# Nanometer-scale studies of nitride/arsenide heterostructures produced by nitrogen plasma exposure of GaAs

R.S. Goldman and R.M. Feenstra
Department of Physics, Carnegie Mellon University, Pittsburgh, Pennsylvania 15213
B.G. Briner<sup>\*</sup>
IBM Research Division, Yorktown Heights, New York 10598
M.L. O'Steen and R.J. Hauenstein
Department of Physics, Oklahoma State University, Stillwater, Oklahoma 74078

## Abstract

We have investigated the nanometer-scale structure and electronic properties of nitride/arsenide superlattices produced by nitridation of a molecular beam epitaxially grown GaAs surface. Using cross-sectional scanning tunneling microscopy and spectroscopy, we find that the nitrided layers are not continuous films, but consist of groups of atomic-scale defects and larger clusters. We identify the defects and clusters as  $N_{As}$  and GaN with dilute As concentration, respectively. Thus, the nitrided regions consist of alloys from both sides of the miscibility gap predicted for the GaAsN system. In addition, spectroscopy on the clusters reveals an upward shift of the band edges and band gap narrowing, with significant change in the conduction band structure. We estimate the contribution of strain to band gap narrowing in terms of an elasticity calculation for a coherently strained spherical GaN cluster embedded in GaAs.

# I. Introduction

Nitride-based III-V compound semiconductor heterostructures are promising for optoelectronic devices, such as blue light-emitting diodes<sup>1</sup> and lasers.<sup>2</sup> In principle, mixed anion nitride/arsenide alloys would enable the fabrication of light emitters operating in the entire visible spectrum. However, for the GaAsN system, calculations predict a limited miscibility of N in GaAs,<sup>3</sup> and experiments have presented conflicting results concerning the formation of GaAsN alloys. Apparently, thick layers (>0.5 µm) of dilute GaAs<sub>1-x</sub>N<sub>x</sub> (x  $\leq 0.03$ ) alloys have been produced by nitride growth,<sup>4,5</sup> and attempts to increase the nitrogen composition in the alloy using GaAs surface nitridation resulted in GaAs/GaN/GaAs thin-layer structures<sup>6</sup> and  $\delta$ -GaAs<sub>1-x</sub>N<sub>x</sub>/GaAs superlattices (0.04  $\leq$  x  $\leq$ (0.33).<sup>7,8</sup> The identification of the nitride/arsenide structures as binary or ternary alloys has relied upon x-ray diffraction (XRD), which has spatial resolution of hundreds of  $\mu m$ and averages over many surface layers parallel to the interfaces. Similarly, crosssectional transmission electron microscopy (XTEM) images may represent an average over many surface layers perpendicular to the interfaces of interest.<sup>9</sup> Thus, standard interpretations may lead to misleading results in terms of ternary alloy formation if the structures are not continuous films of homogeneous material. Therefore, a detailed study of the atomic-scale structure and electronic properties at nitride/arsenide interfaces is essential for the understanding of alloy formation in this materials system.

<sup>\*</sup> Present address: Fritz-Haber-Inst. der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin, Germany.

In this paper, we present cross-sectional scanning tunneling microscopy (STM) and spectroscopy investigations of GaN/GaAs superlattices produced by nitridation of a molecular beam epitaxially (MBE) grown GaAs surface. Our cross-sectional studies indicate that the nitrided layers are not continuous films, but consist of regions with sparse N content and larger clusters. Analysis of x-ray diffraction data in terms of fractional area of clusters and N point defects reveals a cluster lattice constant slightly larger than cubic GaN, indicating that the nitrided regions consist of GaN with a few percent As incorporated in the alloy. Spectroscopic studies on the atomic-scale defects reveal a state in the conduction band associated with an acceptor level of  $N_{As}$  in GaAs, which allows us to identify the defects as  $N_{As}$ . The observed regions with dilute N in GaAs and dilute As in GaN, indicate alloying from both sides of the miscibility gap predicted in the GaAsN system.<sup>3</sup>

In addition, spectroscopy on the clusters reveals an upward shift of the band edges due to band bending at the cluster/GaAs interface and band gap narrowing which may be associated with the few percent As in highly strained GaN. We estimate the band gap narrowing due to strain using an elasticity calculation for a coherently strained spherical GaN cluster embedded in GaAs.

The paper is organized as follows. Section II describes the experimental procedures, including growth conditions. STM images and spectroscopy are presented and discussed in section III. Conclusions are given in section IV. In the Appendix, we present an elasticity calculation for a coherently strained spherical cluster of GaN embedded in GaAs, and a computation of band gap shifts resulting from the strain.

## **II. Experimental Procedures**

The samples were prepared using a combination of solid Ga and As<sub>2</sub> effusion and ECRplasma-excited N<sub>2</sub> sources; details of the growth apparatus have been described elsewhere.<sup>7</sup> Thirty-six period superlattices were produced by a 3-step process, based on the principle of N-As surface anion exchange, which consisted of (1) 4 second exposures of the (001) GaAs surface to a radical-nitrogen flux, (2) 100 second overgrowth of GaAs (simultaneous exposures to Ga, As<sub>2</sub>, and Si fluxes), and (3) 30 second ``As-soak" (As<sub>2</sub> flux only). This sequence was expected to result in monolayers of GaAs<sub>1-x</sub>N<sub>x</sub> separated by spacers of 200 Å Si-doped (N<sub>d</sub>  $\approx$  5 x 10<sup>18</sup> cm<sup>-3</sup>) GaAs. During the growth and nitridation of the samples described in this paper, the substrate temperature typically ranged from 540-560°C. Reflection high energy electron diffraction patterns obtained during surface nitridation revealed a specular, commensurate (3x3) pattern, suggesting coherent growth. Simulations of XRD data suggested that the structures consist of coherently strained superlattices, with monolayer thickness GaAs<sub>0.79</sub>N<sub>0.21</sub> embedded in 192 Å GaAs layers.

For STM studies, the samples were cleaved to expose a (110) surface, in an ultra-high-vacuum chamber with base pressure  $< 5 \times 10^{-11}$  Torr. STM was performed with both electrochemically etched single crystal <111>-oriented W tips. The tips were cleaned by

in-situ electron bombardment and characterized by in-situ field-emission microscopy. Images were obtained with a constant tunnel current of 0.1 nA, and sample bias voltages as described below. Details of the STM design,<sup>10</sup> cleavage procedure,<sup>11</sup> and spectroscopic methods<sup>12</sup> have been described previously.

## **III. Results and Discussion**

Figures 1 and 2(a) show STM topographic images of the GaN/GaAs superlattices, displayed with the growth direction from right to left. In these empty state images, the nitrided regions appear as depressions (darker regions) in the surrounding GaAs (brighter regions). We will show in Fig. 3 that these dark features are not pits in the surface – they correspond to regions with different electronic structure. The large-scale image in Fig. 1, acquired at sample bias voltage of +2.2 V, indicates that the nitrided layers are laterally inhomogeneous, consisting of regions with sparse nitrogen content (N point defects) and larger clusters. In Figs. 2(a) and (b), we present high-resolution topographic and conductance (dI/dV) images (acquired simultaneously) showing one nitrided layer in a region with sparse nitrogen content. In Fig. 2(a), fringes with a spacing of 5.65 Å, corresponding to the (001) lattice planes of GaAs, are observed in the bright regions of the image. In both Figs. 2(a) and (b), it is evident that the point defects are distributed over a thickness > 30 Å. This observation is in agreement with the layer smearing observed by XTEM (in similar samples) and predicted by the model of Bandic et al.<sup>9</sup> However, the XTEM study showed no evidence of clustering. This may be due in part to the insensitivity of TEM to the clusters due to averaging effects, or to differences in the samples due to variations in growth conditions such as substrate temperature.

In Fig. 3, we show a panel of STM topographic and conductance images of the filled and empty states. Each image contains four nitrided layers, displayed with the growth direction from right to left. Figs. 3(a) and (b) correspond to topographic and conductance images of the empty states, acquired simultaneously at +1.8 V sample bias. In these empty state images, the point defects appear dark in both topography and conductance, while the clusters appear dark in topography and bright in conductance. The filled state topographic and conductance images, acquired simultaneously at -2.0 V sample bias, are shown in Figs. 3(c) and (d). In this case, the clusters appear bright in topography and dark in conductance. Since the contrast of the point defects and clusters is dependent on the sign of the bias voltage, both features are of electronic rather than topographic origin. Thus, the dark (bright) features in the empty (filled) state images are not pits protrusions) in the surface but instead regions with different electronic structure.

In order to quantify the nitrogen content in the structures, we have determined the fractional area of clusters and point defects in several large-scale images such as Fig. 1. For the clusters, we used an algorithm to count pixels in regions of the image with tip height below a specified value. We estimated a tip height (depth) criterion based on the tip height profile in the vicinity of a cluster. This is discussed in detail in Ref. 13, where we defined a tip height cutoff as the depth at which the atomic corrugation is not observed, approximately 2 Å below the unperturbed GaAs regions. Here, we have modified our analysis to include the fractional area of N point defects. We limit our

cluster counting to regions with cluster area, > 1 nm<sup>2</sup>, and the modified cluster fractional area is  $f_{1} = 3.80 \pm 0.05 \times 10^{-3}$ . The fractional area of N point defects is determined by assuming each N point defect occupies a single (110) GaAs surface unit cell (5.65 Å x 4.00 Å). The resulting fraction of N point defects is  $f_{pd} = 1.40 \pm 0.05 \times 10^{-3}$ . High resolution x-ray diffraction data of these GaN/GaAs superlattices indicates an average superlattice out-of-plane d-spacing,  $d_{sl} = 5.6436$  Å, previously interpreted in terms of (continuous) coherently-strained monolayers of GaAs<sub>0.79</sub>N<sub>0.21</sub> embedded in 192 Å GaAs layers.<sup>7</sup> With the knowledge of the fractional area of the clusters and point defects, we determine the out-of-plane d-spacing of the clusters from the following

$$d_{sl} = f_{cl} d_{cl} + f_{pd} d_{pd} + (1 - f_{cl} - f_{pd}) d_{GaAs} .$$
(1)

We assume that the clusters are coherently strained, and use linear elasticity to estimate a cluster lattice constant of 4.60  $\pm$  0.05 Å, similar to the lattice constant of cubic GaN, 4.5 Å.<sup>14</sup> Using a linear interpolation of GaAs and GaN lattice constants, this corresponds to 9% As incorporated into the alloy, GaAs<sub>0.09</sub>N<sub>0.91</sub>. Since N point defects distributed over a thickness about 30 Å produce an alloy with very dilute N concentration, and the clusters consist of an alloy with dilute As concentration, we conclude that the nitrided regions consist of alloys from both sides of the miscibility gap.

In order to chemically identify the atomic-scale defects and clusters, we performed spectroscopic measurements on individual defects and clusters of various sizes. In Figs. 4(a) and (b), the normalized conductance versus sample bias voltage are plotted for an atomic scale defect (GaAs:N) and large cluster (lateral extent > 50 Å), respectively, and compared with regions of clean GaAs. The GaAs spectra, shown at the bottom of both figures, display well-defined band edges (the band edge positions are determined by assuming a linear onset in the normalized conductance),<sup>15</sup> with a band gap of  $1.43 \pm 0.10$  eV, comparable to that of bulk GaAs. The nonzero conductance within the GaAs gap in Fig. 4(b) is the "dopant-induced" component, which arises from electrons tunneling out of filled conduction band states.<sup>15</sup> In Fig. 4(a), the spectrum corresponding to atomic scale defects displays well-defined band edges and band gap similar to GaAs. However, in this case, a state is observed at  $0.40 \pm 0.05$  eV above the conduction band edge. The position of this state with respect to the conduction band edge is consistent with the predictions of Wolford et al.<sup>16</sup> for N isoelectronic traps in GaAs. Therefore, we associate the state with an acceptor level of N<sub>As</sub> in GaAs, and identify the atomic-scale defects as N<sub>As</sub>.

In Fig. 4(b), the spectrum corresponding to a large cluster displays several features which are different from the clean GaAs spectrum. The most prominent difference is the reduced band gap of  $1.23 \pm 0.10$  eV, which is significantly smaller than band gaps of GaAs (1.43 eV) and GaN (3.5 eV). Recently, a number of theoretical works have predicted band gap bowing in the GaAs<sub>1-x</sub>N<sub>x</sub> alloy system.<sup>3,17-19</sup> The calculated bowing parameters would suggest that the reduced band gap corresponds to a few percent nitrogen or arsenic in GaAs<sub>1-x</sub>N<sub>x</sub>. However, our analysis of x-ray diffraction data discussed earlier suggests that the clusters are nearly pure GaN. Thus, the band gap reduction is due in part to the few percent As in GaN with additional reduction due to the high lattice-mismatch strain between the clusters and GaAs. For a coherently strained

GaN cluster embedded in GaAs, we estimate a band gap in the range 0 to 1.7 eV (for cluster shape ranging from a rectangular film to a sphere),<sup>20-22</sup> which is also considerably smaller than the bulk GaN band gap. We estimate the band gap of the GaN clusters as follows. We calculate the strains in GaN clusters embedded in GaAs, misfit strain  $\varepsilon_f = (a_{GaAs} - a_{GaN}) / a_{GaN} = 0.26$ , using a Poisson ratio,  $v = C_{12} / (C_{11} + C_{22}) = 0.34$  based on elastic constants calculated for cubic GaN.<sup>20</sup> The details of the strain calculation are given in the Appendix. For a rectangular film of GaN, we find strains  $\varepsilon_{xx} = \varepsilon_{yy} = \varepsilon_f = 0.26$  and  $\varepsilon_{zz} = -[2v/(1-v)]\varepsilon_f = -0.27$ . For a sphere of GaN, we find strains  $\varepsilon_{xx} = \varepsilon_{yy} = \varepsilon_{zz} = [2(1-2v)/3(1-v)]\varepsilon_f = 0.08$ , independent of sphere radius. We calculate the shift of the band gap from that of bulk GaN following Ref. 21, using the shear deformation potential of cubic GaN.<sup>19,22</sup> The details of the band gap computations, including a table of constants, are given in the Appendix.

In addition to the reduced band gap, the band edges of the cluster spectrum are shifted upwardly in comparison to the GaAs spectrum. Similar effects are observed in spatially resolved spectroscopy of a small cluster (lateral extent < 50 Å), as will be shown in Fig. 5, where the band edges are shifted upward as one moves towards the GaAs/cluster interface. The band edge shifts are attributed to electrostatic charging which results in band bending at the cluster/GaAs interface, similar to that observed previously in studies of arsenic precipitates in low-temperature GaAs.<sup>23</sup> The upward shift of the band edges of the cluster is consistent with the contrast observed in the bias-dependent images shown in Fig. 3. Another interesting feature of the cluster spectrum is the reduced slope of the normalized conductance at the conduction band edge, which indicates a reduction in the conduction band density of states.

In Fig. 5, we present spatially-resolved spectroscopy across a small cluster (lateral extent < 50 Å). The data was taken as follows: first, the bottom half of the STM image was acquired; next, a set of spectra (a) - (e) were taken at the points labelled in the image; finally, the top half of the image was acquired. Spectrum (a), which was acquired on clean GaAs, has well defined band edges, with a band gap comparable to that of bulk GaAs. As one moves towards the GaAs/cluster interface, spectrum (b), the band edges shift upward due to the electrostatic charging effect mentioned earlier. Spectrum (c) was taken on the cluster, and has many features similar to those of the large cluster spectrum shown in figure 3(b), including narrowing of the band gap, upward shifting of the band edges, and reduced conduction band density of states (in comparison with clean GaAs). For this small cluster, the appearance of the conduction band edge is somewhat different than that measured on a large cluster. Here, additional states introduced from the conduction band edge narrow the band gap. These states at the conduction band edge appear to be a broadened version of the conduction band state associated with the individual Nitrogen atoms mentioned earlier. It is likely that in this small cluster, the states introduced from the conduction band are forming the beginning of the band of states observed in the large cluster spectrum of figure 3(b). Moving away from the cluster, spectrum (d), located near the cluster/GaAs interface has upwardly shifted band edges. Finally, spectrum (e), acquired on clean GaAs, displays well defined band edges and band gap comparable to bulk GaAs.

#### **IV. Conclusions**

In summary, we have studied the atomic-scale structure and electronic properties of GaN/GaAs superlattices produced by nitridation of a MBE-grown GaAs surface. Our cross-sectional STM imaging reveals laterally inhomogeneous layers, consisting of regions with sparse N content and larger clusters. Using the fractional area of clusters and N point defects (determined from large-scale STM images) to analyze x-ray diffraction data, we identify the clusters as GaN with dilute As incorporation. In addition, using tunneling spectroscopy measurements of the defects, we find a conduction band state associated with an acceptor level of  $N_{As}$  in GaAs, and identify the defects as  $N_{As}$ . These results indicate that the nitrided layers contain alloys from both sides of the miscibility gap predicted for the GaAsN system. In addition, band gap narrowing and band edge shifts are observed, and attributed to lattice-mismatch strain and band bending at the cluster/GaAs interface, respectively. Finally, we estimate the contribution of strain to the band gap narrowing, using an elasticity calculation for a coherently strained spherical GaN cluster embedded in GaAs. The calculation is applicable to any strained-layer materials system with appropriate geometry.

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## Appendix Strain Calculation

We consider the stress and strain produced in a spherical inclusion of one material imbedded in another material with different lattice constant. The boundary conditions between the inclusion and the surrounding material (i.e. the matrix) are such that an equal number of lattice planes of each material are joined together, as pictured in Fig. 6. This problem is a special case of the more general problem of ellipsoidal inclusions considered by Eshelby.<sup>24</sup> However, because of some differences in the definition of starting quantities between his case and ours, we first rederive the result for a spherical inclusion below, and we then demonstrate its equivalence with the result of Eshelby.

We assume isotropic media, with identical elastic constants in the inclusion and the matrix. As an *ansatz* of the solution to the elasticity equations for the displacements in the materials when they are joined, we consider purely radial displacements of the form

$$\vec{u} = Ar^n \, \hat{e}_r \tag{A1}$$

$$=A(x^{2} + y^{2} + z^{2})^{\frac{y}{2}}(x\hat{e}_{x} + y\hat{e}_{y} + z\hat{e}_{z})$$
(A2)

for constants A and n. From Eq. (2) we compute the strains,

$$\boldsymbol{e}_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right), \tag{A3}$$

and from the strains we obtain the stresses  $\mathbf{s}_{ij}$ .<sup>25</sup> The stresses must satisfy  $\sum \partial \mathbf{s}_{ij} / \partial x_j$  =0, from which we find solutions for *n* of *n* = 1 and *n* = -2. The former corresponds to the solution within the inclusion, and the latter to the solution in the matrix.

The boundary condition between inclusion and matrix requires an equal number of lattice planes of each. Referring to Fig. 6(a), we have

$$\Delta R = R \frac{\Delta a}{a} = R \, \boldsymbol{e}_{\mathrm{f}} \tag{A4}$$

where  $\Delta a$  is the difference between lattice constants of matrix and inclusion, a is the lattice constant of the inclusion, and  $\mathbf{e}_{f} \equiv \Delta a/a$  is the misfit strain. Then, the requirement that the inclusion and matrix fill the space between them leads to the equation, to lowest order in  $\Delta a$ ,

$$AR - \frac{B}{R^2} = \Delta R \tag{A5}$$

so that

$$A - \frac{B}{R^3} = \boldsymbol{e}_{\rm f} \tag{A6}$$

where A denotes the prefactor in Eq. (A1) for the inclusion and B denotes the prefactor for the matrix. A second boundary condition is that the normal component of the stress is continuous across the boundary, leading to the equation

$$A = -\frac{B}{R^3} \frac{2(1-2n)}{1+n}$$
(A7)

where  $\boldsymbol{n}$  is the Poisson ratio of the materials. Solving Eqs. (A6) and (A7) we find that

$$A = \frac{2(1-2n)}{3(1-n)} e_{\rm f},$$
 (A8)

which is independent of *R*. The resulting strain in the inclusion is simply  $\boldsymbol{e}_{xx} = \boldsymbol{e}_{yy} = \boldsymbol{e}_{zz} = A$ .

Comparing our solution with that of Eshelby,<sup>24</sup> we note that there are two differences in the way that the problem is defined. His starting point for the inclusion is that it has a size equal to that of the *unstrained* cavity. It then undergoes a "stress-free strain"  $e^{T}$  to transform to the size corresponding to the starting size of our inclusion, Fig. 6(a). Thus, this stress-free strain is related to our misfit strain by

$$\boldsymbol{e}_{ij}^{\mathrm{T}} = -\boldsymbol{d}_{ij} \, \boldsymbol{e}_{\mathrm{f}} \tag{A9}$$

In addition, Eshelby's definition of strain of the inclusion is made relative to the size of the unstrained cavity, whereas we use the natural definition for strain in our case as being relative to the unstrained size of the inclusion. Thus, we expect that the difference between our result and Eshelby's would yield simply  $e_f$ , the misfit between inclusion and matrix. For the spherical inclusion Eshelby finds for the strain

$$\widetilde{\boldsymbol{e}}_{\mathrm{XX}} = \frac{(1+\boldsymbol{n})}{3(1-\boldsymbol{n})} \boldsymbol{e}_{\mathrm{XX}}^{\mathrm{T}}$$
(A10)

and similarly for  $\tilde{e}_{yy}$  and  $\tilde{e}_{zz}$ . Subtracting this result from that given in Eq. (A8), we do indeed find a difference of  $e_f$ .

#### **Band Gap Computation**

We calculate the band gap shifts resulting from strain following Ref. 19. We include the valence band shift

$$\boldsymbol{d} E_{001} = 2b(\boldsymbol{e}_{ZZ} - \boldsymbol{e}_{XX}) \tag{A11}$$

where b is the shear deformation potential. Positive values of  $dE_{001}$  result in an upward shift of the valence band edge, and a reduction in band gap. In addition, we include the band gap shift

$$\Delta E_g = (a_c - a_v) [\boldsymbol{e}_{xx} + \boldsymbol{e}_{yy} + \boldsymbol{e}_{zz}]$$
(A12)

where  $(a_c - a_v)$  is the hydrostatic deformation potential. For this term, positive values of  $\Delta E_g$  result in a larger band gap. The parameters used for these computations, including elastic constants, lattice constants, and deformation potentials are listed in Table I.

#### Table I

Elastic constants, lattice constants, and deformation potentials of cubic GaN, used for strain and band gap computations.

Parameter (units)	Value
C <sub>11</sub> (GPa)	296 <sup>20</sup>
C <sub>12</sub> (GPa)	154 <sup>20</sup>
a (Å)	4.5 <sup>14</sup>
$(a_{\rm c} - a_{\rm v})$ (eV)	-7.32, <sup>19</sup> -8.1 <sup>22</sup>
b (eV)	$-1.6^{20}$

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FIG 1 Large-scale topographic images of GaN/GaAs superlattices, acquired at a sample voltage of +2.2 V. The grey-scale range displayed is 2.1 Å.

**FIG 2** High resolution (a) topographic and (b) conductance images acquired simultaneously at a sample voltage of +2.4 V. The grey-scale range displayed in (a) is 0.6 Å.



FIG 3 Panel of voltagedependent images. The empty state images shown in (a) and (b) are topography and conductance images, acquired at a sample voltage of +1.8 V. The filled state images shown in (c) and (d) are topography and conductance images, acquired at a sample voltage of -2.0 V



**FIG 4** STM spectra acquired on (a) atomic scale defect (GaAs:N) and (b) large cluster (lateral extent > 50 Å), in comparison with regions of clean GaAs. The valence and conduction band edges are marked by  $E_V$  and  $E_C$ , respectively. In (a), the state associated with an acceptor level of N<sub>As</sub> in GaAs is indicated by a downward pointing arrow. The sample voltage corresponds to the energy of the state relative to the Fermi level.



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FIG 6 Illustration of the strain induced in an inclusion when it is epitaxially bonded into a cavity of material with different lattice constant. The radius of the inclusion is R, and the difference in radius between cavity and inclusion is  $\Delta R$ . The lines in the figures represent the position of lattice planes, with (a) showing the structure before joining the two materials, and (b) showing the resulting displacements when they are joined.