Microstructure of GaAs/GaN interfaces produced by direct wafer fusion

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(Received 24 June 2002; accepted 26 August 2002)

Results of a transmission electron microscopy (TEM) study of directly bonded GaAs/GaN structures obtained by wafer fusion are presented. A large fraction of the interface area was found to be well bonded, with the presence of a thin (1–2 nm) amorphous layer of a native oxide at the bonded interface. The dominant defects found in nonbonded areas were cavities elongated along the [110\(_{\text{GaAs}}\)] direction. Plan-view TEM study of well-bonded regions showed the presence of two dislocation networks. The first, formed at the interface to accommodate an unintentional tilt between the fused crystals, consists of a one-dimensional array of wavy dislocations located at interface steps. The second dislocation network, formed to relieve additional strain from the thermal processing of the samples, consists of a two-dimensional, irregularly spaced grid of dislocations formed on the GaAs side that runs parallel to either the [110\(_{\text{GaAs}}\)] or [11\(_0\)]\(_{\text{GaAs}}\) directions.

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Wafer bonding of lattice-mismatched materials has demonstrated great success in producing heterogeneous device structures that could not be formed through alternative methods, such as epitaxial growth. By integrating materials such as GaAs/InP, InGaAs/Si, and GaAs/Si, wafer bonding has produced a variety of devices such as light-emitting diodes, vertical cavity lasers, vertical couplers, and avalanche photodiodes. Recently, GaN wafer fusion has been used to create GaAs/GaN diodes and an n-AlGaAs/p-GaAs/n-GaN heterojunction bipolar transistor (HBT), as well as to integrate GaAs- and GaN-based light-emitting heterostructures. This letter reports transmission electron microscopy (TEM) results of the microstructure of GaAs/GaN interfaces produced by wafer bonding.

The structures used for this study were produced by direct fusion of a GaAs wafer on top of a 2 \(\mu\)m thick GaN layer grown on c-plane (0001) sapphire by metalorganic chemical vapor deposition (MOCVD) (Fig. 1). The GaAs layer was 1 \(\mu\)m thick and it was grown by molecular beam epitaxy (MBE) on a 0.3 \(\mu\)m thick AlAs etch stop layer. Channels 10 \(\mu\)m wide and \(\sim\)100 nm deep were etched into the GaAs substrate, forming a rectangular grid of 150 \(\mu\)m \(\times\)400 \(\mu\)m. These were intended to facilitate the removal of gas or liquid by-products of the fusion process. The GaAs and GaN surfaces were measured to have <0.4 nm root mean square (rms) roughness. The wafers were cleaned with acetone and isopropanol, then underwent two sequential oxidations (first by oxygen plasma then by ultraviolet ozone) followed by steps for oxide removal (in NH\(_4\)OH). Finally, GaN and GaAs were rinsed in methanol, joined together in methanol, and then fused in a nitrogen ambient under uniaxial pressure of 2 MPa. Two different bonding temperatures (550 and 750 °C) and two different bonding times (15 and 60 min) were used to produce four different samples. Further details of the growth conditions of the materials, the fusing apparatus, and conditions can be found elsewhere. Removal of the GaAs substrate by selective wet etching resulted in the following sample structure: GaAs (1 \(\mu\)m)/GaN (2 \(\mu\)m)/sapphire. No attempt was made to optimize the twist angle between the GaN and GaAs layers and therefore each of these four samples has a different, accidental twist angle. Cross-sectional TEM specimens were prepared from the two samples fused at 750 °C and one fused for 60 min at 550 °C. In the sample fused at 550 °C the GaAs layer separated from the GaN during specimen preparation, which suggested very weak bonding. In addition to cross-sectional specimens plan-view TEM specimens were prepared from the sample fused at 750 °C.

All TEM studies indicated that there were no substantial differences in the microstructure of the fused interface between samples bonded at 550 and 750 °C. Details of this microstructure will be described in the following.

The TEM study of cross-sectional specimens showed that most of the interface area was well bonded. A high resolution electron microscopy (HREM) image of this well-bonded interface observed in the sample fused for 15 min at 750 °C is shown in Fig. 2(a). The HREM studies showed that a very thin layer of bright contrast, most likely amorphous material, was visible at the interface even in the well-bonded regions. Its thickness varied between 5 and 10 Å in samples fused at 550 °C.

FIG. 1. Schematic drawing of the (a) starting materials and (b) the structure after fusion and GaAs substrate removal.
bonded at 750 °C and between 15 and 20 Å in the one bonded at 550 °C. Thin layers of residual native oxide have previously been observed in other systems of bonded materials, both by TEM and by secondary ion mass spectroscopy of the fused interface. We also confirmed the presence of oxygen at the GaAs/GaN bonded interface by detailed energy dispersive x-ray (EDX) analysis, details of which are published elsewhere.5 Also observed at the interface were regions with bright contrast, generally identified as “cavities.” As in the case of GaAs/InP or GaN/sapphire bonded materials, these cavities were asymmetric, and extended primarily into one material only. In the case of the InP/GaAs the cavity always extended more deeply into the InP side, whereas cavities formed at the fused GaAs/sapphire interface formed almost entirely in the GaAs and revealed distinct faceting on (001)- and (111)-type GaAs planes.11,12 In these GaAs/GaN samples, the cavities extended almost entirely into the GaAs. These cavities also revealed (001)- and (111)-type facets [Fig. 2(c)], although some cavities were lens like in shape [Fig. 2(b)]. The heights of the cavities ranged between 5 and 20 nm, whereas their horizontal dimension varied from a few tens of nanometers to a few tens of micrometers. The cavities were also evident in the plan-view samples, appearing as bright regions (narrow long strips in Fig. 3) that are distributed between well-bonded areas, with a characteristic line pattern. Most of the cavities were elongated along the [110]GaAs direction. EDX measurements indicated excess oxygen within the cavities, and suggest that the cavity regions are partially empty.5 The formation of such cavities in the GaAs/InP system was correlated with enhanced diffusion processes that took place under the bonding conditions. These cavities may be formed by the migration of small voids that result from surface irregularities of the wafers. During the bonding process, these voids can migrate at the interface and agglomerate to reduce the overall area of nonbonded interface. The asymmetry of the cavity shape observed in the present study can be associated with the fact that, at the fusion temperature, the diffusion of vacancies takes place mainly in GaAs. Reduction of surface free energy of the system is the driving force for the observed faceting of cavity surfaces.

The plan-view samples show a series of dislocation networks that could accommodate the tilt misorientation and thermal mismatch between GaAs and GaN. One of these networks, a one-dimensional array of irregular wavy lines, is clearly visible in Fig. 3(a). These lines are oriented at some average angle relative to the [110]GaAs direction (the direction of the elongation of cavities). The angle varies from sample to sample, and also shows local variation within a sample. The average spacing between neighboring lines of this array is of the order of a few tens of nanometers. We measured average spacing of these lines of about 55 and 35 nm for samples fused for 1 h and 15 min, respectively. We believe that this network accommodates the tilt between the bonded GaAs and GaN. The tilt between two materials brought together in wafer bonding has two principal components: an average, long-scale tilt originating from miscut and local tilts due to surface roughness and irregularities. The “miscut tilt” dislocations will form relatively uniformly distributed steps at the interface. The direction of the dislocation lines is determined by the tilt axis, and the spacing between dislocations depends on the tilt angle. For small tilts ω it can be approximated by $D = b/\omega$ where $b$ is a component of the Burgers vector normal to the bonding plane. Assuming that the Burgers vector of dislocations that form this network is of the order of $a_{\text{GaAs}}$ or less, we estimated that this tilt has a very small value of the order of 1°.

Plan-view TEM also reveals straight dislocation lines along the [110]GaAs and [110]GaAs directions; these features are indicated between the pairs of arrows in Fig. 3. The spacing between these lines varies from place to place but they form a two-dimensional array with an average separation between lines in the range of a few micrometers. We believe that this network results from the thermal mismatch between the GaAs and GaN. Fusion takes place at an elevated temperature and the sample is subsequently cooled down to room temperature. The two-dimensional network of irregularly spaced dislocations forms to accommodate the resulting strain. The average separation between dislocations of this network depends on the magnitude of the strain, which needs to be relaxed. Networks of such dislocations have been reported in the literature for the InP/GaAs system.8,13 They are usually observed some distance from the interface and the average separation between dislocations measured in this system was of the order of a few micrometers. Our material system needs to account for differences in the thermal expansion coefficient of sapphire ($\sim 6.5 \times 10^{-6} \text{ K}^{-1}$),14 GaAs ($\sim 6.5 \times 10^{-6} \text{ K}^{-1}$),14 and GaN ($\sim 5.6 \times 10^{-6} \text{ K}^{-1}$).15 The straight lines (shown in Fig. 3) may belong to such a network of dislocations formed after bonding when the samples were cooled down to room temperature. These dislocations formed in the GaAs, since they are parallel to either the [110]GaAs or the [1-10]GaAs direction.
Finally, we would also have expected to identify a dislocation network that would accommodate the lattice mismatch between GaAs and GaN. When two different materials are fused together lattice mismatch is accommodated by a network of misfit dislocations with an edge component in the bonding plane. If the orientations of the two layers are relatively twisted in plane, dislocations with a screw component will also form to accommodate the twist. Therefore, a two-dimensional network in the form of a regular grid of misfit dislocations with a Burgers vector in the bonding plane will also form to accommodate the twist. Therefore, a two-dimensional network in the form of a regular grid of misfit dislocations with an edge component in the bonding plane should appear at the interface when two twisted, lattice mismatched layers are bonded. Such a grid was observed for bonded cubic crystals.\(^{8,13,16}\) However, in our samples no closely spaced, regular grid of dislocations was observed. This type of dislocation network was also not observed for a bonded sapphire/GaAs interface.\(^{11,12}\) The reasons may have to do with the thin amorphous layer at the interface or with the relative inertness of the component materials. The high melting point of the GaN or sapphire, relative to the bonding temperature, may preclude actual chemical bonding between the GaN (or sapphire) and GaAs. To understand this, further, more detailed studies are necessary.

In summary, the microstructure of the interface formed by direct bonding of GaAs and GaN wafers was investigated using different TEM techniques. The microstructure of the interface of samples fused at 550 and 750 °C did not differ substantially. Most of the interface area was well bonded, with only a thin (1–2 nm thick) amorphous layer present at the interface in these well-bonded areas. Cavities ranging in size from a few tens of nanometers to a few tens of micrometers were also observed at the fused interface. The cavities extended only into the GaAs, and were usually elongated along the \([110]_{\text{GaAs}}\) direction. Plan-view images revealed dislocation networks in the well-bonded areas. One network appeared to arise from unintentional tilts between the fused crystals and the second network formed due to the mismatch in thermal expansion coefficients between GaAs and GaN. We did not observe dislocation networks originating from lattice mismatch or twist between the fused crystals. These and further studies are critical for a detailed understanding of the mechanisms of wafer bonding and the application of this process to device fabrication.

The research at Lawrence Berkeley National Laboratory (LBNL) was supported by AFSOR-ISSA-99-0012 under the sponsorship of Dr. G. Witt and that at the University of California at Santa Barbara (UCSB) by the DoD Multidisciplinary University Research Initiative (MURI) program administered by the Office of Naval Research under Grant No. 14-98-1-0654. The TEM group (J.J. and Z.L.-W.) would like to thank W. Swider for excellent sample preparation, Professor J. Washburn for fruitful discussions, and the National Center for Electron Microscopy (NCEM) at LBNL for the opportunity to use the NCEM’s facilities. The authors would like to thank A. Huntington and L. Coldren, and A. Stonas and S. DenBaars of UCSB for the growth of GaAs and GaN, respectively.