Optical Determination of the Heavy-hole Effective Mass of (In, Ga)As/GaAs Quantum Wells

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CONTENTS

ABSTRACT

We determine the reduced mass of heavy-hole exciton and the heavy-hole in-plane mass for a series of (In, Ga)As/GaAs strained layer quantum wells using the magnetoluminescence measurements of the exciton ground state and the modified perturbation approach. In the theoretical calculation of the magnetoexciton ground state, the exciton reduced mass is considered as an adjustable parameter, and two variation parameters are used in the unperturbed wave function which is expressed in terms of subband wave functions in the growth axis and the product of two-dimensional hydrogen and oscillatorlike wave functions for the in-plane component. We take into account the energy dependence of transverse and in-plane electron masses in the two-band effective mass approximation. The electron effective mass decreases as either quantum-well width or indium composition increases, and so does the heavy-hole in-plane mass down to the value at the decoupling limit ($m_{hh,\rho} = 0.11 m_0$).

I. INTRODUCTION

In recent years, opto-electronic properties of strained (In, Ga)As/GaAs quantum wells have been widely investigated because these structures play pivotal roles in providing basic understanding on low-dimensional systems and new concepts in various device applications such as quantum-well lasers, detactors, optical modulators, and strained quantum well field effect transistors(SQWFET) [1]. The importance of stained (In, Ga)As/GaAs quantum wells is that they provide structures with band gaps in the infrared spectral regions around 0.98μm. The laser chip operating at this wavelength is useful as a pump source for Er-doped fiber amplifier. Furthermore, as the compressive biaxial stain in the (In, Ga)As layer makes a considerable splitting between the heavy-hole ground state and the other light-hole states, the in-plane heavy-hole mass is small, and this also provides an adventage in laser and p-channel SQWFET applications. In making a good device, it is important to understand basic properties of materials such as the carrier effective masses, and many optical investigations employing various techniques have been devoted to determine the carrier effective mass in the doped or undoped (In, Ga)As/GaAs quantum wells[2]-[8] as well as lattice matched quantum well structures such as GaAs/(Al, Ga)As [9]-[12].

In our previous reports on theoretical studies [13], [14], we proposed a method to determine carrier effective masses bases on the diamagnetic shifts of magnetoexciton ground state in the presence of magnetic fields applied in the direction parallel to the growth axis. The binding energy and diamagnetic shifts of the exciton ground state are sensitive to both the confinement effect and exciton reduced mass. In the envelope-function approximation, we calculated magnetoexciton ground state considering the exciton reduced mass as an adjustable parameter and ignoring the valence-band mixing effect on this mass, and compared the calculated diamagnetic shifts for nonzero magnetic fields (B>0) with experimental results. This approach provided an excellent method for obtaining the in-plane carrier masses in both III-VI [13], [14] and IV-VI [15] quantum well structures. If the binding energy of the exciton is known experimentally, the exciton reduced mass can be determined in a rather simple method [14].

The purpose of this paper is to determine systematically the exciton reduced mass for a series of $In_xGa_{1-x}As/GaAs$ strained quantum wells within the indium composition range $x < 0.27$ for quantum well width 2.2 nm$<$ $L_z < 20$ nm. We calculate energy-dependent electron masses of strained (In, Ga)As quantum wells using the two-band effective-mass approximation [16] and determine the heavy-hole in-plane mass from the exciton reduced mass and the electron in-plane mass. The magnetoluminescence data used in this report were supplied by Wimbauer [17], and the detailed experimental setup can be found in [8]. In Section II, we briefly review the modified perturbation method for the magnetoexciton ground state in Type-I quantum well structures and some formula for the effective electron mass in the two-band effective approximation. In Section III, experimental results on a series of (In, Ga)As/ GaAs quantum wells and theoretical determination of carrier effective masses are discussed. Conclusion is given in Section IV.

II. THEORY

1. Modified Perturbation Method

In this section, we review a formalism of magnetoexciton ground state [13] that we developed for the determination of the exciton reduced mass in quasi two-dimensional type-I quantum wells. In our approach, the dispersion of the conduction and valence bands are considered to be parabolic within the effective-mass approximation. The effect of g-factor on the exciton energy is also ignored. We use the Bohr radius of the exciton in three dimensions a_0 as a unit of length, the corresponding Rydberg energy R^* as the energy unit, and the ratio of the cyclotron energy to the Rydberg energy as a dimensionless magnetic field γ:

$$a_0 = \frac{4\pi\epsilon_0\kappa\hbar^2}{\mu e^2}, \quad R^* = \frac{e^2}{8\pi\epsilon_0\kappa a_0}, \quad \gamma = \frac{eB\hbar}{2\mu R^*}, \tag{1}$$

where μ is the in-plane reduced mass of an exciton,

$$\frac{1}{\mu} = \frac{1}{m_{e,\rho}} + \frac{1}{m_{hh,\rho}}. \tag{2}$$

$m_{e,\rho}$ and $m_{hh,\rho}$ denote the in-plane effective masses of the electron and heavy-hole, respectively, and κ represents the mean value of the layer-dependent dielectric constant.

For quantum-well width comparable to the Bohr radius, the confinement effect due to the barrier potential in the growth axis can dominate the effective Coulomb interaction in this direction. In our formalism, the three dimensional Coulomb potential is approximated by a two-dimensional one denoted by V_ρ,

$$V_\rho = -\frac{2\eta}{\rho}. \tag{3}$$

The confinement effect due to the quantum-well potential and other defects may be represented by η the effective coupling constant of the Coulomb interaction between an electron and a hole forming an exciton. Then, η is associated with the structural parameters of the quantum well and represents the dimension of the exciton. We consider that η does not change even in the presence of a magnetic field. This means that once the value of η is calculated, the in-plane Hamiltonian for $B > 0$ does not contain any terms which are z-dependent, so the differential equation is two-dimensional. In other words the exciton diamagnetic shift is uniquely determined for given parameters η, reduced mass of an exciton, and dielectric constant.

In the presence of homogeneous magnetic field $\vec{B} = B\hat{z}$, applied in the direction parallel to the growth axis, the Schrödinger equation of the exciton at rest in two-dimensions may be written by

$$(H_{e,z} + H_{h,z} + H_\rho)\psi = E\psi, \tag{4}$$

where

$$H_{s,z} = \left[-\frac{\partial}{\partial z} \frac{\mu}{m_{s,z}(z)} \frac{\partial}{\partial z} + V_s(z) \right] \tag{5}$$

with $s = e,\ h$ for electron and hole Hamiltonians in the growth direction, respectively. For the exciton ground state, H_ρ, representing the Hamiltonian in the quantum-well plane, can be written in relative coordinates and restricted to the subspace of zero magnetic quantum number,

$$H_\rho = -\frac{\partial^2}{\partial \rho^2} - \frac{1}{\rho}\frac{\partial}{\partial \rho} + \frac{\gamma^2 \rho^2}{4} - \frac{2\eta}{\rho}. \tag{6}$$

As $H_{e,z}$, $H_{e,h}$ and H_ρ in Eq. (4) are independent with each other, the exciton wave function can be decomposed into the z and ρ components in the following form:

$$\psi(z_e, z_h, \rho) = \chi_e \chi_h \phi(\rho), \tag{7}$$

where χ_e and χ_h are eigenstates of

$$H_{s,z}\chi_s(z) = E_s \chi_s(z) \tag{8}$$

with $s = e,\ h$ for electron and hole states, respectively. For single quantum well structure, confined wave functions $\chi_s(z)$ have well-known analytic form consisting of sinusodial and damping exponential functions in the well and barrier regions, respectively. We consider that $\chi_s(z)$ and $(1/m_{s,z})\partial\chi_s(z)/dz$ are continuous at quantum well interfaces. The electron and heavy-hole effective masses in the growth axis are considered as layer dependent. Furthermore, electron effective mass in strained (In, Ga)As quantum wells is dependent on both the stress effect and the subband energy, which will be discussed in the next section. In Eq. (2), $m_{e,\rho}$ are assumed to be uniform in both well and barrier materials, and the following form is used to estimate mean values from the layer-dependent values:

$$\frac{1}{m_{e,\rho}} = \int dz\,|\,\chi_e(z)\,|^2 \frac{1}{m_{e,\rho}(z)}. \tag{9}$$

A similar formula is used for the calculation of the dielectric constant κ in Eq. (1).

Because the 2D Schrödinger equation using Hamiltonian in Eq. (4),

$$H_\rho \phi(\rho) = E_\rho \phi(\rho) \tag{10}$$

is not solved in simple analytic forms, we use a modified perturbation method employing two variational parameters λ and σ. The unperturbed radial wave function of the ground state exciton is given in the form

$$\phi^0(\rho, \lambda, \sigma) = \exp\left(-\frac{\gamma \rho^2}{4\sigma} - 2\lambda\rho \right). \tag{11}$$

After a lengthy calculation, the ground state energy, to be obtained by minimizing $< \phi^0 \mid H_\rho \mid \phi^0 > / < \phi^0 \mid \phi^0 >$ with two parameters, λ and σ, is simplified in the following form,

$$E_\rho = \min \left\{ \frac{\gamma}{2}\left(\sigma + \frac{1}{\sigma}\right) + 4\sigma^2\lambda^2 + 4\lambda^2 \left(1 - \frac{2\eta}{\lambda} - \sigma^2\right) \frac{U(1,\,\frac{3}{2};\,\xi)}{U(1,\,\frac{1}{2};\,\xi)} \right\}, \tag{12}$$

where

$$\xi = \frac{8\sigma\lambda^2}{\gamma} \tag{13}$$

and the confluent hypergeometric function

$U(a,\ b;\ \xi)$ is defined as [13]

$$U(a,\ b;\ \xi) = \frac{1}{\Gamma(a)} \int_0^\infty dt e^{-\xi t} t^{a-1} (1+t)^{b-a-1}. \tag{14}$$

2. Electron Masses in Two-band Effective-mass Approximation

To account for the nonparabolicity effect in the conduction band of a compressively strained (In, Ga)As quantum well grown along the [001] axis, we use energy-dependent longitudinal and in-plane masses of an electron, $m_{e,\ z}(E_e)$ and $m_{e,\ \rho}(E_e)$, obtained by a two-band effective-mass approximation[16] including the conduction and the degenerate valence band but neglecting the spin-orbit interaction and quadratic term in k in $k \cdot p$ Hamiltonian:

$$m_{e,z}(E_e) = m_e' \left(1 + \frac{E_e + \delta V_b}{E_g'}\right), \tag{15}$$

$$m_{e,\rho}(E_e) = m_e' \left(1 + \frac{E_e}{E_g'}\right), \tag{16}$$

where E_e is energy of electron from the bottom of the conduction band of the (In, Ga)As layer. m_e' represents the mass of electron due only to the change in the strained band-gap of bulk (In, Ga)As,

$$m_e' = m_e^0 \frac{E_g'}{E_g}, \tag{17}$$

where m_e^0 is the band-edge mass of untrained bulk (In, Ga)As. As a compressively strained (In, Ga)As layer has the valence band edge consisting of an heavy-hole state ($J_z = \pm 3/2$), the bulk strained band-gap, denoted by E_g', is given in terms of E_g^0, the bulk unstrained band-gap, and δE_g representing the energy shift due to deformation effects:

$$E_g' = E_g^0 + \left[-2a\frac{C_{11} - C_{12}}{C_{11}} + b\frac{C_{11} + 2C_{12}}{C_{11}}\right]\epsilon, \tag{18}$$

where a and b denote the difference between the hydrostatic deformation potentials of the conduction and valence bands and shear deformation potential in the valence band, respectively. ϵ is associated with the biaxial deformation constant of the strained layer, defined as

$$\epsilon = \frac{a_u - a_s}{a_u}, \tag{19}$$

where a_u and a_s are the untrained and strained lattice constants of materials, respectively. δV_b is the energy shift due the change in the cubic symmetry,

$$\delta V_b = -3b\frac{C_{11} + 2C_{12}}{C_{11}}\epsilon. \tag{20}$$

III. DISCUSSION

The material parameters of GaAs and InAs used in theoretical calculations are listed in Table 1. A linear interpolation was used for the $In_xGa_{1-x}As$ values. The band-gap energy at absolute zero temperature (T=0K) of bulk $In_xGa_{1-x}As$ was taken to be $E_g = 1.5192 - 1.45x + 0.35x^2$ eV, and the conduction band offset of (In, Ga)As/GaAs without strain effects was 45%. Ignoring the strain effect on the barrier height of the conduction band at (In, Ga)As/GaAs interfaces resulted the conduction band offset at a strained $In_xGa_{1-x}As$/GaAs interface to be 69% and

Table 1. Material parameters used in calculating the stress-dependent band gaps and electron effective masses in $In_xGa_{1-x}As$.

Material	a_u (Å)	C_{11} ($10^{11} dyn/\text{cm}^{-2}$)	C_{12}	a (eV)	b (eV)	m_e^0 (m_0)	$m_{hh,z}$ (m_0)	ϵ (ϵ_0)
GaAs	5.65325[1)]	11.88[1)]	5.32[1)]	−9.8[2)]	−1.76[2)]	0.0665[2)]	0.34[2)]	12.5[2)]
InAs	6.0583[3)]	8.33[3)]	4.53[3)]	−5.8[2)]	−1.8[2)]	0.023[2)]	0.32[2)]	14.6[2)]

[1)] Reference [19] [2)] Reference [20] [3)] Reference [21]

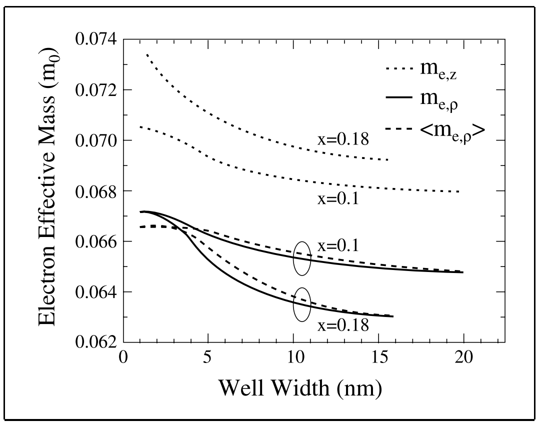

Fig. 1. Calculated electron effective masses as a function of the well width of $In_xGa_{1-x}As$/GaAs quantum wells with $x = 0.1$ and 0.18. $m_{e,z}$ and $m_{e,\rho}$ denote the longitudinal mass and the in-plane mass of the (In, Ga)As quantum well layer, respectively, while $< m_{e,\rho} >$ is the mean in-plane mass obtained by using Eq. (9).

67% for $x = 0.1$ and 0.18, respectively. These results are approximately the same with other reports [4], [22]. As the energy for the electron in a GaAs layer with respect to the band edge of the GaAs barrier can be neglected compared to the band-gap, we take $m_e(E_e) = 0.0665m_0$ in GaAs, where m_0 is the bare electron mass.

In Fig. 1, we display electron effective masses of (In, Ga)As/GaAs quantum wells as a function of well width and indium composition. $m_{e,z}$ and $m_{e,\rho}$ denote electron longitudinal and in-plane masses in (In, Ga)As/GaAs quantum well, respectively, while $< m_{e,\rho} >$ is associated with the mean value of the in-plane electron mass calculated using Eq. (9). As the well width decreases, both the longitudinal and in-plane masses increase due to increasing nonparabolicity in the conduction band. As (In, Ga) As well width approaches to zero, the electron in-plane mass becomes approximately equal to that of GaAs ($0.0665m_0$). This is understood by that subband wave functions spread into the GaAs barrier layer as well width decreases and therefore the contribution of the GaAs layer on the electron mass increases. As δV_b in Eq. (20) is positive for a compressively strained (In, Ga)As quantum well, the longitudinal mass of electron is heavier than the in-plane mass and the difference between the two increases as indium composition increases. It is noted that the electron in-plane mass decreases as indium composition increases, while the reverse is true for the electron longitudinal mass for $In_xGa_{1-x}As/GaAs$ quantum wells for $x = 0.1$ and 0.18 with well width within 20nm. Calculated electron effective masses at the conduction band edge of unstrained bulk $In_xGa_{1-x}As$ layer for $x = 0.1$ and 0.18 are $0.0662m_0$ and $0.0587m_0$, respectively. We find that, for $In_xGa_{1-x}As/GaAs$ quantum wells with $x = 0.1$ and $L_z \geq 8$ nm, theoretically obtained in-plane effective mass of electron can be smaller than that of strain-free bulk $In_xGa_{1-x}As$ layer. However, for quantum wells of $x = 0.18$, the electron in-plane mass is greater than the bulk effective mass. This result demonstrates that the effect of strain on electron effective mass is evident.

In the rest of this section, we analyze low temperature(T $=$ 6 K) magnetoluminescence data of two undoped (In, Ga)As/GaAs multi-quantum well samples with indium composition $x = 0.1$ and 0.18. Each sample contains four isolated quantum wells with well width between 2.3 nm to 20 nm. Fig. 2 shows the diamagnetic shift of the heavy-hole exciton ground state (1*s*) as a function of magnetic field up to 11 tesla. Of quantum wells with well width of 16 and 20 nm for $x = 0.1$ and 0.18, respectively, the magnetoexciton state reveals well-resolved spin splittings, while that

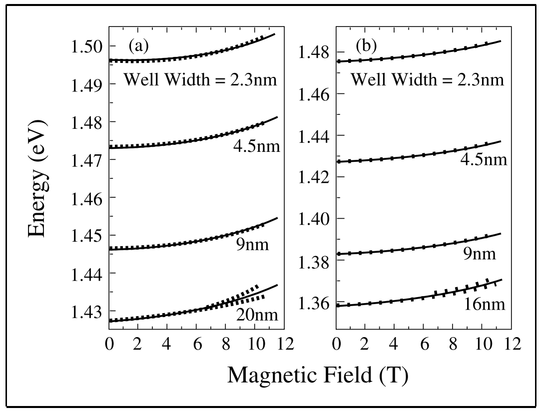

Fig. 2. Transition energies of the magnetoexciton ground state in a series of $In_xGa_{1-x}As$/ GaAs quantum wells with (a) x= 0.1 and (b) 0.18. The dots denote the experimental data, while the solid lines represent the calculated results, which is shifted within a few *meV* for the comparison of the calculated diamagnetic shifts with the experimental results.

of other quantum wells in the figure remain single curves. The drawn lines represent the theoretical fit based on our formalism. As we did not consider the spin splitting in our formalism, diamagnetic shifts showing this property were fitted by a single curve at the mid points. We note that the calculated result at $B = 0T$ were shifted within ± 3 *meV* for the comparison of the calculated diamagnetic shifts with the experimental results. It is noted that Wimbauer et al. [8] found that the spin splitting is dominated by the heavy-hole valence band splitting and determined the electron as well as heavy-hole g-factor.

Fig. 3 displays the in-plane reduced mass of the heavy-hole exciton ground state in

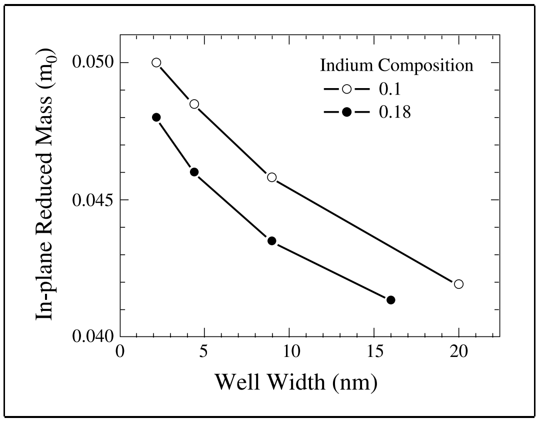

Fig. 3. The dependence of the reduced mass of the heavy-hole exciton on the indium composition and quantum well width. The drawn lines are guides to the eye.

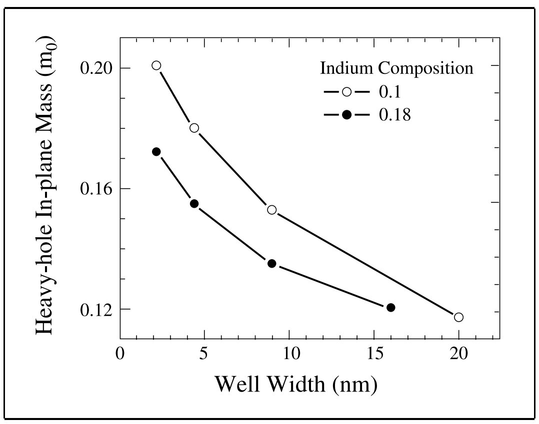

Fig. 4. The dependence of the heavy-hole in-plane mass on the indium composition and quantum well width. The drawn lines are guides to the eye.

$In_xGa_{1-x}As/GaAs$ quantum wells as a function of well width, determined from the fit of theoretical calculations to the experimental results in Fig. 2.Exciton reduced mass shows a strong dependence on both the well width and indium fraction. As well width decreases from the high value limit, the reduced mass increases due to increasing penetration of the exciton wave function into GaAs barrier layers. For instance, $\mu = 0.042m_0$ and $0.05m_0$ for $In_{0.1}Ga_{0.9}As/GaAs$ quantum wells with well width L_z = 20 nm and 2.3 nm, respectively. On the other hand, for increasing indium composition in the (In, Ga)As quantum-well layer, the exciton reduced mass decreases, because the electron in-plane mass decreases as shown in Fig. 1 and so does the heavy-hole in-plane mass, whose behavior will be shown in Fig. 4. We note that Zhou et al.[7] determined the exciton reduced mass from a theoretical fit of using a simple parabolic curves to the diamagnetic shifts measured by magnetoreflectance spectroscopy and obtained a bit heavier values (e.g. $0.051m_0$ for $In_{0.1}Ga_{0.9}As/GaAs$ quantum well with well width of 9 nm). However, it should be pointed out that a simple parabolic approximation of magnetoexciton energy is not suitable for high magnetic fields greater than a few tesla (B $>$ 3 T) for an exciton state having a light reduced mass (e.g. $\mu < 0.06m_0$). We also like to mention that the localization of an exciton is affected considerably by the confinement effect introduced by the quantum-well width, barrier potential energy, and interface roughness. Especially, the effect of interface roughness on the exciton binding energy and the diamagnetic shift cannot be negligible if well width decreases below the Bohr radius of the exciton. If one is not very careful on this effect for samples having rough quantum well interfaces, the calculated reduced mass will result to be heavier than real one.

In Fig. 4, we plotted the heavy-hole in-plane mass versus $In_xGa_{1-x}As$ well width, determined from μ and $m_{e,\rho}$. The figure shows that the heavy-hole in-plane mass decreases as well width increases. For instance, for $x = 0.1$ and well width $L_z = 2.3$ nm, $m_{hh,\rho} \sim 0.2m_0$ which is quite close to those of GaAs/(Al, Ga)As quantum well, $0.22m_0$, while for quantum wells with ($x = 0.1$ and $L_z = 20$ nm) and ($x = 0.1$ and $L_z = 16$ nm), we find $m_{hh,\rho} \sim 0.12m_0$ which is nearly equal to 0.11 m_0, the calculated result in the decoupled limit between heavy- and light-hole subbands. The effective masses of holes are significantly reduced from those found in unstrained bulk (In, Ga)As [20]. From other analysis on spin splitting of the diamagnetic shift on the latter two samples, Wimbauer at al. [8] obtained slightly higher $m_{hh,\rho} = 0.143m_0$ and $0.121m_0$, respectively. It is also noted that, for two different indium compositions $x = 0.1$ and 0.18, the heavy-hole in-plane mass increases as x decreases. For quantum wells with $L_z = 2.3$, 4.5, and 9 nm, the $m^*_{hh,\rho}$ increases about 15 percent from $x = 0.18$ down to 0.1. These results demonstrate that the hole mass is dramatically altered in the presence of strain [23], and its dependence on the additional confinement effect of quantum well is also significant. Although it not indicated in Fig. 3, we find that the fitting error of μ is within $0.0005m_0$ for all the data, and therefore, that of the in-plane heavy-hole mass is within $0.006m_0$.

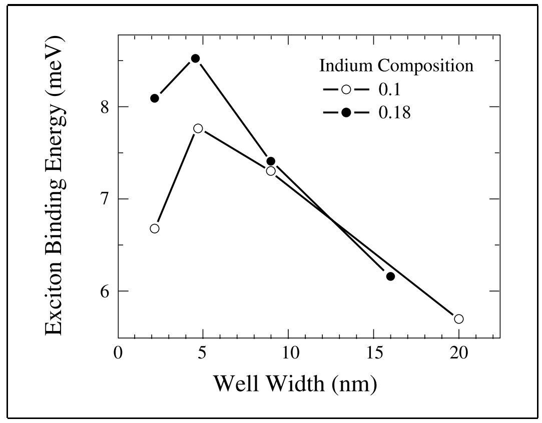

Fig. 5. Calculated binding energies of the heavy-hole exciton ground state mass at zero magnetic field as a function of indium composition and quantum well width. The drawn lines are guides to the eye.

In Fig. 5 we displayed the calculated binding energy of the heavy-hole exciton ground state at zero magnetic field as a function of well width for indium compositions $x = 0.1$ and 0.18. Exciton binding energy shows a strong dependence on both the well width and indium composition. As well width decreases from the high value limit, the binding energy is enhanced due to the increasing confinement effect. However, if the quantum well is too narrow, the energy difference between the barrier energy and the subband energy level becomes small, and the wave function spills into the barrier layer. Consequently, the confinement effect on the exciton wave function by the barrier potential energy is reduced. For the quantum well samples discussed in this report, the calculated exciton binding energy has a maximum value at 4.5 nm for $x = 0.1$ and 0.18. Competing effects between the reduced mass of the exciton and quantum well potential is found to be important to understand the crossing of the two linearly interpolated lines at around 7.5 nm. For increasing indium composition x in the (In, Ga)As quantum well layer, the reduced mass of an exciton decreases. The smaller reduced mass tends to decrease the exciton binding energy, while the effect of higher barrier potential energy due to the larger indium composition tends to increase it. For quantum wells with relatively larger width ($\geq$ 7.5 nm), the effect of the reduced mass of a heavy-hole exciton against the confinement effect due to the barrier potential with $x = 0.18$ becomes larger than that with $x = 0.1$.

IV. CONCLUSION

In the present work, we determined carrier effective masses in a series of (In, Ga)As/GaAs quantum wells by comparing theoretical calculations with magnetoluminescence measurement of the heavy-hole exciton ground state. The effective mass of both electron and heavy-hole in strained (In, Ga)As/GaAs quantum wells increases as quantum-well width or indium composition deceases. The heavy-hole effective mass is dramatically reduced in the presence of strain, and its dependence on the additional confinement of quantum well is also significant. Finally, we demonstrated that the diamagnetism of the magnetoexciton ground state can provide an excellent means to characterize both the exciton dimensionality and a number of physical properties of carriers in semiconductor nanostructures.

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