Band gaps of the dilute quaternary alloys GaN$_x$As$_{1-x-y}$Bi$_y$ and Ga$_{1-y}$In$_y$N$_x$As$_{1-x}$

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We report strong band gap photoluminescence at room temperature in dilute quaternary GaN$_x$As$_{1-x-y}$Bi$_y$ alloys ($x \leq 1.6\%$, $y \leq 2.6\%$) grown by molecular beam epitaxy. The band gap of the alloy can be approximated by the band gap of GaAs minus the reduction in gap associated with the effects of N and Bi alloying individually. A one-parameter method for fitting the composition dependence of the band gaps of dilute quaternary semiconductor alloys is proposed which is in excellent agreement with data for Ga$_{1-y}$In$_y$N$_x$As$_{1-x}$. © 2005 American Institute of Physics.

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The photoluminescence (PL) and electroreflectance (ER) data for one of the samples, Ga$_{0.0085}$As$_{0.9775}$Bi$_{0.014}$, are shown in Fig. 1. The band gap of the sample is 1.10 eV as measured by ER, in good agreement with the PL emission at 1.08 eV. Qualitatively, the photoluminescence is strong, especially given the absence of a capping layer and the fact that no attempt was made to optimize the growth conditions.

800 W/cm$^2$. The electroreflectance was measured as discussed earlier. The photoluminescence (PL) and electroreflectance (ER) data for one of the samples, Ga$_{0.0085}$As$_{0.9775}$Bi$_{0.014}$, are shown in Fig. 1. The band gap of the sample is 1.10 eV as measured by ER, in good agreement with the PL emission at 1.08 eV. Qualitatively, the photoluminescence is strong, especially given the absence of a capping layer and the fact that no attempt was made to optimize the growth conditions.

Figure 2 presents the (004) x-ray diffraction pattern for this sample (upper pattern), as well as a dynamical simulation indicating that it is nearly lattice matched to GaAs. Previous RBS results$^5$ for this sample showed that the Bi content was not uniform but increased with depth below the surface, which may account for the absence of pendellosung fringes in the experimental data. Experimental and simulated x-ray spectra are also presented for a second sample, Ga$_{0.0155}$As$_{0.9725}$Bi$_{0.012}$. The position of the diffracted peak corresponding to this layer indicates that it is under tensile strain relative to the GaAs substrate, consistent with the higher nitrogen content of this sample.

Conventional fits to the composition dependence of the band gaps of ternary III–V semiconductor alloys, with quadratic bowing parameters, do not accurately describe the bandgap of the dilute nitride alloy GaN$_{1−x}$As$_x$Bi$_y$ as a function of N content. Although band gaps can be calculated from underlying physical properties by theoretical methods such as the band-anticrossing model,$^5$ tight binding theory$^1$ or density functional theory,$^2$ these methods typically involve multiple parameters and relatively complex computations that are inconvenient or not sufficiently accurate for device design. As a simple fitting procedure we propose the following mathematical expression with one adjustable parameter, which parameterizes the bandgap of the dilute nitride quaternary alloys as a function of composition in an intuitive way:

\[ E_{\text{aN}}(x,y) = E_{\text{GaAs}} - \Delta d(x) - \gamma \Delta N(x) \Delta d(y). \] (1)

In this expression $E_{\text{aN}}(x,y)$ is the band gap of the quaternary alloy Ga$_{1−x}$In$_x$N$_y$As$_{1−y}$Bi$_z$ ($a=$In) or Ga$_{x}$N$_{1−x}$As$_y$Bi$_z$ ($a=$Bi), $E_{\text{GaAs}}$ is the band gap of GaAs, and $\Delta d(x)$ is the reduction in the band gap of GaAs associated with N alloying for concentration $x$. Similarly, $\Delta N(x)$ or $\Delta b(y)$ represents the change in band gap associated with In (or Bi) alloying of GaAs, and $\gamma$ is an adjustable coupling parameter used to match the experimental data.

If $\gamma=0$, then in the case of In and N alloying for example, the band gap of the quaternary alloy GaInNAs will be equal to the band gap of GaAs minus the sum of the reductions associated with In and N alloying measured independently in the corresponding ternary alloys. Similarly, if $\gamma>0$, then the effect of the two alloying elements will be greater than the sum of the two elements separately. A feature of Eq. (1) is that it maintains the same shape for the concentration dependence of the band gap as the ternary compound if the concentration of one of the elements is held fixed. The $\Delta$-functions are determined from fits to the experimentally determined composition dependence of the band gaps of the ternary alloys.
wavelength devices can be grown lattice matched to GaAs with relatively low concentrations of Bi and N.

A positive coupling parameter for co-alloying with Bi and N was previously predicted theoretically by Janotti et al., although they used a rather different form for the composition dependence which does not translate into the coupling parameter in Eq. (1). Their theoretically predicted bandgap for a sample with 2% Bi and 2% N is 1.22 eV at 0 K, somewhat larger than the 0.95 eV predicted for room temperature in Fig. 4. The ~300 K temperature difference should account for almost half of the difference between the two values.

In summary, the dilute nitride-bismide alloy Ga0.97In0.03As1−yBi, grown by MBE on GaAs substrates, shows strong band gap photoluminescence at room temperature. We fit the composition dependence of the band gap of the quaternary alloy with a parameterization scheme based on the band gaps of the corresponding ternary alloys, and a single adjustable parameter. This parameterization scheme is in excellent agreement with experimental data on the Ga0.97In0.03As1−y dilute nitride alloys, and predicts optical emission at 1.55 μm for a Ga0.97In0.03As1−yBi alloy lattice matched to GaAs, with x=2% and y=3.5%.

14G. E. Pikus and G. L. Bir, Sov. Phys. Solid State 1, 1502 (1960). The modification of the band gap due to strain (e) was taken to be (2πC11−C12)/C11−b(C11+2C12)/C11 e, where a and b are the hydrostatic and tetragonal-shear deformation potentials respectively and C11 are the appropriate elastic constants. Parameter values were obtained by linear interpolation from GaAs and InAs data published by I. Vurgaftman, J. R. Meyer, and L. R. Ram-Mohan [J. Appl. Phys. 89, 5815 (2001)]. Compressive strain was defined to be negative.