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The effect of reactor pressure on selective area epitaxy of GaAs in a close-coupled showerhead reactor

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Abstract

Selective area epitaxy (SAE) is an established means to control the lateral size and height of epitaxial features. An enhanced growth rate is observed to be a function of mask dimensions. In this study, the effects of reactor pressure and configuration on the SAE of GaAs were studied. Using a SiO_2 mask in a dual stripe configuration, the growth rate enhancement and mesa shape were measured at reactor pressures ranging from 50 to 600 Torr. Results are obtained using a close-coupled showered (CCS) reactor design and compared to a conventional horizontal reactor. The CCS reactor demonstrates a wide range of pressure for stable operation, which has notable advantages for SAE.

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1. Introduction

Selective area epitaxy (SAE) is the controlled deposition of material in well-defined regions on a substrate. In the SAE of GaAs using MOVPE this is most often achieved by the use of a dielectric mask patterned in appropriate dimensions. Under typical epitaxy conditions using suitably narrow mask dimensions, the SAE is perfect and no deposition occurs on the mask. This situation gives rise to an additional concentration gradient in the region adjacent to the mask and leads to the well-known growth rate enhancement (GRE) near the mask edges. The dielectric mask can be patterned in ways to control the GRE to produce novel optoelectronic devices [1,2].

SAE of GaAs has been studied both theoretically and experimentally [3–5]. SAE occurs by a combination of gas phase and surface diffusion, each occurring over an appropriate length scale. Surface diffusion plays a role in forming enhanced ridge features adjacent to the mask edge. Gas phase diffusion dominates the main characteristics of SAE, particularly for the center regions of wider mask openings. Several groups [3–6] have modeled GREs as a function of mask geometry by calculating the reactant concentration profile above a masked surface. This requires the solution of the 2-D Laplace equation for diffusion, assuming specific boundary conditions at various points

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within the calculation cell. The reactant concentration gradient ($\delta N/\delta z$) in the vertical direction is non-zero and zero above the window region and the mask region, respectively, corresponding to epitaxial growth in the window and no deposition on the mask surface. A boundary layer thickness is defined as the height where the gas-phase concentration is held constant. The presence of masked features in the lateral direction introduces a lateral component to the otherwise transverse concentration gradient in the region surrounding the mask features, which must be solved numerically. Simulations [3–6] rely on the use of fitting parameters such as the ratio of the diffusion coefficient to the reactant incorporation rate constant, D/k, to correlate calculated concentration profiles to experimental data. D/k values obtained in this manner range from 110 to 238 μm for a TMGa precursor at 150 [6] and 760 [5] Torr, respectively.

There have been reports of reactor pressure dependence of SAE for GaAs and InP. The pressure range under investigation is typically limited to small excursions (<100 Torr) in the low-pressure MOVPE regime [7,8]. In different studies, a completely different reactor was used to compare low pressure to atmospheric pressure results [9,10]. Using a CCS reactor, it is possible to vary the reactor pressure over a much larger range than traditional reactor geometries, and still retain acceptable uniformity. This paper presents a parametric study of reactor pressure, carrier flow, and temperature to illustrate the dependencies of SAE on a CCS reactor platform.

2. Experimental procedure

GaAs (1 0 0) substrates were patterned with SiO_2 using a dual-stripe configuration shown in the inset of Fig 1. In these experiments, the oxide opening, or "*s*", values range from 2 to 20.4 μm and the oxide width, or "*w*", values range from 6 to 25 μm. The stripes are oriented in the [0 1 1] direction and are positioned on 400 μm centers.

MOVPE of undoped GaAs was performed on the patterned substrates in a CCS reactor. A parametric study of SAE dependence on reactor pressure, growth temperature, and carrier flow rate was performed. The reactor pressure was varied between 100 and 600 Torr, the growth temperature range was 680–750°C, and the carrier gas flow rate was varied by a factor of two in some experiments. Selected experimental conditions were repeated on a conventional horizontal reactor at 38 and 150 Torr at 700°C.

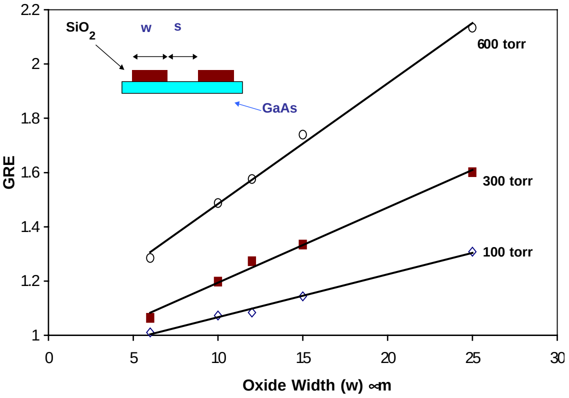

Fig. 1. GRE as a function of oxide width, w, for $s = 8$ μm. Data for three reactor pressures are presented.

The SAE mesa height and shape were measured using surface profilometry and SEM cross-sections following mask removal. The growth rate enhancement (GRE) is defined as the total mesa thickness between the oxide stripes divided by the nominal thickness. The nominal growth rate is measured using an in-situ reflectance tool on planar substrates and correlates well with the thickness measured in regions far away from the masked areas on the SAE wafers. Nominal thickness ranged from 150 to 500 nm depending on the experiment. No changes in SAE characteristics were observed as a function of thickness.

3. Results

Fig. 1 shows the GRE as a function of oxide width for three different pressures with a fixed oxide opening, $s = 8$ μm. In this case, only the reactor pressure was varied, by adjusting the throttle valve setpoint. As expected, as the masked area increases, the GRE increases. In Fig. 1 this is demonstrated for a fixed s and increasing oxide width. Other data show that as the opening, s, increases, the GRE decreases. Fig. 1 also shows that as the reactor pressure is increased, the amount of GRE increases for a given mask geometry. The nominal growth rate is only weakly affected by growth pressure, changing by no more than 5% over the pressure range investigated. The GRE dependence on pressure is due to gas phase diffusion effects above the masked regions. Increasing the reactor pressure enhances the effects due to the decreased diffusion length.

Fig. 2 shows SEM cross-section images of SAE GaAs mesas oriented in the [0 1 1] direction at 600 and 300 Torr. The nominal thicknesses are 200 and 500 nm, respectively. The GaAs mesa grown at either pressure shows a well-defined mesa with little, if any, edge enhancement adjacent to the mask. This demonstrates that SAE of GaAs can be performed at 600 Torr to take advantage of the high GRE. Smooth, uniform mesas are important for subsequent epitaxial regrowth for the fabrication of optoelectronic devices.

Fig. 3 shows the effect of growth temperature on the GRE in the range of 680–750°C. Several oxide geometries are included and the nominal growth rate is plotted for comparison. The nominal growth rate is about 1 nm/s and changes by less than 5% over the temperature range investigated as measured by in-situ reflectance. Fig. 3 shows that the growth rate enhancement increases with increasing temperature for a given mask dimension. Between 680°C and 750°C, there is a systematic 45–60 nm increase in the SAE thickness. This suggests that the modeling parameter D/k is temperature and pressure dependent, which has been previously proposed [4].

The effect of changing carrier flow and reactant mole fraction at 300 Torr was investigated. Three conditions were evaluated: (a) decrease the carrier flow by half but maintain all other flow rates, (b) decrease all flow rates by half, and (c) double only the TMGa flow rate. Fig. 4 plots the GRE vs. oxide width for each of these conditions, comparing this data to the baseline condition at 300 Torr. In these cases, the nominal growth rate is affected by the change in conditions. For example, a decrease in the carrier flow by half increases the growth rate by $\sqrt{2}$. The GRE is unaffected by these changes in nominal growth rate. Fig. 4 shows that the maximum thickness difference between

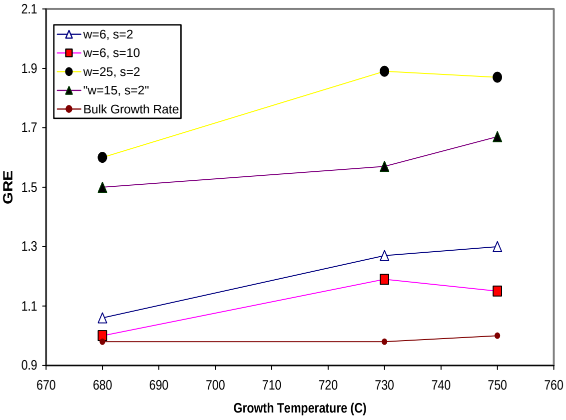

Fig. 3. Effect of growth temperature on growth rate enhancement of SAE of GaAs. At higher temperatures more GRE is observed. The bulk growth rate changes less than 5% over this temperature range. The trend lines are added to guide the eye.

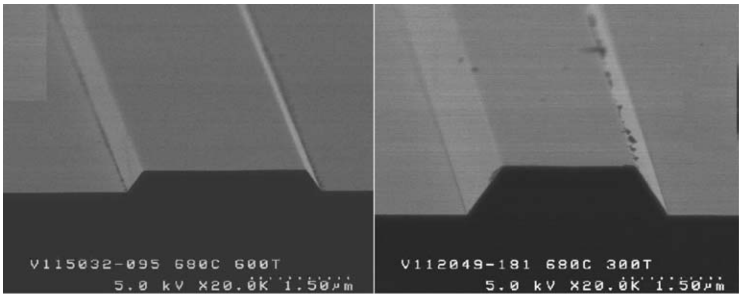

Fig. 2. SEM micrographs of SAE GaAs at 600 and 300 Torr. Nominal thicknesses are 200 nm and 500 nm, respectively. The mesas are uniform and do not exhibit measurable edge enhancement under these conditions.

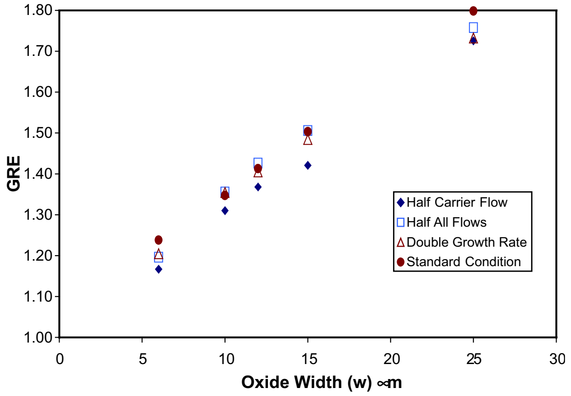

Fig. 4. SAE of GaAs at 300 Torr ($s = 2\,\mu m$) using various growth rate conditions. The GRE is not affected by changes in the nominal growth rate or flow conditions.

conditions is at most 14 nm, but less for most masks dimensions. The GRE for these cases are identical, suggesting that the growth rate enhancement is unaffected by flow rate or mole fraction of column III source, and is affected only by the mask geometry.

The pressure dependence of SAE was also performed on a conventional, horizontal reactor at 38 and 150 Torr. Fig. 5 shows the results from this configuration compared to the CCS reactor. It is found that while the GRE trends with temperature and mask dimension are similar, the absolute magnitude of the GRE is greater for the conventional horizontal chamber at low pressures.

4. Discussion

Several observations can be made concerning SAE from this study. The growth rate enhancement is increased at higher growth pressures and temperatures for a given mask geometry. These effects can be described in terms of the fitting parameter D/k used frequently in SAE calculations.

Most literature simulations [4–6] calculate D/k values using fixed conditions of reactor pressure and temperature. D and k cannot be independently determined in this manner. The parameter D/k is varied in order to converge the calculated concentration profile to the experimental data, using variable mask dimensions to verify consistency. In one report [6], calculated GRE profiles are shown that demonstrate that as D/k decreases, the GRE increases. No comment is made regarding the physical reason for a D/k decrease, however it is clear that a reduced diffusion length and a larger incorporation constant should increase the GRE.

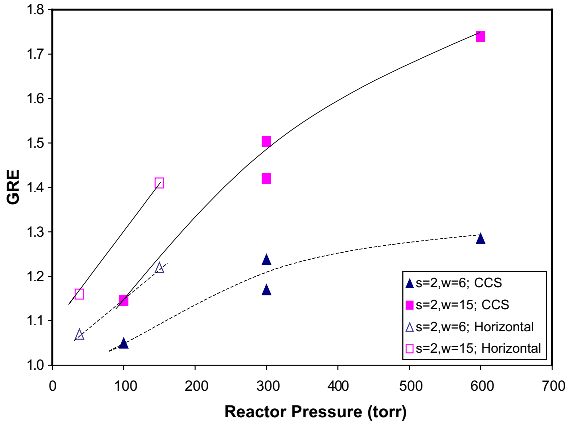

Fig. 5. GRE as a function of reactor pressure in a CCS (closed symbols) and conventional horizontal reactor (open symbols). The trends are similar, but the absolute magnitude of GRE is different between the two platforms. The lines are added merely as a guide for the eye.

The increase in GRE with reactor pressure can be described in terms of a decreased diffusion length leading to more incorporation within the oxide opening. For TMG in H_2 the diffusion coefficient has the following form [11]

$$D = \frac{2.23 \times 10^{-5}(T^{1.73})}{P} \tag{1}$$

which predicts a reduced diffusion coefficient at higher pressures. The data in Fig. 5 support this trend between 50 and 600 Torr. Therefore, as pressure increases, D/k decreases and the GRE increases.

Ultra-high vacuum deposition of InGaAs on InP shows no growth rate enhancement for any mask geometry at pressures of 4×10^{-4} Torr [12]. Under those conditions, the diffusion length is expected to be very long (D/k large) and the epitaxy is catalyzed by heterogenous reactions. These conditions will virtually eliminate any effect of the mask on the GRE. These observations indicate that gas-phase diffusion plays the dominant role in SAE.

Over a practical range of growth temperatures, the temperature increases the GRE less than the reactor pressure. The diffusion coefficient will increase with temperature according to Eq. (1). The incorporation factor, k, governs an activated process with an Arrenhius temperature dependence. The increase in GRE as a function of reactor temperature implies that D/k decreases with temperature. Our calculations indicate that D/k should decrease with temperature for effective activation energies of greater than 0.15 eV.

The horizontal reactor configuration appears to have a larger GRE at lower pressures than the CCS reactor, for the conditions used. The reason for the difference is unclear, since the GRE should normalize most differences between reactor variables. A comprehensive study on the horizontal reactor was not performed so the impact of other variables cannot be established.

The trend of decreasing D/k with increasing pressure is not supported by the published TMGa D/k values mentioned above [5,6]. However, the trend is consistent with published values for TMIn, where $D/k = 15$ and $30\,\mu\text{m}$ for 150 [4] and 15 [6] Torr, respectively. It is not reasonable to suspect the calculations since each set of D/k values for TMGa and TMIn have been used successfully to predict ternary compositions [4–6]. The difference between horizontal and CCS GREs may suggest that the magnitude of D/k may depend on certain reactor-specific variables, making the direct comparison of D/k values unreliable. Direct modeling of D/k values as a function of pressure and temperature would resolve the problem. It is also possible that using pressure dependent GRE data would allow the independent determination of D and k.

The reactor pressure variation produces the largest range of GREs, second to the mask geometry. This makes the reactor pressure range a useful parameter for implementing SAE into devices. It is often advantageous to achieve the largest possible GRE difference between two regions in an integrated device. One common method is to adjust the width of the oxide stripes to achieve the desired growth rate enhancement. At low pressures, with the concomitant small GREs, very wide oxide widths might be necessary to achieve the desired GRE. This can lead to interaction between adjacent elements if the oxide width comprises a significant fraction of the wafer surface area. Another problem commonly observed with wide oxide features is nucleation on the mask.

Alternatively, a higher reactor pressure can achieve larger GREs while keeping the oxide widths reasonably narrow. Fig. 6 shows the GRE as a function of oxide width for 2 μm openings at 100 and 600 Torr. The shaded box represents two boundary conditions that might be imposed for a practical device fabricated using SAE. The first condition is the desired GRE. If a GRE = 1.4 × or greater is needed between two regions, then an oxide width of 8 μm (30 μm) is needed at 600 Torr (100 Torr). In order to minimize long-range interactions between cells and avoid nucleation on the mask, mask coverage of less than 20% might be required. For devices on 400 μm centers the oxide width would be less than 40 μm. The maximum mask coverage limits the utility of low pressure SAE since at 100 Torr, only a small region of the total phase space is covered. The shaded area is accessed more readily by using 600 Torr. The CCS reactor allows SAE at 600 Torr which can hit the GRE target. This additional flexibility, in addition

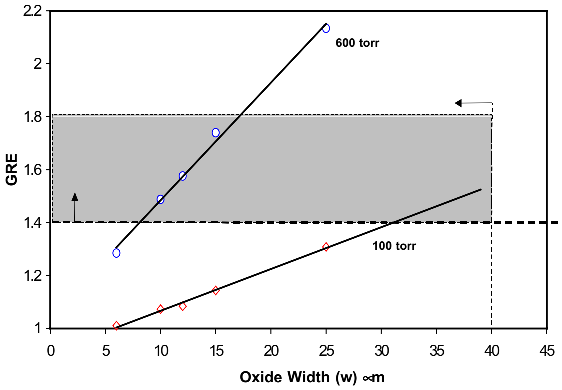

Fig. 6. GRE as a function of oxide width at various reactor pressures. The shaded area represents practical design constraints for SAE. Using higher pressure may be necessary to create optoelectronic devices with dimensions in the design window.

to the exceptional uniformity maintained at higher pressures, makes the CCS reactor well suited for selective epitaxy.

5. Conclusion

A parametric study of SAE on a CCS reactor was performed. The reactor pressure has the largest impact on the GRE of GaAs, with temperature showing only a modest effect. The CCS reactor can be used in a wider pressure range than conventional horizontal reactors, which allows a greater achievable range of GREs for a given mask geometry. This has several advantages for optoelectronic device design using selective epitaxy.

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