Excitonic energies and inhomogeneous line broadening effects in InAlAs/InGaAs modulator structures

S. Hong and J. Singh
Department of Electrical Engineering and Computer Science, The University of Michigan, Ann Arbor, Michigan 48109-2122

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The exciton problem in the $In_{0.52}Al_{0.48}As/In_{0.53}Ga_{0.47}As$ quantum well in the presence of static transverse electric field is studied. We report results on variation of exciton size, binding energies, and emission energies as a function of electric field and well size. Inhomogeneous line broadening of exciton lines due to interface roughness and alloy disorder is also calculated. Alloy disorder in the well and barrier regions is found to be very important and its control may be critical in the performance of this system as a high efficiency modulator.

I. INTRODUCTION

The study of excitonic properties in quantum wells in the presence of a static transverse electric field has drawn considerable interest due to the new physics concepts involved and potential applications for optical modulators and switches.[1-6] Although a considerable effort has focused on the AlGaAs/GaAs system,[7-10] much less experimental or theoretical work has been done on the InAlAs/InGaAs modulator structure. The primary reason for this appears to be lack of sharp excitonic features in the InAlAs/InGaAs quantum-well structures due to inhomogeneous line broadening effects presumably arising from the alloy and interface quality. For example, while excitonic features with linewidths ~ 0.1 meV have been observed in the AlGaAs/GaAs quantum wells,[11] typical excitonic features in InAlAs/InGaAs quantum wells have linewidths of ~ 10 meV.[12-15] An important area of technology where excitonic transitions play an important role is the area of optical modulation and switching. Exciton lines which have large inhomogeneous broadening will have obvious detrimental effects on the device performance. For example, if the exciton linewidth is of the order of the energy shifts produced by static electric fields used in optical modulators, the modulator efficiency will be extremely poor.

In this paper we address the exciton problem in an InAlAs/InGaAs quantum well in presence of a static transverse electric field. In particular, we focus on the exciton binding energy, exciton emission energy, electron and hole tunneling rates, exciton radius, and volume, as well as the inhomogeneous line broadening of excitonic transitions. These basic properties of excitons are extremely important for applications of quantum wells in high-speed modulation and as nonlinear optical elements. A number of different approaches have been used to address the problem of excitons in a quantum well in the presence of transverse static electric field. We use an approach which can be used not only for square quantum well, but for arbitrarily shaped quantum wells as well. The exciton problem is solved using the following approach: (i) the solution of the electron (hole) subband levels is obtained by either numerically integrating Schrodinger equation or by a variational approach based on Monte Carlo techniques; (ii) the exciton problem is solved variationally using the electron and hole states obtained from (i) above; (iii) the inhomogeneous broadening of the exciton transition is calculated for interface roughness and alloy disorder. In this paper, we present results for the square well, although the method is applicable to an arbitrarily shaped well. In Sec. II, we describe the exciton problem and our approach, and in Sec. III we present the results. Discussions and conclusions are presented in Sec. IV.

II. THE EXCITON PROBLEM

The Hamiltonian of an exciton in electric field in a $In_{0.53}Ga_{0.47}As$ slab between two $In_{0.52}Al_{0.48}As$ layers grown along the (001) direction can be expressed as[16,17]

$$H = -\frac{\hbar^2}{2\mu_\pm}\left(\frac{1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho}+\frac{1}{\rho^2}\frac{\partial^2}{\partial\phi^2}\right) - \frac{\hbar^2}{2m_e}\frac{\partial^2}{\partial z_e^2} - \frac{\hbar^2}{2m_h}\frac{\partial^2}{\partial z_h^2} - \frac{e^2}{\epsilon|r_e - r_h|} + V_{ew}(z_e) + V_{hw}(z_h) + eEz_e - eEz_h . \quad (1)$$

Here we use the effective mass approximation, neglecting the heavy-hole and light hole coupling and effective mass mismatch between well and barriers, which is valid when well size is larger than 50 Å. m_e and m_h are the effective mass of the conduction-band electron and the valance-band hole, respectively. These two exciton systems are nondegenerate since the degeneracy of the valance band of GaAs is removed due to reduction in symmetry along the z axis. $\mu_\pm$ is the reduced mass corresponding to heavy-hole (+) or light hole (−) bands in the plane perpendicular to the z axis. $\mu_\pm$ can be expressed in terms of the well-known Kohn–Luttinger band parameters.[18,19] In the above equation we have not accounted for the kinetic energy of center of mass because we are only interested in the state which can be accessed optically. We have also assumed the same values for the static dielectric constant in the two semiconductors. The appropriate dielectric constant is taken to be $\epsilon = \sqrt{\epsilon_\omega \epsilon_b}$, where ϵ_ω, ϵ_b are the dielectric constants of the well and barrier, respectively. This comes from a consideration of the equivalent dielectric continuum for thin wells and barriers of equal width. The potentials such as $V_{ew}(z_e)$ for electron and $V_{hw}(z_h)$ for hole can be arbitrarily confining potentials, which give rise to bound or quasibound states. The energy due to the electric field on electrons (eEz_e) and holes (eEz_h) can be treated as additional potentials. It is clearly impossible to solve directly for the Schrodinger equation associated with exciton Hamiltonian [Eq. (1)] either analytically or numerically. Therefore, we assume that the exciton trial wave function can be factored as[20]

$$\Psi = \Phi_e(z_e)\Phi_h(z_h)\exp(-\rho/\lambda) , \qquad (2)$$

where $\Phi_e(z_e)$, $\Phi_h(z_h)$ are determined exactly by applying numerical methods to the one-dimensional potential well problem describing z axis confinement of electrons and holes. The exponential factor is an envelope function which we choose to be a simple 1s like orbital in-plane radial motion of the exciton. Previous calculations have indicated that this simple trial function is accurate for the well thickness of our interest ($\geqslant$50 Å).[19] Here λ is a variational trial parameter for calculating the exciton binding energy. To determine $\Phi_e(z_e)$ and $\Phi_h(z_h)$, we use numerical techniques. Since we have already described the Monte Carlo approach,[21,22] we briefly outline the ordinary differential equation solving approach.

Inital and final conditions are chosen in a region $-L$ to $+L$ surrounding the well [($\Phi(-L)=0$, $\Phi'(-L)=0$ and $\Phi(L)=0$, $\Phi'(L)=0$, respectively]. Here L has a value larger than the extent of the function (we use $L\sim 2.5$ W). A quasibound level is then determined by solving the Schrodinger equation

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(\mathbf{k},z) + [V(z) \pm eEz]\Psi(\mathbf{k},z) = E\Psi(\mathbf{k},z) . \qquad (3)$$

It is important to realize that both these methods are straightforward methods and do not assume any starting wave functions.

We have applied the above techniques to calculate the electron and hole state and associated exciton wave functions for $In_{0.52}Al_{0.48}As/In_{0.53}Ga_{0.47}As$ quantum wells. We assume that the total band discontinuity of 650 meV across the interface is distributed in the conduction band and valence band in the ratio of 70% and 30%, respectively. In our calculations, we assume the electron, heavy-hole, and light hole masses to be $0.044m_0$, $0.44m_0$, and $0.036m_0$ (m_0 is free electron mass).[22] The reduced masses in the x-y plane for heavy hole and light hole are $0.023m_0$ and$0.032m_0$, respectively. Due to anisotropic nature of the kinetic energy, the reduced mass associated with the heavy-hole band is less than that of the light hole band in the direction perpendicular to the interface. The problem is solved in absence and presence of electric field.

A. Exciton binding energy

If a quantum well is exposed to light with energy above the effective band gap, electron and hole pairs are produced. The absorption energy is given by

$$E_{\rm ph} = E_e + E_h + E_g - E_b , \qquad (4)$$

where E_e and E_h are electron and hole subband energies in a quantum well, respectively; E_g is the band gap of the well material, i.e., $In_{0.53}Ga_{0.47}As$, and E_b is exciton binding energy. The electron and hole pairs form excitons due to the Coulombic interaction. The exciton can collapsed to produce photons with energy $E_{\rm ph}$. In the presence of an electric field, the electrons and holes are spatially separated so that electron and hole interaction reduced. This causes E_b to decrease. However, the change of E_b which is controlled by the overlap of the electron and hole wave functions is an order of magnitude smaller than the change produced in the values of E_e and E_h. To get exciton binding energy by variational method, first the expectation value of Hamiltonian [Eq. (1)] has to be calculated by calculating

$$E = \int\int\int \Psi^* H\Psi \times dz_e\, dz_h\rho\, d\rho \Big/ \int\int\int \Psi^*\Psi\, dz_e\, dz_h\rho\, d\rho \qquad (5)$$

and minimizing as a function of the trial parameter λ. The binding energy E_b is then obtained by subtracting $E_{\rm min}$ from total ground-state energy of electron and hole.

B. Tunneling rate of electron and hole

In the presence of a transverse electric field, the electron and hole states of the quantum well are only quasibound states and have a nonzero probability of tunneling out of the well. These tunneling rates are important because (a) the electrons and holes that tunnel out cannot contribute to the exciton collapse and hence to photoluminescence and (b) the tunneling, which effectively removes the space charge from the quantum well and consequently "resets" the well in the optical modulation of a pulse stream of an optical signal, can eventually control the speed of optical modulation.

We have calculated the electron and hole subband levels and the associated energies and wave functions which allow us to calculate the tunneling probabilities. The tunneling rates can be evaluated either by WKB method (for the Monte Carlo approach which is variational in nature) or by the wave function in the numerical solution of the Schrodinger equation.[23]

C. Exciton volume

It is important to determine the spatial extent of the exciton in the quantum well. This information is important in understanding the broadening of the exciton line due to structural fluctuations in the quantum well. It is also important in calculating the light intensity at which excitons start overlapping with each other and causing very strong optical nonlinearities.

$$\Theta = \int\int\int \rho\, d\rho\, d\phi\, dz |\Psi|^2 \rho^2 |z| |\cos\theta\,|\sin\theta\,| . \qquad (6)$$

It is also useful to consider the fraction of the exciton volume in the barrier region versus the volume inside the well. The exciton in the barrier sees the material quality of the barrier which is often an alloy and causes broadening of the excitonic transition linewidth. With this motivation we have calculated the exciton volume in the barrier region and inside the well.

D. Inhomogeneous broadening of exciton transitions

The general method to treat the inhomogeneous line broadening is discussed in Ref. 24. The line broadening arises due to spatially localized fluctuations which are capable of shifting the exciton emission energy. In general, one may describe these fluctuations by concentration fluctuations in the mean compostions C_A^0, C_B^0 of the structure. For example, C_A^0 and C_B^0 may represent the height of the islands and the valleys representing interface roughness, or the mean composition of the alloy in the treatment of alloy broadening.

The probability of a concentration fluctuation C_A occuring over a region β, which is the exciton area for interface roughness studies and exciton volume for alloy disorder effects where β is used as a variational parameter, is

$$P(C_A,\beta,C_A^0) = \exp\left[-\frac{\beta}{\alpha}\left(C_A \ln \frac{C_A}{C_A^0} + C_B \ln \frac{C_B}{C_B^0} \right)\right], \quad (7)$$

where α is the smallest region over which the fluctuation can take place(= area of two-dimensional islands describing the interface roughness and the smallest cluster size for the alloy disorder. For a perfectly random alloy α is the Wigner Seitz cell volume.) The full width half maximum of the probability distribution of Eq. (7) is

$$\delta P = 2\sqrt{1.4 C_A^0 C_A^0 \alpha/\beta}\,. \quad (8)$$

The shift in the excitonic energy due to this fluctuation is then the linewidth of the exciton transition,

$$\sigma(\beta) = \delta P\,|\Psi|_\beta^2 \,\frac{\partial E_{\rm ex}}{\partial C}, \quad (9)$$

where $|\Psi|_\beta^2$ is the fraction of the exciton sensing the region β, and $\partial E_{\rm ex}/\partial C$ represents the rate of change in the exciton energy with concentration. To obtain the linewidth of the excitonic emission (absorption) one has to maximize $\sigma(\beta)$ allowing β to vary. Using the expression for the exciton wave function, it is straightforward to see that to a very good approximation we have for interface roughness:

$$\sigma_{\rm IR} = 2\sqrt{\frac{1.4 C_A^0 C_A^0 a_{2d}}{3\pi\lambda^2}\,\frac{\partial E_{\rm ex}}{\partial W}\bigg|_{W_0}\,\delta_0}\,, \quad (10)$$

where α_{2d} is the areal extent of the two-dimensional islands representing the interface roughness, δ_0 is their height, and λ is the exciton Bohr radius in the lateral direction parallel to the interface. $\partial E_{\rm ex}/\partial W$ is the change of the exciton energy as a function of well size. For alloy broadening due to composition fluctuations inside the well (for $W_0 \leqslant \sim 200$ Å),

$$\sigma_{\rm alloy}^{\rm internal} = 2\sqrt{\frac{1.4 C_A^0 C_A^0 V_c}{3\pi\lambda^2 W_0}\,\frac{\partial E_{\rm ex}}{\partial C_A}\bigg|_{C_A^0}}\,. \quad (11)$$

For large wells, the W_0 in the equation approaches 3λ. For alloy broadening due to fluctuations outside the well,

$$\sigma_{\rm alloy}^{\rm internal} = 2\sqrt{\frac{1.4 C_A^0 C_A^0 V_c}{3\pi\lambda^2 L_{\rm eff}}\,\frac{\partial E_{\rm ex}}{\partial C_A}\bigg|_{C_A^0}\,\delta_0}\,, \quad (12)$$

where $L_{\rm eff}$ is an effective length to which the exciton wave function penetrates in the barrier and has to be calculated numerically. $L_{\rm eff}$ is approximately equal to twice the distance over which the exciton wave function falls to $1/e$ of its initial value. Typically, this is of the order of a few monolayers.

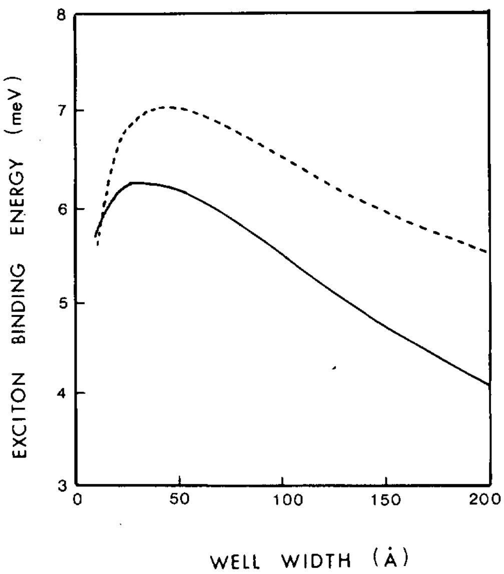

FIG. 1. Variation of light (dashed) and heavy (solid) hole exciton binding energy as a function of well size in a $In_{0.52}Al_{0.48}As/In_{0.53}Ga_{0.47}As$ quantum well.

For the calculations reported here, we use $C_A^0 = C_B^0 = 0.5$ assuming that there are equal fractions of islands and valleys at the interface. For the well region $C_A^0 = 0.53$, $C_B^0 = 0.47$ corresponding to $In_{0.53}Ga_{0.47}As$ for the barrier region corresponding to $C_A^0 = 0.52$, $C_B^0 = 0.48$ corresponding to $In_{0.52}Al_{0.48}As$.

III. RESULTS AND DISCUSSIONS

In this section we will present the results of our calculations and discuss these results. In Fig. 1 we present the results for the variation of light (dashed) and heavy (solid)

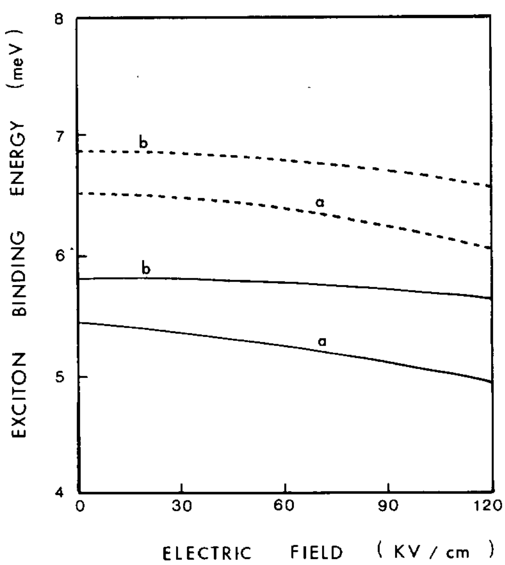

FIG. 2. Effect of electric field on the exciton binding energies of the light (dashed) and heavy hole (solid) excitons. Cases (a) and (b) are for a 100- and 70-Å well.

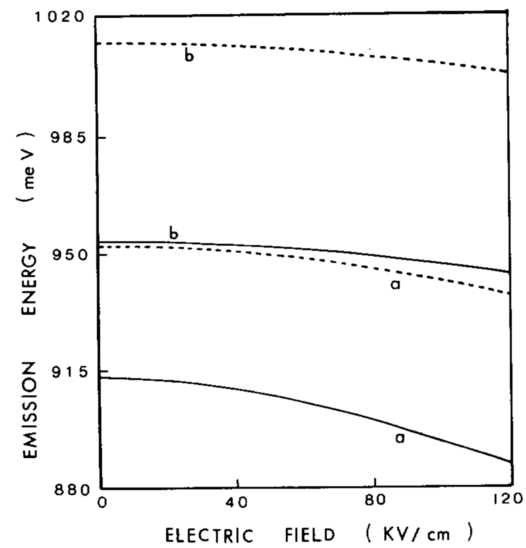

FIG. 3. Variation of light (dashed) and heavy (solid) exciton emission energy as a function of electric field. Cases (a) and (b) are for a 100- and 70-Å well.

exciton binding energies as a function of well size in absence of electric field in the $In_{0.52}Al_{0.48}As/In_{0.53}Ga_{0.47}As$ square well. Such variations have been reported by a number of workers for the AlGaAs/GaAs system. Note that the exciton binding energies in the InGaAs and GaAs systems are 2.01 and 4.2 meV for heavy-hole and 2.79 and 5.0 meV for light hole excitons, respectively. The maximum binding energy enhancement for the $Al_{0.3}Ga_{0.7}As/GaAs$ well occurs at ~40-Å well size is a factor of ~2.5 for the heavy-hole exciton.

For the InAlAs/InGaAs system the enhancement is much higher (~factor of 3) and the exciton binding energies are almost as high as for the AlGaAs/GaAs quantum wells for narrow wells even though in the large well limit there is a big disparity in the binding energies of the two systems. This greater enhancement is due to the higher band-gap discontinuity in the InAlAs/InGaAs system and is responsible for a number of other quantitative differences between the excitonic features of the two systems.

In Fig. 2 we show the effects of electric field on the exciton binding energies in a 100 Å (case a) and 70 Å (case b) quantum wells. By comparing these with the results of Fig. 3, it is clear that the variation in the emission energy is primarily due to the variation of the electron and hole subband levels. We find that variations of ~20 meV are observed for a 100 kV/cm field. These variations must be large compared to the excitonic linewidths if the structure is to function well as an optical modulator.

In Fig. 4 we plot the variation of exciton transverse radius as a function of electric field in a 100 Å (case a) and 70 Å (case b) quantum well. It is important to point out that the exciton radii for the large barrier limit case are 288 and 206 Å for the heavy and light hole excitons. The strong reduction of exciton size is again related to the large band discontinuity. As the electric field is increased, the exciton radius becomes larger due to the weaker Coulombic interaction between the electron and the hole states.

Figure 5 shows the tunneling rates for the electron and hole quasibound states. The higher band discontinuity lowers the electron and hole tunneling rates as compared to the $Al_{0.3}Ga_{0.7}As/GaAs$ modulator structure rates.[22] This suggests that a much higher electric field swing is required to remove the charges from the well region in the InAlAs/InGaAs system. This may have detrimental effect for the modulators where high-speed pulses are to be produced which will affect the exciton absorption.

In Fig. 6 we show the exciton linewidth in the InAlAs/InGaAs system well due to interface roughness ef-

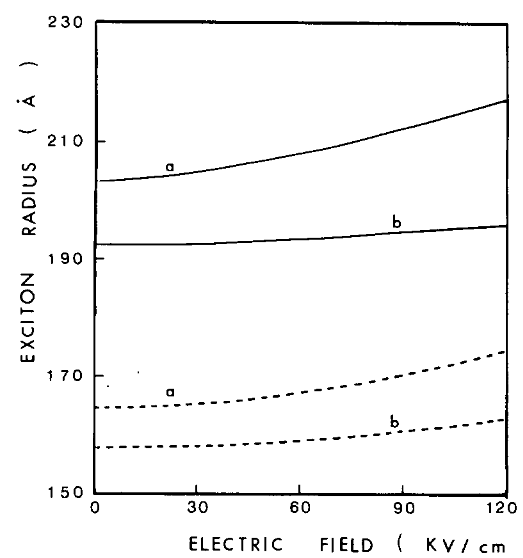

FIG. 4. Variation of light (dashed) and heavy (solid) hole exciton Bohr radius as a function of electric field for a 100-Å (case a) and 70-Å (case b) well.

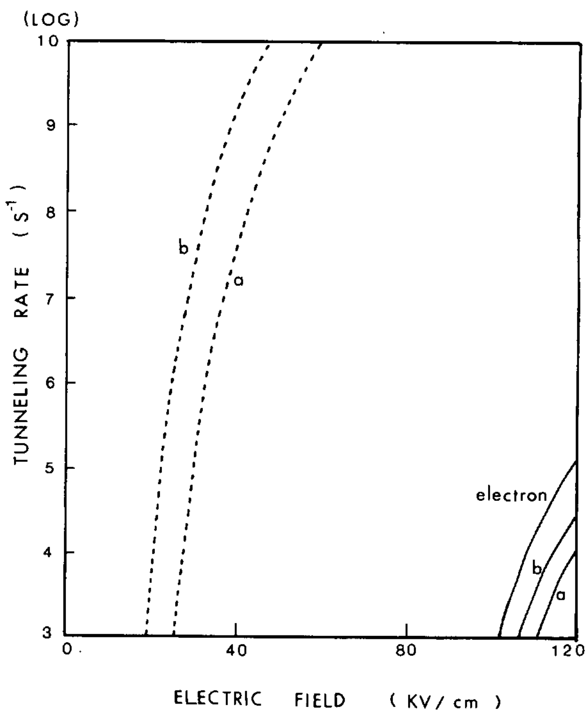

FIG. 5. Electron and hole tunneling rates vs transverse electric field. Solid lines stand for heavy hole and dotted lines for hole a for 100-Å well and b for light 70 Å.

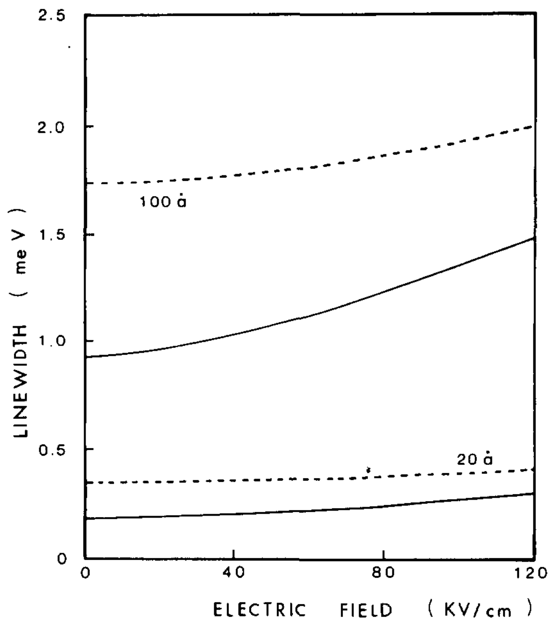

FIG. 6. Exciton linewidths due to interface roughness in a 100-Å well. Results are shown for one monolayer roughness with $2d$ island sizes of 20 and 100 Å.

fects. The results are shown for interface islands which are one monolayer ($\sigma = 1$ monolayer) and (a) 20-Å radius and (b) 100-Å radius. The solid and dashed lines are for heavy and light hole excitons. Note that even though the exciton radius increases with electric field, it increases faster so that the broadening increases with increased electric field. We note that lifetime broadening is much smaller than the interface roughness broadening. The interface broadening is very sensitive to the size of the islands and valleys, as can be expected from Eq. (10). Finally, in Fig. 7 we show the effect of alloy disorder on the heavy (solid) and light (dashed) excitonic linewidth. The results are shown for the broadening

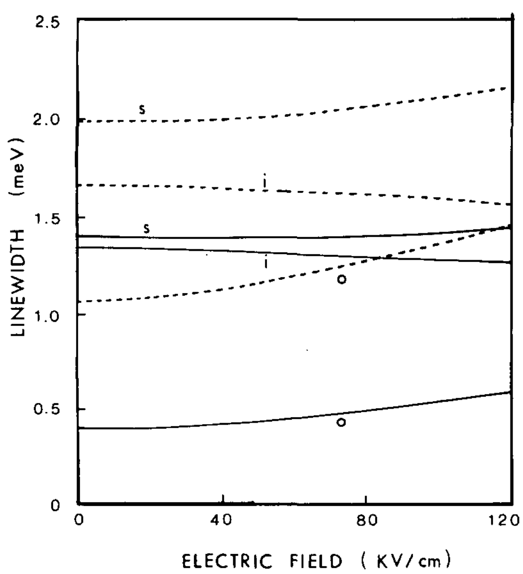

FIG. 7. Exciton linewidth due to alloy disorder assuming a perfect alloy. The solid and dashed lines represent the heavy and light hole excitons. The indices i, o, and s represent the inside contribution, outside contribution, and the total linewidth, respectively.

due to alloy disorder inside (i), and outside (o) the well region, and the sum (s). Here we assume that no clustering is present so that V_c is the Wigner Seitz cell volume. It is important to note that even for a 100-Å well there is a strong contribution of the barrier material to the inhomogeneous broadening. This is in fact quite disturbing because the InAlAs appears to show alloy clustering.[25] If InAlAs is clustered and V_c is larger than the Wigner Seitz cell, the inhomogeneous broadening will be much larger. Even for the perfect system, the linewidth due to alloy disorder is quite large and will smear out fine structure in the excitonic spectra. As noted earlier, the values of barrier contribution to the exciton linewidth are reported for perfectly random $In_{0.52}Al_{0.48}As$. If one uses instead the best available linewidth reported in bulk MBE grown $In_{0.52}Al_{0.48}As$ in the literature (which is ~ 15 meV in contrast to a theoretical limit of ~ 3 meV), one gets linewidths which are ~ 10 meV or more. The need for growth of high quality ternaries is thus obvious.

IV. CONCLUSIONS

In this paper we have discussed the exciton problem in the $In_{0.52}Al_{0.48}As/In_{0.53}Ga_{0.47}As$ system. An important difference between this system and the $Al_{0.3}Ga_{0.7}As/GaAs$ system (a widely studied system) is the higher band discontinuity and the presence of a ternary (InGaAs) in the well region. The enhancement in the exciton binding energy is substantial ($\sim$maximum factor of 3.0 from the bulk value). The exciton sizes in the narrow well case are comparable to those in the AlGaAs/GaAs system suggesting the strong exciton lines and optical nonlinearities. The tunneling rates for electrons and holes in the presence of a transverse electric field are low compared to the $Al_{0.3}Ga_{0.7}As/GaAs$ system, due to the higher band-gap discontinuity.

The contribution of interface quality and alloy disorder in the well and barrier region have also been studied in the modulator structure. Alloy disorder is found to be a very important source of line broadening. In particular we find that the quality of InAlAs is quite important. Even for a perfect system, the total inhomogeneous linewidth for a 100-Å well is ~ 1.5 meV so that the kind of fine structure seen in the photoluminescence of the AlGaAs/GaAs well may only be observed for extremely abrupt heterostructures. Finally, we note that use of thin period superlattices such as $(InAs)_m(AlAs)_m$ or $(InAs)_n(GaAs)_n$ with $n,m \leqslant 4$ monolayers may reduce the alloy disorder and lead to sharp exciton lines.

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