Chapter 3. Wafer-fused GaAs - GaN Heterojunctions

3.1. Overview

This chapter describes the wafer fusion of an n-GaAs/n-GaN heterostructure (henceforth called the “n-n” structure) and a p-GaAs/n-GaN heterostructure (henceforth called the “p-n” structure), achieved over a wide range of fusion process conditions (500-750°C for 0.25-2 hours). These simple fused structures were fabricated and characterized, in order to determine the starting points of the fusion process for the more complicated HBT structures. Two principal characterization methods were used to assess the quality of the fused junctions: electrical current-voltage (I-V) characteristics, and secondary ion mass spectrometry (SIMS) analysis of the chemical composition. I-V characteristics alone suggested that elevated process times or temperatures were more optimal fusion conditions. However, SIMS
data revealed substantial inter-diffusion of dopants and contaminants, especially with elevated process times and temperatures. The details of the characterization are described in this chapter.

3.2. Design and Fabrication

Starting materials are depicted in Figure 3.1.i. In the p-n structure, both carbon and beryllium were investigated independently as p-GaAs dopants. Both dopants had been used successfully in high-performance AlGaAs-GaAs HBTs. However, beryllium exhibited a much higher diffusivity, and beryllium out-diffusion from the base was problematic.[1, 2] For the fused HBTs (Chapters 4-6) carbon was chosen, rather than beryllium, in order to minimize dopant diffusion during the high-temperature fusion process.

Samples were fused using the process described in Section 2.2. I-V test structures are depicted in Figure 3.1.iii. Simulated energy band diagrams are shown in Figure 3.2.

3.3. Electrical Analysis

Figure 3.3.a displays I-V data for various samples of an identical n-n structure (Figure 3.1.a.iii). All samples were formed via wafer fusion for two hours, but each was fused at a different temperature (650-750°C). I-V curves became more linear and less resistive with elevation in process temperature. Data for the same n-n
structure fused at shorter times (1 hour), but over the same range of temperatures (650-750°C), demonstrated the same trend. Figure 3.3.b revealed that a similar trend resulted from various samples of the same n-n structure, all fused at 750°C but each fused for a different time (0.5-2 hours); I-V curves became more linear and less resistive with elevation in process time. The simulated band diagram (Figure 3.2a) suggested that, ideally, the I-V characteristics of the n-n structure would have been nearly ohmic. Thus, the increased linearity of the I-V results suggested that a higher fusion time (2 hours) and temperature (750°C) were more optimal. This trend correlated well with cross-sectional TEM results (Figure 2.7), which revealed a thinner disordered interlayer at junctions fused at a higher temperature. (The interlayer thickness varied from 0.5-1nm in samples fused at 750°C, to 1.5-2nm in a sample fused at 550°C.) SIMS data, discussed in Section 3.4, also provided additional insight.

As of the date of this dissertation study (2004), UCSB was the only group that reported GaAs-GaN fusion.[3-9] However, a few groups were developing the heteroepitaxial growth of cubic GaN on a cubic GaAs substrate via MOCVD, plasma-assisted MBE, or radio-frequency magnetron sputtering.[10-14] Given the large lattice mismatch between GaAs (lattice constant of 5.65A) and GaN (3.19A), in light of the discussions of Section 1.1, the crystalline quality of the grown heterojunctions was less than perfect. To achieve a layer of cubic GaN on cubic GaAs, a thin (20nm), undoped, and highly dislocated low-temperature buffer layer was required between the GaN and the GaAs. The I-V data of a grown cubic
n\textsuperscript{+}GaN(4x10\textsuperscript{19} cm\textsuperscript{-3})-nGaAs(2x10\textsuperscript{18} cm\textsuperscript{-3}) junction were shown to be rectifying, with a turn-on voltage of 0.4V. [12] Since the buffer layer of the grown junction (20nm) was much thicker than the disordered layers of our junctions fused at 750\textdegree C (0.5-1nm), this may explain why our fused junctions exhibited more ohmic I-V characteristics (Figure 3.3) when fused at sufficiently high temperature and time (750\textdegree C for 2 hours). Similarly, since the disordered layer at our junction fused at 550\textdegree C (1.5-2nm) was thicker than at our junction fused at 750\textdegree C (0.5-1nm), this may explain why the higher fusion temperatures corresponded to more ohmic I-V characteristics.

Figure 3.4 displays a subset of I-V data for various samples of the same p-n structure (Figure 3.1.b.iii). All samples were formed via wafer fusion for one hour, but each was fused at a different temperature (650-750\textdegree C). All p-n samples had an identical material structure, except that two different p-GaAs dopants were investigated: beryllium (Figure 3.4.a) and carbon (Figure 3.4.b). In reverse bias, the leakage current varied with voltage. In forward bias, the threshold turn-on voltage was low. At higher fusion temperatures, diodes demonstrated softer breakdown in reverse bias, higher turn-on in forward bias, and lower ideality factors (n). For example, for Be-doped diodes formed via fusion for 1 hour, n=1.4 for a fusion temperature (T\textsubscript{f}) of 750\textdegree C, n=1.5 for T\textsubscript{f}=700\textdegree C, and n=1.7 for T\textsubscript{f}=650\textdegree C. The improved breakdown and ideality factor, with increasing fusion temperature, may have been due to the decrease in interfacial disorder observed via cross-sectional
TEM (Figure 2.7). SIMS data, discussed in Section 3.4, also provided additional insight.

Compared to the Be-doped structure, the C-doped structure exhibited more uniform turn-on and lower resistance in forward bias. Differences between Be-doped and C-doped samples may have arisen from differences in dopant diffusivity during the high-temperature fusion anneal. Hence, SIMS analysis was used in conjunction with I-V analysis, in order to monitor dopant migration.

### 3.4. Chemical Analysis

SIMS was used to profile dopants and impurities from the GaAs layer, through the fused interface, into the GaN layer. As with the electrical data, comparisons were made among the systemically varied fusion conditions (time, temperature) and the different p-GaAs dopants (Be, C). Be, like Zn, is a more conventional p-GaAs dopant. However, C is known to have a higher solubility and lower diffusivity than Be and Zn. C may more readily provide the thin, sharp dopant profiles required for bipolar transistor operation, especially when these dopant profiles can be expected to broaden due to dopant and impurity diffusion at the high fusion temperatures (500-750°C, 0.25-2 hours).

Regardless of fusion condition and sample material structure, SIMS data consistently revealed high dopant and impurity signals (Si, Be, C, H, O), which peaked at the fused interface (as shown, for example, in Figures 3.5-3.9). This
aggregation at the interface was expected, as disordered interfaces were known to act as gettering sites for dopants and impurities, especially with strain due to thermal expansion mismatch.\cite{15} The presence of dopants, impurities, or defects (at or near the fused interface) may be detrimental to the electrical quality of the fused interface, which acts as the base-collector junction of the HBT. For instance, n-type and p-type dopants may act to compensate each other. Additionally, impurities may act as unintentional dopants or passivating agents. Finally, defect-assisted diffusion (such as vacancy-assisted diffusion) has been observed previously near fused interfaces. By enhancing diffusion, defects associated with the fused interface were seen to degrade overall device characteristics.\cite{16}

Also as expected, more extensive diffusion was observed in Be-doped samples as compared to C-doped samples, as suggested by SIMS data for the two different structures fused under the same process conditions. After fusion at 650°C for one hour, the Be-doped structure displayed broader and larger SIMS signals of Si, C, O, and H (Figure 3.5), suggesting that (during the fusion anneal) the Be-doped structure underwent more diffusion than the C-doped structure. However, it is interesting to note that, after fusion at a higher temperature of 750°C for one hour, the SIMS signals were comparable between the two structures (Figure 3.6).

Figure 3.7 shows the Si, C, O, and H profiles of different samples of the same Be-doped p-n structure (Figure 3.1.b.ii), all formed via fusion for one hour but each fused at a different temperature (650 and 750°C). Although the Si, C, O, and H peak values were greater with the higher fusion temperature, the overall signals (areas
under the signal curves) were greater with the lower fusion temperature, suggesting the increased diffusion of species away from the fused interface with increasing fusion temperature. Figure 3.8 shows the Si, C, O, and H profiles of different samples of the same C-doped p-n structure (Figure 3.1.b.ii), all formed via fusion for one hour but each fused at a different temperature (650 and 750°C). For n-n samples and C-doped p-n samples, it was generally observed that higher SIMS signal peaks were observed at interfaces fused with lower times or temperatures. With increased fusion time or temperature, peak concentrations diminished in height and broadened into the surrounding materials. All these data suggested that Si, C, O, and H were present at the fused interface prior to fusion (in some chemical form, perhaps including hydrocarbons), and/or the species readily diffused to the gettering fused interface early in the bonding process. With continued thermal treatment, the high concentrations of Si, C, O, and H at the interface may have driven the redistribution of these species into the surrounding materials.

It is interesting that elevated fusion times and temperatures induce improvements in both electrical performance (Figures 3.3 and 3.4) and interface contamination (Figures 3.7 and 3.8). However, more detailed studies would be helpful in correlating the chemical composition, electronic trap density, and electrical performance of interfaces fused under various conditions, especially in consideration of numerous complications. For example, Figure 3.8 shows large concentrations of hydrogen at the fused interface between n-GaN and C-doped p-GaAs. In C-doped p-GaAs, hydrogen and carbon have been shown (via infrared absorption analysis) to
bond together into complexes, passivating the electrical activity of the C dopant.[17] The observed reduction of H concentration may help to explain why the C-doped p-n diodes exhibited better electrical performance if formed via fusion at higher temperatures (Figure 3.4.b).

Despite the previous discussion, it is not recommended that fusion temperature be elevated, with the goal of minimizing interface contamination. Diffusion effects are quite complicated, given that numerous species are driven to diffuse by several factors: large concentrations, exposure to high fusion temperatures for long times, and the nearby presence of the fused interface (which can act as both a source and sink for diffusion). For example, in contrast to the general trend described previously, C and O signals were sometimes observed to broaden and increase with increasing fusion time or temperature (Figure 3.9). Although C and O may have originated from residual surface impurities on the constituent wafers (prior to intimate contact and fusion), an increase of these signals with elevated fusion time or temperature suggested that O and C may have also emerged as they diffused from deep in the bulk starting materials. Because C and O can serve as dopants in GaN and GaAs, their diffusion aggravated the issues of dopant compensation and disruption of the thin, sharp dopant profiles required for bipolar transistor operation. In summary, the SIMS data suggested that the fusion temperature and time should be reduced as much as possible, in order to mitigate complicated diffusion effects.
SIMS data were obtained in collaboration with one of three service providers:
Yumin Gao at Applied Microanalysis Labs, Inc., Patrick van Lierde at Charles Evans & Associates, or Tom Mates at the University of California at Santa Barbara.
Figure 3.1. The fabrication process for fused (a) n-GaAs/n-GaN (“n-n”) heterojunctions and (b) p-GaAs/n-GaN (“p-n”) diodes: (i) starting materials, (ii) samples after fusion and GaAs substrate removal, and (iii) I-V test structures after mesa etching and contact metallization.
Figure 3.2. Simulated energy band diagrams for (a) the n-n and (b) the p-n wafer-fused material structures depicted in Figure 3.1.
Figure 3.3. Current-voltage (I-V) data for various samples of the same n-n structure shown in Figure 3.1.a.iii: (a) all samples were formed via fusion for two hours, but each sample was fused at a different temperature (650-750°C), and (b) all samples were formed via fusion at 750°C, but each sample was fused for a different duration (0.5-2 hours).
Figure 3.4. I-V data for various p-n samples, all formed via fusion for one hour but each fused at a different temperature (650-750°C). The two p-n materials structures (Figure 3.1.b.iii) were identical, except two different p-GaAs dopants were investigated: (a) beryllium and (b) carbon.
Figure 3.5. SIMS profiles in various samples of both the C-doped and Be-doped p-n structures (Figure 3.1.b.ii), all fused at 650°C for one hour. Profiles are shown for (a) silicon, (b) carbon, (c) oxygen, and (d) hydrogen. These SIMS data were obtained in collaboration with Yumin Gao at Applied Microanalysis Labs, Inc.
Figure 3.6. SIMS profiles in various samples of both the C-doped and Be-doped p-n structures (Figure 3.1.b.ii), all fused at 750°C for one hour. Profiles are shown for (a) silicon, (b) carbon, (c) oxygen, and (d) hydrogen. These SIMS data were obtained in collaboration with Yumin Gao at Applied Microanalysis Labs, Inc.
Figure 3.7. SIMS profiles in various samples of the same Be-doped p-n structure (Figure 3.1.b.ii), all fused for one hour but each fused at a different temperature (650-750°C). Profiles are shown for (a) silicon, (b) carbon, (c) oxygen, and (d) hydrogen. These SIMS data were obtained in collaboration with Yumin Gao at Applied Microanalysis Labs, Inc.
Figure 3.8. SIMS profiles in various samples of the same C-doped p-n structure (Figure 3.1.b.ii), all fused for one hour but each fused at a different temperature (650-750°C). Profiles are shown for (a) silicon, (b) carbon, (c) oxygen, and (d) hydrogen. These SIMS data were obtained in collaboration with Yumin Gao at Applied Microanalysis Labs, Inc.
Figure 3.9. SIMS profiles in various samples of the same C-doped p-n structure (Figure 3.1.b.ii), all fused at 550°C but each fused for a different duration (0.25-1 hour). Profiles are shown for (a) silicon, (b) carbon, and (c) oxygen. The double peak of the O signal is discussed in Section 2.4. These SIMS data were obtained in collaboration with Tom Mates at the University of California at Santa Barbara.
3.5. References


