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Enhancement of the Excitonic Effects in Semiconductor Thin Quantum Boxes with Large Lateral Size

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We discuss the enhanced excitonic effects found in thin quantum boxes based on a rigorous theoretical analysis which takes excitonic confinement effects into account. These enhanced effects occur in boxes that have lateral widths larger than the Bohr radius. The calculated results explain well the unique optical phenomena recently observed in semiconductor microdisks. We also discuss the useful excitonic electric-field effects found in these boxes and propose novel optical device applications.

1. Introduction

Densely-packed and self-organized disk-shaped semiconductor nanostructures, or "quantum disks", 30 to 100 nm in size, can be fabricated by a single crystal growth procedure.[1] The novel optical properties observed in the quantum disks are attracting interest in disk structure research.[1,2] For example, sharp and intense photoluminescence (PL) emissions with spectral widths half that of quantum wells, and much smaller than that of the thermal energy kT, has been measured in InGaAs quantum disks at room temperature.[1] Extremely narrow PL and photoluminescence excitation (PLE) spectra can be obtained at cryogenic temperature, although the disk lateral size obviously is distributed, causing considerable inhomogeneous line broadening.[2,3] The physical origin of these peculiar optical phenomena has been disputed, and remains an important issue to clarify.

Regarding carrier-confinement, we can categorize quantum disks as thin quantum boxes with lateral widths larger than their height. In thin quantum box structures, the quantum confinement dimension is between 2D and 0D, and can be tuned by changing the box lateral width. The behavior of excitons in the regime between 2D and 0D is one of the most interesting areas of research in exciton optics,[4] and a few theories have been examined.[5,6] These studies, however, are based on the assumption of the lateral parabolic potential, and cannot compare directly with experimental results in the quantum disks.

In this paper we theoretically examine excitonic optical properties of thin GaAs quantum boxes that have intermediate dimensionality between 0D and 2D. The exciton behavior is simulated, taking into account the potential distributions and the boundary conditions of the thin quantum boxes. We discuss the fundamental optical properties of the exciton in the intermediate dimension in relation to the unique photoluminescence properties reported in the quantum disks. Considering device application, we also calculate the excitonic electroabsorption in thin quantum boxes by applying an electric field in the lateral direction along the box. And finally, we propose optical device application for these electric field effects.

2. Calculation Model and Method

Let us consider an electron and a hole are confined in a thin GaAs quantum box by an infinitely high energy barrier (Fig. 1). Assume that the potential distribution inside the quantum box is uniform. We can analyze numerically the quantum states bound in the quantum box by an orthogonal function expansion method based on effective mass theory to treat not only ground excitonic states but also higher energy states, and thus clarify the absorption properties near the bandedge. To analyze the optical properties, we need to know the electron-hole wavefunctions of the thin box, which can be found by solving the Schrödinger equation. The Hamiltonian H for the electron-hole system, in which an electron and a hole interact with each other via the Coulomb force, is given as the sum of the electron and hole kinetic energy terms and the Coulomb potential term V:

$$H = -\frac{\hbar^2}{2m_e}\nabla_e^2 - \frac{\hbar^2}{2m_h}\nabla_h^2 + V\ , \quad (1)$$

Here, m_e refers to the electron's effective mass and m_h refers to the hole's effective mass. Assuming that the dielectric constant ε has the same value inside and outside the box, we can express the Coulomb potential V as

$$V = -\frac{e^2}{4\pi\varepsilon\left[(x_e - x_h)^2 + (y_e - y_h)^2 + (z_e - z_h)^2\right]^{1/2}}\ , \quad (2)$$

where e is the elementary charge. In our formula, the wave function Ψ for the electron-hole system is expanded by using the electron and hole orthogonal functions as follows:

$$\Psi = \sum_{l_e,m_e,l_h,m_h} D_{l_e,m_e,l_h,m_h}\psi_{l_e,m_e}(x_e,y_e,z_e)\psi_{l_h,m_h}(x_h,y_h,z_h)\ . \quad (3)$$

Here, D_{l_e,m_e,l_h,m_h} represents the expansion coefficients, and l_e, l_h, m_e and m_h refer to indices of the orthogonal base functions in the x and y directions. We adopt the sin functions as electron and hole base sets. We only consider the lowest-order expansion function in the z direction, because we assume that an electron and a hole are strongly

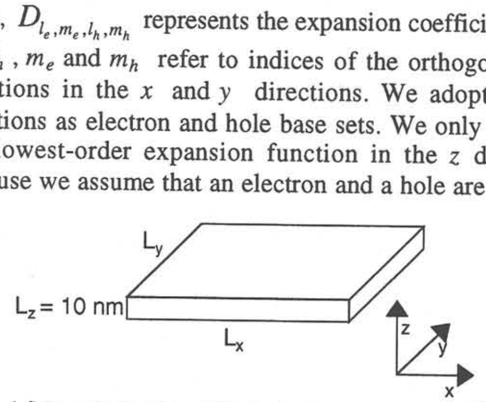

Fig. 1 Schematic drawing of the GaAs thin quantum well. The energy barrierof the cladding region is assumed to be infinitely high and the dielectricconstant has the same value inside and outside of the box. The box thickness L_z is assumed to be 10 nm in the numerical calculations.

confined in this direction. By substituting Eqs. (1)-(3) into the Schrödinger equation $(H - E)\Psi=0$, we have a $l_e \times l_h \times m_e \times m_h$ secular equation, or the Wannier equation, in the thin quantum box:

$$D_i^p\left(H^{kin} - E^p\right) + \sum_i D_i^p V_{i,j}^{eff} = 0 \ . \qquad (4)$$

The term $V_{i,j}^{eff}$ is the Coulomb energy obtained by performing an integral over the box volume, and i and j represent combinations of l_e, l_h, m_e and m_h.

Solving the secular equation, Eq. (4), by the matrix diagonalization method, we obtain the p-th eigenenergies E^p and the corresponding eigenvectors D^p for both the ground state and the higher energy excitonic states. The absorption spectra can be calculated by using the eigenvalues and eigenvectors, and the usual numerical procedures.[7]

3. Enhancement of the Excitonic Effects

Figure 2 illustrates how the binding energy of the first heavy-hole exciton varies as a function of the box lateral width $L_x(=L_y)$. Compared with the exciton binding energy of a 2D quantum well, the exciton binding energy of a thin quantum box with a 30 nm lateral width is enhanced twofold due to quantum confinements from the three directions. The exciton binding energy tends to decrease with increasing lateral width and to approach the binding energy of the 2D exciton in the quantum well as the lateral width approaches infinity. Note that the exciton binding energy is found to be substantially enhanced compared with that in the quantum well even in a box where the lateral width is much larger than the Bohr radius. Figure 3 shows optical absorption spectra for a thin box with a 50 nm width and a 10 nm thickness, calculated with (solid curves) and without (broken curves) Coulomb interaction. In these calculation both heavy-hole and light-hole related transitions have been considered separately. Since the lateral width of the box is much longer than its height, we can ignore the mixing of the heavy-hole and light-hole states. When we include the Coulomb interaction, the absorption edge shifts to the lower energy side and the absorption coefficient of the lowest energy peak increases. The energy shift of the absorption peak corresponds to the binding energy of the first heavy-hole exciton ($Ex1_{hh}$). The increase in the optical absorption of the first heavy-hole exciton is caused by the concentration of the oscillator strength of each inter-sublevel transition to the lowest excitonic transition due to Coulomb interaction (the Coulomb enhancement effect). Note that in the spectra

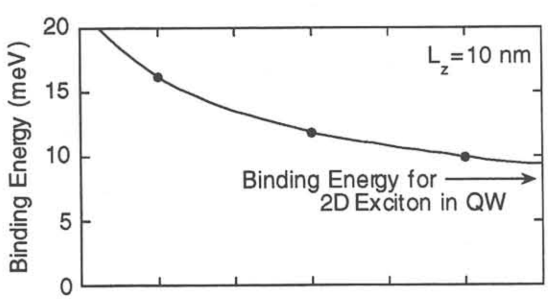

Fig. 2 Binding energy of the first heavy-hole exciton as a function of quantum box lateral width $L_x(=L_y)$

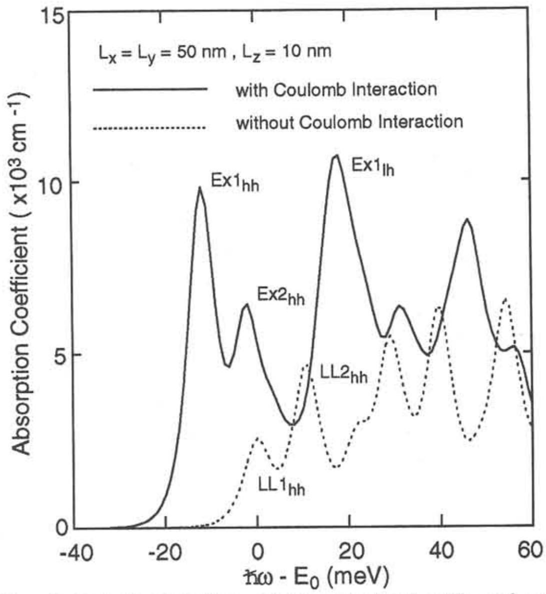

Fig. 3 Optical absorption spectra calculated with and without Coulombinteraction between an electron and a hole. Ex and LL respectively denoteexciton transition and inter-sublevel transition. The abscicca is the photonenergy with respect to the energy E_0 for lowest inter-sublevel transition $LL1_{hh}$.

calculated with the Coulomb interaction, the absorption peaks found above the bandedge all correspond to the discrete excitonic transitions produced by the quantum confinement from three directions. The narrow PL and PLE spectra observed in quantum disks[1,2] can be explained by (i) the enhancement of the ground ($Ex1_{hh}$) exciton binding energy and the concentration of oscillator strength to the ground excitonic state and (ii) the spectral discreteness of the ground exciton state, well separated from the higher energy exciton states by the lateral quantization.

4. Excitonic Electric Field Effect

We consider the external electric-field effects on excitonic optical transitions for thin quantum boxes, where we apply the electric field along the lateral (x) direction. We modify the Hamiltonian H of the electron-hole system to include external electric field E_w. The exciton electric-field effects can be clalified by solving Eqs. (2)-(4) using the modified Hamiltonian. The results are shown in Figs. 4(a) and (b). Fig. 4(a) shows the shift of 1st heavy-hole exciton resonance and the change in the 1st exciton oscillator strength induced by the electric field. As shown in Fig. 4(a), when the lateral width of the box L_x is 20 nm, both the red shift of the exciton resonance and the decrease in the oscillator strength contribute almost equally to the change in the excitonic absorption. The main feature of this field effect is essentially the same as that of the well-known quantum confined Stark effect in 2D quantum wells.[8,9] In quantum boxes with a larger lateral width (30 nm and 50 nm), the change in the exciton absorption caused by the change in the oscillator strength dominates that induced by shift of exciton resonance. The large change in the oscillator strength, which occurs in a field regime lower than 10^4

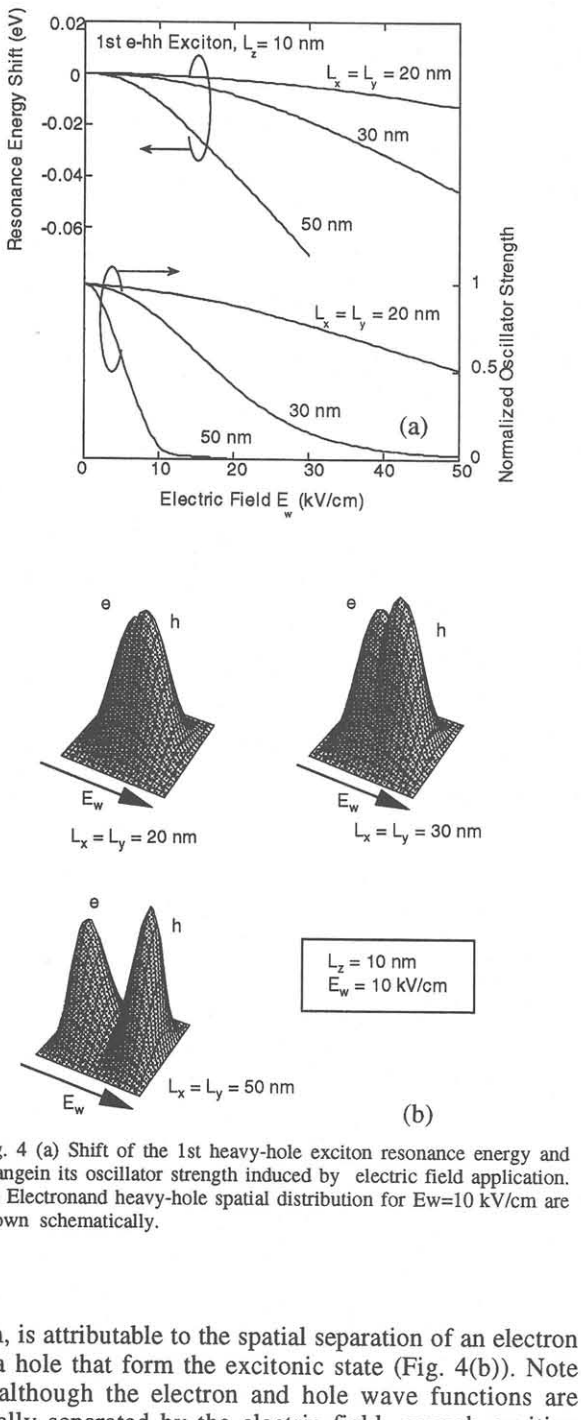

Fig. 4 (a) Shift of the 1st heavy-hole exciton resonance energy and changein its oscillator strength induced by electric field application. (b) Electronand heavy-hole spatial distribution for Ew=10 kV/cm are shown schematically.

V/cm, is attributable to the spatial separation of an electron and a hole that form the excitonic state (Fig. 4(b)). Note that although the electron and hole wave functions are spatially separated by the electric field, enough excition binding energy to maintain a stable excitonic state is preserved. Thus an exciton electric field effect an order of magnitude greater than that in quantum wells can be expected in the quantum box with a lateral width of 50 nm. This improvement in exciton electroabsorption offers new possibilities for novel optical modulation and switching devices.

5. Conclusion

We have discussed excitonic optical properties in the thin quantum box, based on a rigorous theory that takes into account the excitonic confinement effect. The theory demonstrates that the binding energy of the ground-state heavy-hole exciton is found to increase considerably in a thin box whose lateral width is up to 5 times larger than the Bohr radius. Confinement of the exciton by the lateral boundary, which restricts the exciton center-of-mass motion in the box, also modifies the envelope of the exciton relative motion, giving rise to an increase in the exciton binding energy. The loose confinement of the exciton in the thin box was found to result in the concentration of optical oscillator strength to the lowest excitonic transition. The quantum confinement of an exciton from three directions also generates novel electroabsorption properties that are different in character from well-known QCSE. Particularly in a box of larger than 30 nm, a strong electric-field dependence of excitonic absorption is expected due to the spatial separation of the electron and the hole, preserving enough binding energy to stabilize the exciton state. These results clearly demonstrate that weak lateral confinement in a thin quantum box enhances excitonic effects and thus brings about novel optical phenomena that are interesting from the stand points of device application.

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