Variation of refractive index in strained $In_xGa_{1-x}As$-GaAs heterostructures

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$In_xGa_{1-x}As$-GaAs heterostructures and strained-layer superlattices can be used as optical waveguides. For such applications it is important to know explicitly the refractive index variation with mismatch strain and with alloying in the ternary layer. Starting from the Kramers–Kronig integral dispersion relations, we have developed a model from which the refractive index change in the ternary layer of $In_xGa_{1-x}As$-GaAs heterojunctions can be calculated. The results are presented and discussed. The expected changes in a superlattice have been qualitatively predicted.

I. INTRODUCTION

Since the demonstration of optical waveguiding in GaAs beneath a stripe window due to built-in strain by Kirkby and co-workers,[1] interest has been focused on the strain-induced change of refractive index in heterojunction epilayers and double heterojunction structures. Ongoing work is mainly related to $In_xGa_{1-x}As_yP_{1-y}/InP$[2–5] and $Al_xGa_{1-x}As/GaAs$[6–8] since they can be easily grown as near-lattice-matched epitaxial layers. Linear relationships between strain and the refractive-index step were obtained by Olsen *et al.*[4] for a $InP/In_xGa_{1-x}As_yP_{1-y}/InP$ structure. However, since larger strains were not considered by them and other authors, the change in refractive index has been attributed almost entirely to the change in alloy composition. Broberg and Lindgren[5] have observed that a lattice mismatch, Δ_a/a_0, of $+10^{-3}$ corresponds to an increase of refractive index of roughly 0.02 compared to that in a perfectly matched layer. The change of composition with mismatch could not be measured accurately enough by these authors, and no definite conclusion regarding the role of strain on the change of refractive index was made. On the other hand, in a strained-layer superlattice (SLS) it is relatively easy to change the strain in the layer for a fixed alloy composition by varying the layer thickness. Thus it is possible to obtain the change of refractive index due to strain alone when the alloy composition remains unchanged.

Strained-layer superlattices are of particular interest for opto-electronic device applications because it allows tailoring of the effective band gap by proper selection of superlattice parameters without the constraint of working with lattice-matched materials, within certain limits. Opto-electronic devices such as lasers, LEDs, solar cells and detectors using InGaAs/GaAs SLS have been fabricated recently.[9–12] Photoluminescence measurements made on them indicate good structural integrity.[13] Therefore strain guides using intentionally strained single layers or superlattices would be useful materials for passive optical components to be coupled with active devices in an optically integrated circuit. Calculations for asymmetric waveguides[14] show that a refractive index step of ~ 0.001 is necessary for optical confinement at a wavelength of ~ 0.89 μm with a guide thickness of 3 μm. However, for higher wavelengths and smaller thicknesses the refractive index step necessary is at least one order higher. This is not easily achieved with a striped geometry structure. $In_xGa_{1-x}As/GaAs$ SLS are potentially excellent materials for this purpose as InAs has the highest refractive index amongst the common III-V binary semiconductors. Marzin and Rao[15] have performed absorption measurements on $In_xGa_{1-x}As/GaAs$ strained quantum well heterostructures, and an analysis was performed to fit the data. However, the change in refractive index with strain was not presented. Moreover, the effect of strain in the GaAs layer was neglected in their analysis. This approximation is not valid for very thin SLS structures.

We have calculated the refractive index change in single $In_xGa_{1-x}As$-GaAs strained heterostructures caused by alloying and by strain. To our knowledge, the explicit determination of these two components has not been done before. It is found that the contribution to the index change due to strain is much smaller than that due to alloying. It should be realized, however, that any suitable thickness of a single $In_xGa_{1-x}As$ strained layer on a GaAs substrate for use in guiding or modulation cannot be grown. This is made possible by a SLS, where higher x values in the well regions can be used. We have used the same theoretical approach to calculate the refractive index steps in single heterojunctions where the GaAs and strained $In_xGa_{1-x}As$ layers have thicknesses comparable to that in a SLS. The effects of quantization in such a superlattice have not been included in the model, but have been qualitatively discussed.

II. THEORETICAL CONSIDERATIONS

Previous theoretical work with strained-layer heterostructures and superlattices[12,16,17] indicates that strain decreases the band gap of the lower band-gap material and increases the band gap of the higher band-gap material. Applying a similar reasoning to $In_xGa_{1-x}As/GaAs$ strained layers the change in the different band gaps, as shown in Fig. 1, are given by[16]

$$\Delta E_0(1) = \left[-2a\left(\frac{C_{11}-C_{12}}{C_{11}}\right) + b\left(\frac{C_{11}+2C_{12}}{C_{11}}\right)\right]\epsilon, \tag{1a}$$

$$\Delta E_0(2) = \left[-2a\left(\frac{C_{11}-C_{12}}{C_{11}}\right) - b\left(\frac{C_{11}+2C_{12}}{C_{11}}\right)\right]\epsilon, \tag{1b}$$

and

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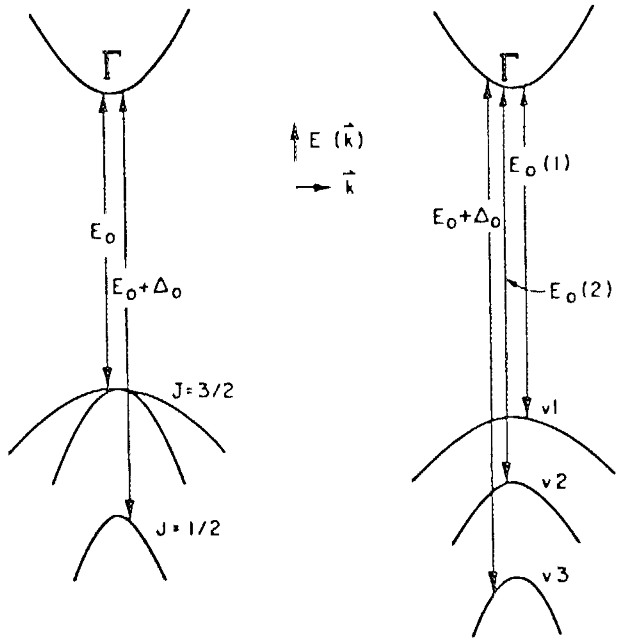

FIG. 1. Upper valence bands and lowest conduction band in diamond (zincblende) crystals in the absence (left) and in the presence (right) of uniaxial stress.

$$\Delta(E_0+\Delta_0) = -2a\left(\frac{C_{11}-C_{12}}{C_{11}}\right)\epsilon \qquad (1c)$$

where $\Delta E_0(1)$, $\Delta E_0(2)$, and $\Delta(E_0+\Delta_0)$ are the shifts of the heavy-hole, light-hole, and spin-orbit-split valence bands, respectively, due to the combined effects of hydrostatic and shear stress, with respect to the conduction band. ϵ is the biaxial strain parallel to [100] and [010] directions, and a and b are the hydrostatic and shear deformation potential constants, respectively. The strain in the layers is calculated using

$$\epsilon = (S_{11}+S_{12})\sigma, \qquad (2)$$

where σ is the compressive biaxial stress and S_{ij} is the compliance constants of the material. The stress in the two layers were calculated from[18]

$$\sigma_1 = 2G_1\left(\frac{1+\gamma_1}{1-\gamma_1}\right)f^2\left(\frac{a_1}{a_2}+\frac{a_2}{a_1}\frac{G_1h_1}{G_2h_2}\right)^{-2}, \qquad (3a)$$

$$\sigma_2 = 2G_2\left(\frac{1+\gamma_2}{1-\gamma_2}\right)f^2\left(\frac{a_2}{a_1}+\frac{a_1}{a_2}\frac{G_2h_2}{G_1h_1}\right)^{-2} \qquad (3b)$$

where G_i are the shear moduli[19] given by

$$G_i = 2\left(C^i_{11}+C^i_{12}-\frac{2(C^i_{12})^2}{C^i_{11}}\right) \qquad (4)$$

and a_i, h_i, γ_i are the lattice constant, thickness, and Poisson's ratio, respectively, in the layers and C_{ij} is the material stiffness constant. Here, $i=1$ and 2 represent (InGa)As and GaAs, respectively, and f is the misfit factor. The parameters a and b for (InGa)As were linearly interpolated from available data for GaAs[20,21] and InAs.[22,23] Values of a_i, C^i_{11}, and C^i_{12} were also obtained from similar interpolation.[24]

For relatively pure materials the effect of dispersion of the real part of the dielectric constant due to free carriers will be small and, as shown by Itoh *et al.*,[25] the discrete excitonic contribution to the real part of the dielectric constant is small for GaAs and InAs. Thus for GaAs and InAs, which have a M_0 critical point at $k=0$, the real part of the dielectric constant can be written as[26]

$$\epsilon_r(\omega) = A\left[f(\chi_0)+\frac{1}{2}\left(\frac{E_0}{(E_0+\Delta_0)}\right)^{3/2}f(\chi_{s0})\right]+B, \quad (5)$$

where

$$\chi_0 = \frac{\hbar\omega}{E_0}, \quad \chi_{s0} = \frac{\hbar\omega}{(E_0+\Delta_0)},$$

and

$$f(\chi_i) = \frac{1}{\chi_i^2}\left[2-(1-\chi_i)^{1/2}-(1+\chi_i)^{1/2}\right].$$

Here, $i=0$ and $s0$ for the minimum band gap and the spin-orbit-split band gap at $k=0$,

$$A \sim \frac{4}{3}\frac{e^2\hbar^{1/2}}{m_0^2\epsilon_0}\left(\frac{2\mu}{\hbar}\right)^{3/2}P^2E_0^{-3/2}$$

and B is a nondispersive contribution from the higher lying bands similar to ϵ_∞. ω is the angular frequency of the incident radiation, $\hbar$ is the reduced Planck's constant, m_0 is the free-electron mass, ϵ_0 is the permittivity of free space, μ is the combined density of states mass, E_0 is the minimum direct band gap, Δ_0 is the spin-orbit-splitting, and P^2 is the average matrix element squared.[27] Due to splitting of the $J=3/2$ valence band with shear stress, Eq. (5) can be modified with a third term in the square brackets. The modified equation will reduce to the form of Eq. (5) as the shear is reduced to zero. The value of A calculated for GaAs[26] was found to be four times lower than that obtained by fitting Eq. (5) to experimental data of $\epsilon_r(\omega)$. In view of this discrepancy we have used values of A and B obtained by fitting Eq. (5) to the $\epsilon_r(\omega)$ data for GaAs[28] and InAs.[3] The values of A and B for (InGa)As were then obtained from an interpolation of the binary data. Bowing parameters were used to calculate the values of E_0 and $(E_0+\Delta_0)$ for different alloy compositions of (InGa)As. The values used in the analysis are listed in Table I.

In the region near and below the band gap, absorption can be neglected, and the refractive index can be expressed by

$$n(\omega) \simeq [\epsilon_r(\omega)]^{1/2}. \qquad (6)$$

Using this equation the refractive indices for GaAs and $In_xGa_{1-x}As$ were obtained for different wavelengths of the

TABLE I. Binary data used in the calculations.

Parameter	GaAs	InAs
E_0(eV)	1.425	0.36
$E_0+\Delta_0$(eV)	1.76	0.796
C_{11}(dyne/cm^2)	11.88×10^{11}	8.329×10^{11}
C_{12}(dyne/cm^2)	5.38×10^{11}	4.526×10^{11}
C_{44}(dyne/cm^2)	5.94×10^{11}	3.96×10^{11}
a_0(Å)	5.64191	6.0584
a(eV)	−9.8	−5.0
b(eV)	−1.76	−1.8
A	6.64	4.36
B	9.2	10.52

incident radiation. The difference gives the refractive index step. It should be remembered that the evaluation of this parameter is only valid when the band gap is close to but higher than the incident photon energy.

III. RESULTS AND DISCUSSION

The variation of refractive index, compared to that in GaAs, in a single $In_xGa_{1-x}As$ layer is shown in Fig. 2. Two cases have been considered. In the first it is assumed that the ternary layer is strain-free, and in the second the effect of mismatch with a GaAs substrate (infinite thickness) is considered. It is seen that strain causes an additional increase of refractive index, though the effect is small compared with that for alloying.

It is known that even for $x = 0.2$, the thickness of the ternary layer that can be grown on GaAs is only a few hundred angstroms, before dislocations are generated in the strained layer. Therefore to use the large change in refractive index, as demonstrated in Fig. 2, in a practical waveguiding structure, it is necessary to use multiple layers of GaAs and $In_xGa_{1-x}As$ in a superlattice configuration. As a starting point we have therefore considered GaAs-$In_xGa_{1-x}As$ heterostructures in which the respective layers are of thicknesses similar to those in a strained-layer superlattice. Figures 3(a) and 3(b) depict the calculated values of strains in the ternary and binary layers of the heterostructure for different combinations of layer thickness. These thicknesses are indicated in the caption and are represented by various data points. It is seen that the strain in one type of layer in a heterostructure decreases with an increase of the layer thickness, when the thickness of the other type of layer is held constant. This trend agrees with the results of Osbourn[17] obtained from a study of $GaAs_yP_{1-y}$ SLS. The corresponding refractive index steps as a function of layer thickness are shown in Fig. 4.

From linear interpolation between GaAs and InAs, it can be seen that a 1% lattice mismatch exists between GaAs and $In_{0.14}Ga_{0.86}As$. The data of Fig. 4 indicate that for this amount of mismatch and the corresponding x value, the refractive index step at a wavelength of 1.13 μm is $\sim$0.06, which is slightly greater than that obtained by Olsen *et al.*[4] for a InP-(InGa)(AsP) lattice-matched heterostructure. The data in Figs. 3(a) and 4 indicate that a refractive index step greater than 0.02 due to strain alone can be achieved for $x = 0.2$ with a change in strain of 8×10^{-3} in the $In_{0.2}Ga_{0.8}As$ layer. On the other hand, Fig. 4 also shows that for $x = 0.2$ the total refractive index step is $\sim$0.14. Thus the contribution to the change in refractive index by alloying alone and that due to added strain are explicitly obtained. Laidig *et al.*[29] have shown that defect-free epitaxial growth of $In_xGa_{1-x}As$ is possible up to $x = 0.38$ for layer thicknesses $\sim$100 Å. This would give higher values of the refractive index step with the transparent region near a wavelength $\sim$1.5 μm.

It should be stressed that the usefulness of ternary lay-

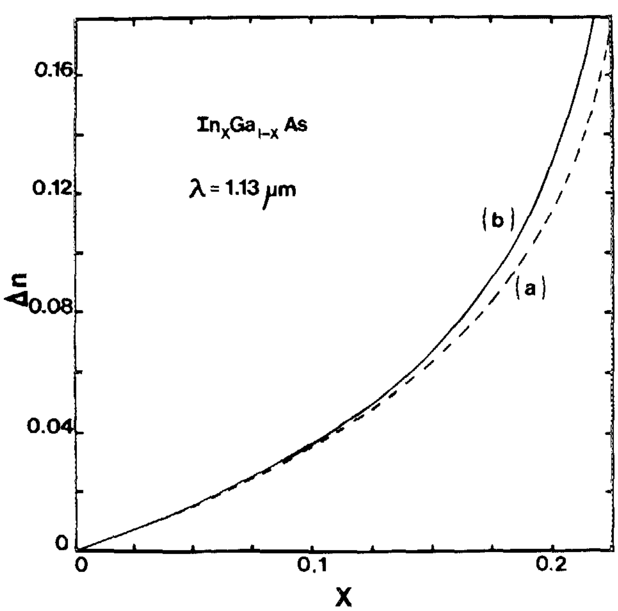

FIG. 2. Variation of refractive index with composition in (a) a strain-free layer of $In_xGa_{1-x}As$ and (b) in the same layer grown with mismatch induced strain on a GaAs substrate. In case (b) it is assumed that the thickness of the ternary layer is less than the critical value above which dislocations are induced.

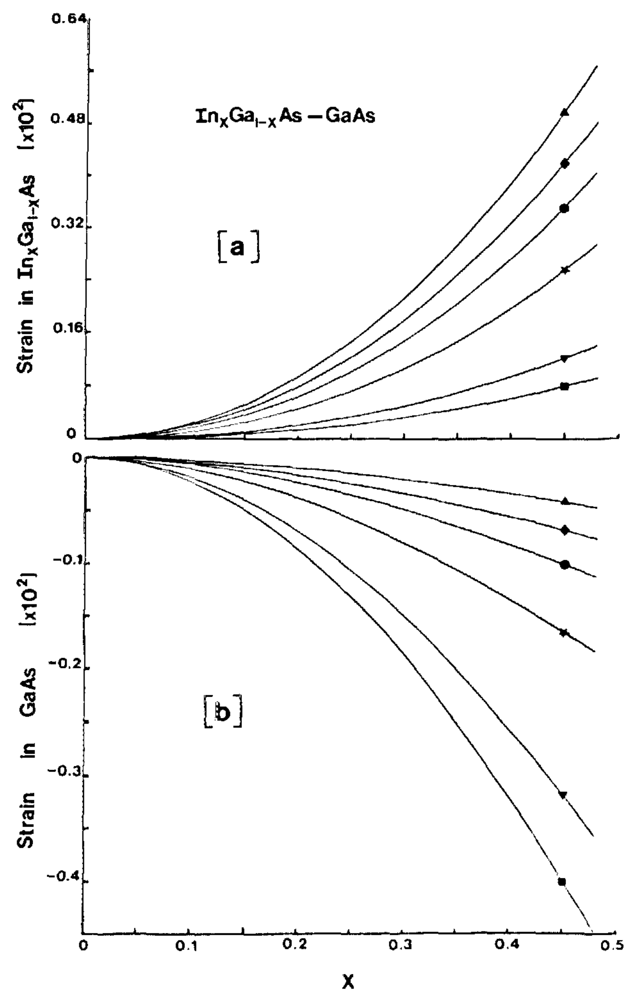

FIG. 3. Strain in the $In_xGa_{1-x}As$ layer (a) and GaAs layer (b) for the following combination of thicknesses indicated by representative symbols: (▲) (InGa)As = 25 Å, GaAs = 70 Å; (◆) (InGa)As = 50 Å, GaAs = 100 Å; (*) (InGa)As = 70 Å, GaAs = 70 Å; (▼) (InGa)As = 100 Å, GaAs = 50 Å; (■) (InGa)As = 70 Å, GaAs = 25 Å; and (●) (InGa)As = 30 Å, GaAs = 45 Å.

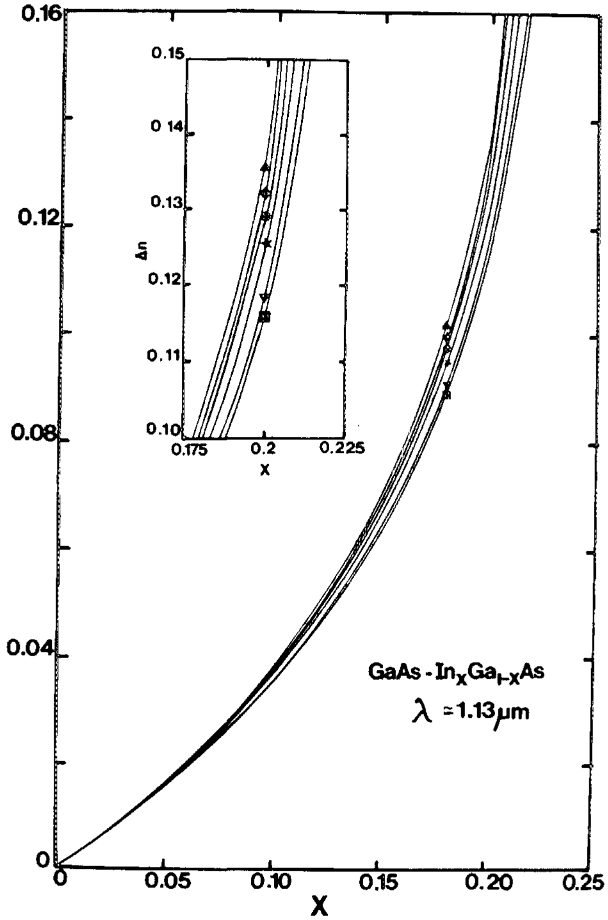

FIG. 4. Refractive index step between $In_xGa_{1-x}As$ and GaAs for different values of x as indicated by the representative symbols: (▲) $In_xGa_{1-x}As$ = 25 Å, Ga As = 70 Å; (◆) $In_xGa_{1-x}As$ = 50 Å, GaAs = 100 Å; (*) $In_xGa_{1-x}As$ = 70 Å, GaAs = 70 Å; (▼) $In_xGa_{1-x}As$ = 100 Å, GaAs = 50 Å; (▩) $In_xGa_{1-x}As$ = 70 Å, GaAs = 25 Å; and (●)$In_xGa_{1-x}As$ = 30 Å; GaAs = 45 Å. The inset shows an enlarged view of the characteristics around $x = 0.2$.

ers with large x, giving a large refractive index change, can only be realized in a superlattice structure. It is not clear how meaningful the parameter Δn, as calculated here, remains for a superlattice. It can only be said, with some caution, that the calculated Δn will be a measure of the effective refractive index in a superlattice. Size quantization effects also need to be taken into account in a superlattice. Leburton and Hess[30] have recently calculated the average refractive index in GaAs-AlAs superlattices. They have shown that the refractive index $\bar{n}$ increases with the decrease of superlattice composition defined by $\bar{x} = L_B/(L_B + L_Z)$, where L_B and L_Z are barrier and well thicknesses, respectively. The order of the variation in $\bar{n}$ is less than the values of Δn calculated by us. However, their results indicate that quantization effects may play a more dominant role than strain effects in changing the refractive index.

IV. CONCLUSIONS

The effects of alloying and strain on single mismatched $In_xGa_{1-x}As$-GaAs heterostructures have been calculated. Calculations for $0 \leqslant x \leqslant 0.25$ indicate that the effect of alloying is more pronounced. For example, at $x = 0.2$, the effect of alloying produces a change in refractive index which is $\simeq 10$ times that produced by mismatch strain. The mismatched ternary layers can be used in strained-layer superlattices to constitute efficient optical guiding layers. Size quantization effects in superlattices need to be taken into account.

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