45 needed to maintain selectivity on such masks are examined.

2. Experimental

The concept of the growth is shown in Fig. 1(a). The substrates for growth were thermally oxidized Si (100) wafers, with a SiO_2 thickness of 200 nm. For growth of GaN on this surface, the channel structure designed was prepared by
50 first depositing a layer (650 nm) of AlN by rf-magnetron sputtering. This AlN film exhibits a c-axis preferred orientation towards the sample normal, with a distribution of 2° (XRD (0002) rocking curve FWHM). Standard photolithography and reactive-ion etching was performed to define the shape of the AlN (for the growth channel - here, rectangular channels are used with widths between 2
55 and 8 μm), which was subsequently covered by a layer of conformal SiO_2 (1 μm , PECVD). Another photolithography step was performed to open the end of the

Figure 1: a) Concept of channel confined selective area growth. The SiO_2 channel is fabricated to confine the extent of the growth in the vertical and one of the lateral directions. The channel, in conjunction with the use of a textured AlN seed on the amorphous SiO_2 , enables the application of the evolutionary growth process to obtain single crystal GaN material. Tilt-view scanning electron microscopy images of b) the fabricated dielectric channel mask before the AlN undercut etch, and c) the GaN crystal grown within the mask shown after mask removal by a buffered oxide etch.

growth channel and expose a portion of the AlN, and wet chemical undercut etching was performed to partially remove AlN from within the channel. The amount of AlN removed is controlled by both etch temperature and etch time, allowing control over the growth channel depth (the distance from the opening to the seed). Thus, the AlN serves as both a cast to define the channel shape, and as the seed for the final step GaN ES growth. The final structure fabricated is shown in Fig. 1(b). More details of the sample preparation can be found in Ref 15.

GaN growth was performed in a horizontal low pressure MOCVD reactor. Trimethylgallium (TMGa) and ammonia (NH_3) were used as precursors for GaN growth, and H_2 was used as the carrier gas. Growth commenced at 1030°C , after thermal cleaning and desorption under H_2 and NH_3 at the same temper-

Figure 2: EBSD characterization of single crystal GaN grown by ES-SAG. a) Kikuchi pattern and b) fit, c) SEM and inverse pole figure mapping.

ature. Here, the TMGa precursor molar flow rate was in the range of 30 to 132
 70 $\mu\text{mol}/\text{min}$, and growth was performed under a V/III ratio of 350 or 1400. The
 chamber pressure was varied between 30 and 400 mbar.

3. Results and discussion

3.1. Characterization of GaN on SiO_2

An example of the resulting GaN is shown in Fig. 1(c), and Fig. 2(c). In
 75 this case, the GaN follows the channel dimensions of $2\text{ }\mu\text{m}$ in width, and 650
 nm in height, and the MOCVD growth duration of 1 hr results in a length of
 approximately $10\text{ }\mu\text{m}$. After removing the top covering SiO_2 with a buffered
 oxide etch, the grown GaN crystal is characterized using electron back scatter
 diffraction (EBSD). A typical Kikuchi pattern collected near the tip of the
 80 crystal is shown in Fig. 2(a). This pattern clearly displays the symmetry of
 the wurtzite crystal lattice (fit shown in Fig. 2(b)). The features in the pattern
 show sharp contrast and include higher order lines suggesting high crystalline
 perfection.

EBSD maps are collected by scanning the electron beam across the sample,
85 and collecting and fitting the Kikuchi patterns to determine the orientation at a
given beam position. In Fig.2(d), an inverse pole figure is plotted, showing the
different grains and evolution of GaN starting from the AlN seed. As is seen, at
the resolution of EBSD measurement (estimated at <100 nm perpendicular to
the beam direction), GaN nucleates on the AlN seed with five different orienta-
90 tions. These orientations all have the polar c-axis perpendicular to the sample
surface, following the AlN grains on which they nucleate on, but have various in-
plane orientations. As growth progresses, each grain extends in both dimensions
until they interact with the SiO_2 sidewall or neighboring grains, where they are
separated by grain boundaries and gaps, some of which are visible under top
95 view SEM. It is seen that the center grain in this case extends the fastest in the
growth direction, and blocks the other grains from propagating further, which is
the manifestation of the ES growth principle. In this way, in each growth tunnel
a single oriented crystalline GaN layer eventually dominates. More details of
the ES-SAG process can be found in Ref 15, 19.

100 In the following, the growth process is analyzed, particularly the param-
eters which are of general concern in the different manifestations of channel
confined SAG. The model system described above and used here share primary
characteristics and requirements with other recently developed growth configu-
rations, such as that for aspect ratio trapping of defects,[1] embedded photonic
105 crystals,[9, 10] thin III-V lateral overgrowth,[12] and InP on Si heterogeneous
integration.[14]. All of these configurations rely on selective MOCVD growth on
a crystalline seed through a multi-dimensional dielectric channel mask character-
ized by a submicron length scale. Here, the three main practical considerations
in the confined growth scheme are discussed to enable the predictive design
110 of the growth process. While the system we study here is specifically for the
growth of GaN, the general principles can be extended to the MOCVD growth
of other III-V materials. The first influence of growth conditions is on the
transport of precursors through the confined channel, determining the growth
rate and the maximum length of GaN growth in the tunnel in a given growth

115 time. The second consideration is the control of nucleation on the AlN seed. The ability to control the growth conditions during the nucleation of GaN on the lattice-mismatched polycrystalline seed will determine the material quality which results from the process. [20] Additionally, the ES growth mechanism scales as the density of the initial nucleation, thus the evolution rate will be
120 scaled as well. [15] The third consideration is the necessity of selective growth to prevent unwanted nucleation on the SiO₂ growth surface. While these polycrystals can be removed with subsequent etching of the SiO₂ mask, these large GaN clusters act as sinks for the precursors and grow at a much faster rate since they are not confined within tunnels. Given the large areas of SiO₂ mask,
125 or equivalently very low fill-factors, the growth conditions must be carefully selected to not exceed the nucleation barrier on the inert mask. The balance between these three considerations will determine the growth conditions used, each of which is discussed in the following.

3.2. Mass transport analysis

130 The transport of precursors during growth on planar 2D masks has been analyzed in detail, [8, 16, 21, 22, 23, 24] however the use of three dimensional masks, i.e. confinement of growth in both in-plane and out-of-plane directions, has been the subject to fewer studies.[5, 9, 14] Typically during MOCVD growth, a combination of surface and lateral gas phase diffusion takes place, each acting
135 dominantly over different characteristic length scales. In planar selective-area growth, gas phase transport has been shown to be the dominant process due to the large length scale ($>5 \mu\text{m}$) of SiO₂ masks. Growth profiles have been accurately predicted by gas phase diffusion models over a wide range of mask sizes and growth reactor conditions by use of D/k_s ratio[8], or the Damköhler
140 number. [16]

Here, we consider the transport of the precursor (MMGa, which is obtained by the fast pyrolysis of the initial TMGa molecules) in a mixture of H₂ and NH₃ gases through a channel confined mask. First, the problem is analyzed in the framework of the kinetic theory of gases. The length scales of the geometry here

145 is applicable to this theory, since while the relevant characteristic lengths (size of opening, depth of channel) are small (0.65 μm and 5 to 20 μm , respectively), they represent lengths many orders of magnitude greater than the molecular diameters of the constituent gases (H_2 : 0.2915 nm, [25] NH_3 : 0.29 nm, [26] MMGa: 0.429 nm [26]). The regime of flow, continuum or free-molecular, can
 150 be characterized by the Knudsen number, Kn , which is the ratio between the mean free path and the relevant length scale [27]. The mean free paths in the conditions studied here (i.e. a mixture of H_2 and NH_3 , pressures of 30 to 400 mbar, temperature of 1030°C), is calculated to range from 0.17 μm to 2.8 μm , using the expression given for a mixture[17]

$$\lambda_{MMGa,H_2/NH_3} = \frac{1}{\pi} \left(\sqrt{2} n_{MMGa} \sigma_{MMGa}^2 + \sqrt{1 + \frac{m_{MMGa}}{m_{H_2}} n_{H_2} \sigma_{MMGa,H_2}^2} + \sqrt{1 + \frac{m_{MMGa}}{m_{NH_3}} n_{NH_3} \sigma_{MMGa,NH_3}^2} \right)^{-1}. \quad (1)$$

155 This average distance between molecular collisions is on the same order of magnitude as the height of the confined mask, yielding a Knudsen number Kn of ~ 1 . This regime of transport (the intermediate regime) is perhaps the least well modeled, as momentum transfer between particles must be accounted for by the use of the Navier-Stokes equations, but at the same time ballistic motion
 160 and collisions with the mask walls could appreciably alter the characteristics of the gas.[17] The model of mass transport in the continuum and free-molecular regimes, Fick's law diffusion and Knudsen diffusion, respectively, offer a testable difference in behavior and will be the subject of the following experiments.

A description of the growth geometry is given to discuss the experiment
 165 aimed to characterize the regime of transport through the confined mask. At the reactor scale, transport of precursors to the sample surface has been shown to be by diffusive transport across a boundary layer; outside the boundary layer reactants move via convective transport due to laminar flow of the gases. For

standard growth, the flux of precursors is given by[18]

$$J = D \frac{C_i - C_s}{\delta}, \quad (2)$$

where C_i is the inlet precursor concentration, C_s is the surface at the concentration, D is the diffusivity, and δ is the boundary layer thickness. Essentially, a concentration gradient is built up between the constantly supplied reactants and the surface where a fast reaction rate depletes the concentration to C_s . The diffusion constant through the multicomponent mixture is calculated by Chapman-Enskog theory, with the following expression for the diffusion constant D [28],

$$D_{MMGa,H_2/NH_3} = \left(\sum_{j=1}^n \frac{x_j}{D_{i,j}} \right)^{-1}, \quad (3)$$

$$D_{i,j} = \frac{0.00266T^{3/2}}{PM_{i,j}^{1/2} \sigma_{i,j} \Omega}, \quad (4)$$

where x_j is the mole fraction of component j , T is the temperature in Kelvin, P is the pressure, $M_{i,j} = 2[(1/M_i) + (1/M_j)]^{-1}$, and Ω is the diffusion collision integral obtained by the analytical approximation for the Lennard-Jones potential [28].

The purpose of the experiments is to look within the boundary layer and determine the mechanism of mass transport into the confined mask channel. If the precursor molecules exhibit many collisions in the gas phase ($Kn \ll 1$), a concentration gradient within the channel will exist, and an expression for the flux of precursors to the growing surface similar to the Eq. 2 will model the transport process. Finite element modeling software (COMSOL) was employed to numerically solve the diffusive transport governed by the Laplace equation, showing the concentration gradient surrounding and within the channel as shown in Fig. 3(a) and Fig. 3(b). For an analytic solution, the structures are modeled in one dimension as channels of changing depth, where one side is the growing GaN surface (which extends through the channel during growth decreasing the depth

of the channel), and the other side is the source concentration of precursors. This can be analytically modeled as a simple compartment model, described by the reaction-diffusion differential equation. The solution of such a system has
195 been given, by Deal and Grove,[29] to be

$$\frac{dx}{dt} = \frac{B}{2x_i + A}, \quad (5)$$

where x is the distance from the tunnel opening to the growth front, and the constants A and B are defined by $A = 2D/k$, $B = 2DC_s/N$, where D is the diffusion constant calculated by Chapman-Enskog theory, k is the reaction rate constant, C_s is the surface concentration of precursors outside the tunnel,
200 and N is the number of precursor molecules incorporated in a unit volume. To compare with the experimental results at a pressure of 100 mbar, 1030°C, and a precursor flow rate of 30 $\mu\text{mol}/\text{min}$, the parameters are calculated to be $D = 29 \text{ cm}^2/\text{s}$, $k = 15850 \text{ cm}^3/\text{s}$ (following Ref 16), and $C_s = 1 \times 10^{-9} \text{ mol/L}$ [30]. Of course, the actual C_s cannot be probed directly, so an estimate is used
205 given the TMGa flow rate, typical reactor gas velocity of 10 cm/s, the volume of the reactor, and the decomposition ratio as analyzed by computational fluid dynamic simulations, [30] which yields this order of magnitude. The value of the surface concentration C_s will be related to the inlet concentration C_i as discussed later, but is also an uncertainty in the subsequent modeling. The
210 value of the boundary layer thickness is obtained through fit to the data, with a physically reasonable value of 0.5 cm for the flow rates used here.[16] The resulting curve is plotted in Fig. 3(c) for continuum flow.

If the collisions the molecules undergo are dominated by those with the structure walls rather than with each other, the flux of molecules reaching the
215 growing surface will be largely determined by the geometry of the channel, specifically the length to opening dimension ratio. The flow of gas through long tubes where the mean free path is greater than the tube radius has been thoroughly investigated, beginning with Knudsen in 1909.[31] Essentially, the transmission probability of molecules in the gas can be calculated for a given

Figure 3: Diffusion modeling of SAG within tunnel masks. a) Iso-concentration profile in a control volume above mask, and b) the linear concentration gradient within the tunnel, computed through finite element modeling. c) Growth models by kinetic theory of continuum (dashed lines) and free-molecular (dotted line) with experimental growth rates as a function of channel depth and d) pressure dependence on the GaN horizontal growth length from the AlN seed as compared to models.

220 tube geometry, as the molecules undergo a number of collision with the tube walls and the Knudsen (cosine) law is used to express the velocity distribution of molecules as the cosine of the emission angle.[32] Analytic methods, integral equation theory and Monte Carlo simulations have been used to describe the geometric dependence on the transmission probability.[33] The solution by Pol-
 225 lard and Present [34] is used here, which is that the transmission probability can be expressed as

$$\eta = \frac{4d}{3L} \left(1 - \frac{3d}{8L} \right), \quad (6)$$

where the transmission probability, η , modifies the Knudsen diffusivity as a function of the geometric parameters of length, L , and diameter, d . The results of the variation in growth rate as a function of tunnel depth in the free-molecular
 230 transport regime are plotted in Fig. 3(c).

As can be seen, experimental data of growths in many channels etched to different depths lie between the theoretical trends of growth rate for the two cases, as plotted in Fig. 3(c). Both models predict a decreasing growth rate as the depth of the tunnel increases due to the increased diffusion distance, or
 235 increased number of collisions of the precursors. However, an appreciable growth rate ($>1 \mu\text{m/hr}$) is still possible with tunnel depths of $100 \mu\text{m}$ and greater. It is noted that with long growth times, a buildup of concentration of the reaction byproducts within the channel may eventually affect precursor incorporation and crystal growth.[35]

240 The dependence of diffusivity on pressure is different for the continuum and free-molecular regimes. This allows us to experimentally probe the differences between the regimes more definitively. While D calculated through the Chapman-Enskog theory is inversely proportional to pressure (Eq. 4), diffusivity in the molecular regime is constant.[27] In fact, by measuring the growth
 245 rate as a function of pressure, a marked difference in growth behavior is observed even as compared to planar growth (as shown in Fig. 3(d)). It is known that growth rates for typical planar MOCVD growths are relatively constant as

pressure is changed with a fixed flow rate.[36] However, it can be seen that the range of growth rates varies widely as reactor pressure is changed from 30 mbar to 400 mbar. It is evident that the use of a large area selective growth mask and transport within the channels are defining a growth behavior that differs from typical planar growth.

Again, to explain this variation in growth rate, we appeal to the continuum and free-molecular transport models described above. Starting again from the reactor scale, Eq. 2 is used to describe the mass transport of reactants across the boundary layer. As pressure is varied, the diffusion constant changes as $1/P$ (Eq. 4), while the gas flow velocity and partial pressure of precursor is proportional to P . The boundary layer thickness, δ , is constant.[18] For standard MOCVD growth with the entire substrate exposed, the relatively fast reaction rate constant of GaN allows the approximation of a very small surface concentration of unreacted species, typically negligible in analysis. This results in the constant growth rate typically observed, since opposing tendencies of partial pressure and diffusivity compensate. [36] However, for the ES-SAG substrates which are covered in a large majority with inert SiO_2 , the average surface concentrations become non-negligible, reducing the total diffusive transport of species to the sample surface at low partial pressures. Thus, as pressure increases, the partial pressure of the precursor dominates the trend in growth rate, which can be seen by the $2.3\times$ increase in growth rate as pressure is increased from 30 mbar to 200 mbar.

This can be considered more precisely by linking the reactor scale mass transport with the transport through the confined mask. The flux of precursors through the boundary layer (Eq. 2) should be related to amount of material deposited inside the channel (Eq. 5) by dividing out N , the number of molecules incorporated in a unit volume. Equating the two, we can relate the inlet concentration to the surface concentration by,

$$C_s = C_i \left(\frac{kx + D}{k\delta + 1} \right). \quad (7)$$

Since the inlet concentration is proportional to P , the diffusivity D is inversely proportional to P , and the average reaction rate over the surface is small because of the very low fill factor, the surface concentration will be approximately constant.

280 Using this model, and the diffusivity calculated with Eq. 3 and Eq. 4, the rough trend of growth rate as a function of pressure is obtained. This C_s is the concentration of precursors outside the tunnel, used in the modeling of growth rate as a function of tunnel depth in Fig. 3(c).

Next, we note the difference between the pressure dependence of the continuum and free-molecular diffusion coefficients, where the molecular (Knudsen) 285 diffusion coefficient is given by the pressure independent expression [32]

$$D_K = 97r \left(\frac{T}{M} \right)^{1/2}, \quad (8)$$

where r is the diameter of the channel. Thus, with a pressure independent D within the channel, the growth rate curve is plotted in Fig. 3(d). The modification may serve to explain several points about the growth rates measured 290 within the intermediate regime. In linear scale, this curve is linear with pressure, with a growth rate approaching zero for low pressures due to decreasing flux of precursors with decreased partial pressure. In the range of pressures below about 80 mbar, the molecular transport predicts a lower rate than the diffusive one, which is also displayed by the experimental data. At these lower pressures, 295 Kn is reduced by several times, which means the growth rate is further influenced by collisions with the channel walls rather than between molecules. With increase of pressure, it is seen that the growth rate drops off from the trend predicted in the molecular flow regime, due to enhanced gas phase collisions. The experimental growth rates may be enhanced from the purely diffusive regime by 300 some fraction of ballistic transport to the growth seed. The diffusion constants in the intermediate regime can be interpolated by the Bosanquet formula in the

form [34]

$$\frac{1}{D_e} = \frac{1}{D_F} + \frac{1}{D_K}, \quad (9)$$

where D_e is the effective diffusion coefficient, D_F is calculated by Chapman-Enskog theory from Eq. 3 and Eq. 4, and D_K is the Knudsen diffusion coefficient
 305 calculated from Eq. 8. It is seen that by the use of this effective diffusion coefficient, the experimental data can be described accurately.

Having verified the transport of precursors into the channel, the conditions at the AlN seed must be controlled in order to have successful nucleation of GaN material. In particular, the balance between the partial pressure of the
 310 Ga-containing species, H_2 partial pressure, and temperature is required. It has been shown that for planar two-step GaN growth on sapphire and GaN on LT-AlN buffer layers, [20, 37] the growth conditions determine nuclei density, grain size and spacing. In particular, growth at increasing H_2 partial pressures and decreasing TMGa flow rates change the growth mode to discontinuous island
 315 growth, and finally to no film growth. The influence of H_2 partial pressure, in particular, on the MOCVD growth of GaN nucleation has been analyzed and high partial pressures have been shown to suppress nucleation, resulting in large nuclei grain sizes and discontinuous islands. [20] In addition, a change of V/III ratio during initial GaN growth has a direct effect on the dislocation density of
 320 the material. [38] While adjustment of the parameters to control nucleation and growth in planar MOCVD growth is straightforward, it is not clear whether the same principles will apply within the channel confined mask.

3.3. Control of nucleation density

Here, we demonstrate control of the nucleation density of GaN on the AlN
 325 seed by the H_2 partial pressure. In Fig. 4(a) and Fig. 4(b), growth conditions of 300 mbar and 500 sccm NH_3 are used (high pressure, low NH_3 flow condition). The EBSD analysis shows GaN nuclei density in the range of $(1.75 - 2.5) \times 10^4 \text{ cm}^{-2}$ on the AlN seed. In Fig. 4(c) and Fig. 4(d), growth conditions using the same TMGa flow but under 100 mbar and 2000 sccm NH_3 (low pressure, high

Figure 4: Control of nucleation density of GaN on AlN seed in ES-SAG. GaN grown in a), c) 2.6 μm wide channel and b), d) 4 μm wide channel at a), b) 300 mbar, 500 sccm NH_3 or c), d) 100 mbar, 2000 sccm NH_3 .

330 NH_3 flow condition), the nuclei density increases to $(2.5 - 4) \times 10^4 \text{ cm}^{-1}$. Here, reactor flow rates are maintained under constant total flow, such that reduction of NH_3 flow is compensated by an increase in H_2 flow to maintain laminar flow conditions in the reactor. Additionally, increase in total reactor pressure will also result in an increase in H_2 partial pressure. These two factors combined
 335 result in the noticeable increase in nucleation density for the initial ES growth stages.

3.4. Selectivity on large area dielectric masks

Finally, the control of selectivity on the large area dielectric mask is discussed. Under typical growth conditions of GaN, temperatures and supersaturation are in ranges where heterogeneous nucleation of GaN on dielectric or
 340 refractory metal masks (such as SiO_2 , SiN , Ti , W) is suppressed. The precise kinetic behavior of precursors depends on the type of mask, [39] due to differences in affinities of the Ga precursor to the different mask materials resulting in changes in mean residence times, desorption rates, and surface diffusion
 345 lengths. For SiO_2 and the typical GaN growth temperature used here, unwanted

nucleation is prevented even with the large mask areas due to reevaporation of adatoms. In addition, decomposition of nuclei clusters is aided by etching from H_2 . The trends of selectivity of GaN growth on SiO_2 masks have been analyzed with respect to supersaturation of precursors over the mask, as a function of pressure and flow rate. [23] As opposed to Ref [23], the flow rates here are not
350 adjusted to maintain the same partial pressures of TMGa and H_2 .

In Fig. 5, the selectivity on the mask is shown for a wide range of growth conditions. For each growth condition, the surface was observed under Nomarski optical microscopy, and large clusters (as shown in Fig. 5(b)) are counted to
355 determine the density of unwanted nucleation, and the size for each cluster is measured to determine an equivalent planar thickness. It can be seen that the selectivity behavior can vary widely as a function of growth condition when these measurements are plot as a function of TMGa flow (Fig. 5(c)) and pressure (Fig. 5(d)). At low TMGa flow, and at high pressures, the unwanted nucleation
360 can be eliminated completely. At high TMGa flows, the equivalent thickness of the unwanted nucleation can approach 80 % of the expected planar growth thickness. It is consistent with these trends that the supersaturation of TMGa and partial pressure of H_2 determine the selectivity behavior on the large area selective-growth masks used here.

365 4. Conclusion

It has been shown that MOCVD growth has the flexibility and control to achieve the selectivity and nucleation conditions necessary to achieve channel confined growth enabling single crystal GaN on amorphous SiO_2 . In this paper, we have analyzed three of the main practical considerations in designing growth
370 processes that utilize non-planar masks in selective area growth. First, the understanding of the transport properties in these structures was built from the kinetic theory of gases. Given the typical pressures used in MOCVD and the size scale of the mask features, it was found the growth results are described by intermediate Knudsen numbers. This modeling has accurately described precursor

Figure 5: Selectivity of samples grown. Nomarski microscope images of samples grown under a) 7 sccm, 200 mbar and b) 30 sccm, 200 mbar. Density and equivalent planar thickness of unwanted nucleation as a function of c) TMGa flow and d) reactor pressure.

transport through the masks, and explained the effectiveness of changing reactor pressure to increase growth rates and reach deeper channel depths. Secondly, we observed significant changes in the nucleation behavior within the channel by the control of H_2 partial pressure. Finally, the conditions to achieve complete selectivity on low fill factor masks, such as the 0.1% fill factor mask used here, are shown. This includes limitations on precursor flow rates, and increased reactor pressure. The full understanding and control of channel confined growth, as presented here, is expected to enable a scalable and effective method for integration of device quality semiconductor crystals with non-crystalline substrates. Further applications requiring novel growth configurations are envisioned using channel confined masks, to achieve new designs in semiconductor electronic and optoelectronic devices.

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