

## Enhanced Exciton Effects in Dielectric Quantum Well (DQW)

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A novel QW structure called Dielectric Quantum Well, or DQW, is proposed. This structure enhances excitonic properties such as binding energy and oscillator strength. The barrier material of DQW has a smaller dielectric constant than that of the well material. The barrier material dilutes the effective dielectric constant of the QW and reduces the screening effect. The Coulomb interaction between an electron and a hole is thereby forced to yield a large exciton binding energy. It is shown theoretically that excitons in the DQW structure are stable even at room temperature, and that the oscillator strength of the excitonic transition is also enhanced. Various combinations of materials which look promising for application to optical devices are discussed.

In recent years, excitons in semiconductors have been studied intensively because of their characteristic spectra and applicability to optical functional devices.<sup>1)</sup> They show sharp, high peaks in absorption and luminescence spectra, reflecting their atomic-like energy structure. In III/V compound semiconductors, however, the binding energy of excitons is only a few meV - smaller than room temperature energy (26 meV). In the Quantum Well (QW) structure, exciton binding energy is enhanced to as much as 4 times that in bulk semiconductors at the 2 dimensional limit (thin limit).<sup>2)</sup> For example, exciton binding energy in GaAs QW becomes 20 meV at the 2 dimensional limit, while that in bulk GaAs is 5 meV. This value, however, is still smaller than room temperature energy, and is expected to be enhanced more. Exciton binding energy originates from the Coulomb interaction between an electron and a hole. In semiconductors, Coulomb interaction between carriers is screened and weakened by the host material.

Exciton binding energy for bulk material is given by:

$$E_{bind}(bulk) = \frac{e^2}{2\epsilon_1 a_B} = \frac{\mu e^4}{2\epsilon_1^2 \hbar^2}$$

where  $a_B$  is the exciton Bohr radius,  $\epsilon_1$  is the dielectric constant of the material, and  $\mu$  is the exciton reduced mass

( $= \frac{m_e \cdot m_h}{m_e + m_h}$ ). From this equation, exciton binding energy is expected to be enhanced by reducing the dielectric constant or increasing the exciton reduced mass of the host material. Dielectric constant and exciton reduced mass can be effectively modulated by forming a QW structure using appropriate barrier material.

In this work, the Dielectric Quantum Well (DQW) structure is proposed as a material with enhanced Coulomb interaction, and its characteristic features are analysed theoretically. Two mechanisms independently enhance the Coulomb interaction between carriers in this structure and yield a large exciton binding energy: the confinement effect in conventional QW, and the reduction of the screening effect.<sup>3)</sup>

Figure 1 shows the structure of the Dielectric Quantum Well. To enhance the Coulomb interaction (*i.e.*, reduce the screening effect),  $\epsilon_2$  is taken to be smaller than  $\epsilon_1$ . Theoretical calculations are performed using the variational method. In this calculation, the difference in the dielectric constant between well and barrier is taken into account in terms of induced image charges. The variational wave function is defined as,<sup>4)</sup>

$$\Psi(r_{\parallel}, z_e, z_h) = A f_e(z_e) f_h(z_h) \exp\left(-\sqrt{\alpha^2 r_{\parallel}^2 + \beta^2 (z_e - z_h)^2}\right)$$

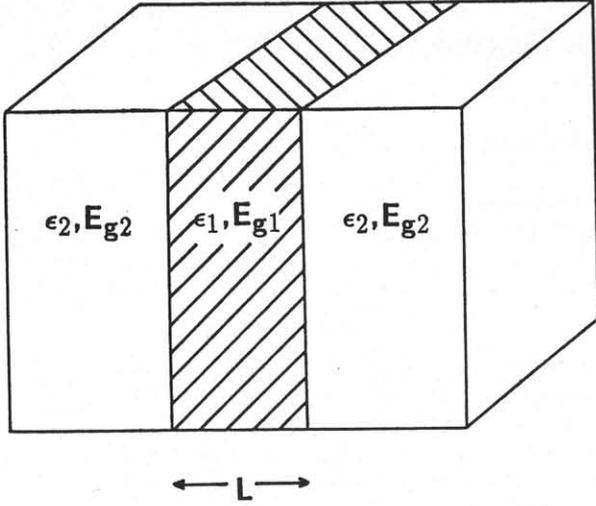


FIG.1 Schematic diagram of the DQW structure.

where  $f_e(z_e)$  and  $f_h(z_h)$  are the solutions of Schrödinger equations for an electron and a hole, respectively, and  $\alpha$  and  $\beta$  are the variational parameters describing the relative motion of an electron and a hole.

The variational parameters are determined by minimizing the total energy of the system using the equation,

$$E_{total} = \min_{\alpha, \beta} \langle \Psi | H_{total} | \Psi \rangle$$

with

$$H_{total} = H_{K\parallel} + H_{K\perp} + H_{pot.} + H_{image} + H_{self} + E_g$$

The factors in the second equation are as follows:  $H_{K\parallel}$  and  $H_{K\perp}$  are kinetic energy terms in the directions parallel and perpendicular to the quantum well interface, respectively;  $H_{pot.}$  is the Coulomb interaction energy between an electron and a hole;  $H_{image}$  is the Coulomb interaction between an electron (a hole) and images of a hole (electron);  $H_{self.}$  is the Coulomb interaction energy between an electron (a hole) and its own images, and  $E_g$  is the band gap energy of the well material. These are given as follows,

$$H_{K\parallel} = -\frac{\hbar^2}{2\mu} \nabla_{r\parallel}^2,$$

$$H_{K\perp} = -\frac{\hbar^2}{2m_e} \frac{\partial^2}{\partial z_e^2} - \frac{\hbar^2}{2m_h} \frac{\partial^2}{\partial z_h^2},$$

$$H_{pot.} = -\frac{e^2}{\sqrt{(\mathbf{r}_{e\parallel} - \mathbf{r}_{h\parallel})^2 + (z_e - z_h)^2}},$$

$$H_{image} = -e^2 \sum_n \frac{q_n}{\epsilon_1 \sqrt{(\mathbf{r}_{e\parallel} - \mathbf{r}_{h\parallel})^2 + (z_e - (-1)^n z_h - nL)^2}},$$

$(n = \pm 1, \pm 2, \dots),$

$$H_{self} = -e^2 \sum_n \frac{q_n}{\epsilon_1 \sqrt{(z_e - (-1)^n z_h - nL)^2}},$$

$(n = \pm 1, \pm 2, \dots),$

$$q_n = q_{-n} = \left( \frac{\epsilon_1 - \epsilon_2}{\epsilon_1 + \epsilon_2} \right)^n,$$

where  $H_{pot.}$ ,  $H_{image}$  and  $H_{self}$  are given for the case of infinite potential barrier. Hereafter, only results for the infinite barrier case are presented, because the gross features are the same for both infinite and finite barrier cases. Simple cosine functions are employed for  $f_e$  and  $f_h$ . The optimized wave function  $\Psi_{min.}$  given by the variational equation shown above is used to calculate the exciton binding energy and oscillator strength of excitonic transition.

Exciton binding energy is defined by the difference between the exciton energy and the sum of conduction and valence subband energies. It is given by

$$E_{bind} = \langle \Psi_{min} | H_{total} | \Psi_{min} \rangle - (\Delta E_{c1} + \Delta E_{v1})$$

where  $\Delta E_{c1}$  and  $\Delta E_{v1}$  are lowest conduction and valence subband energy, respectively. It is very important to have large exciton binding energy to utilize the excitonic transition. In particular, it is desirable for device applications that the binding energy exceeds room temperature energy.

Calculated exciton binding energy is shown in Fig. 2. It can be seen from the figure that binding energy increases monotonically as the barrier dielectric constant decreases.

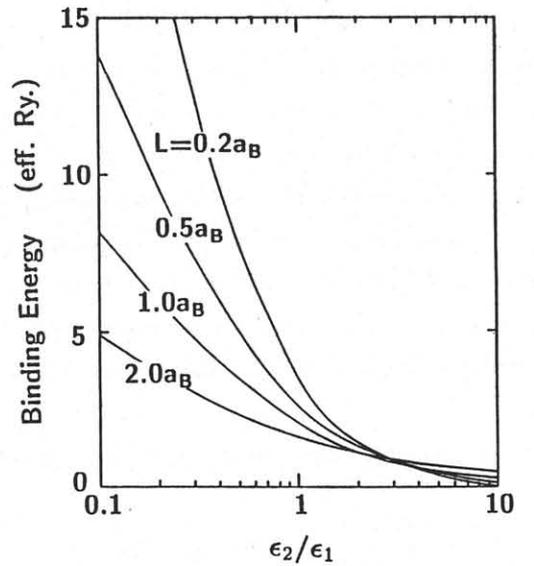


FIG.2 Structure dependence of the exciton binding energy. Exciton binding energy and quantum well width are scaled by effective Rydberg energy and effective Bohr radii of the bulk state well material, respectively.

It must be noted that well-width dependence of the binding energy is the same as that of a conventional QW but more effective enhancement of binding energy can be obtained.

Oscillator strength represents the optical activity of the material and is one very important characteristic in optical device application. Oscillator strength for excitonic transition is given by

$$f_{ex} = \frac{2}{m_0 \hbar \omega_{ex}} |\langle ex | M | g \rangle|,$$

where  $M = (p \cdot e^{iK \cdot r} + e^{iK \cdot r} \cdot p)/2$ ,  $m_0$  is the free electron mass,  $|ex\rangle$  is exciton state,  $|g\rangle$  is ground state and  $\omega_{ex}$  is the transition energy between ground and exciton state.

Figure 3 shows the calculated oscillator strength of the excitonic transition. In this figure, oscillator strength is normalized by bulk oscillator strength. Oscillator strength depends on the barrier dielectric constant, and a larger value is obtained for smaller values of the barrier dielectric constant. These results show that this material is suitable for optical device application, because it simultaneously shows larger exciton binding energy and greater oscillator strength than the conventional QW.

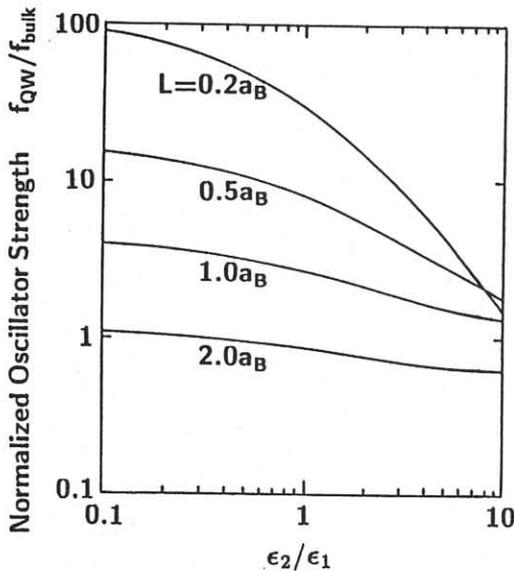


FIG.3 Structure dependence of the excitonic oscillator strength in the unit volume. Units are the same as Fig. 2.

Realistic examples for DQW are given below.

1) GaAs/ZnSe QW: ZnSe is a nearly lattice matched material for a GaAs system and has a small dielectric constant ( $\epsilon_2/\epsilon_1 \approx 0.6$ ). This system yields binding energy exceeding room temperature energy; for example, calculated binding energy is 30 meV for  $L=25 \text{ \AA}$ , while room temperature energy is 26 meV. This is thought to be the most realistic and effective example of DQW.

2) GaAs/CaF<sub>2</sub> QW: CaF<sub>2</sub> has a very small dielectric constant. Although it has a different crystal structure from GaAs, the lattice constant is similar. This system is being given a great deal of attention using the SOI technique,<sup>5)</sup> and is expected to be realized in the near future.

3) GaAs/vacuum: This system is one of the limiting cases of GaAs DQW, because vacuum has the smallest dielectric constant. Even when the well width is as large as 100  $\text{\AA}$ , binding energy easily exceeds room temperature energy. Although this system is very difficult to fabricate, the largest effect can be expected from it.

4) CuCl/CaF<sub>2</sub> QW: CuCl has a very large binding energy in itself ( $\approx 190 \text{ meV}$ ), and this energy can be enhanced by the DQW structure. Extremely large binding energy will be obtained with this system.

In all these systems, only DQW structures are discussed, however, single hetero interfaces (surface) are available for enhancement of binding energy through the reduced screening effect, though they have not the QW confinement effect. Multi-dimensional quantum well structures are also available.

In conclusion, a DQW structure is proposed which modulates the Coulomb interaction between carriers in semiconductors. Theoretical calculations show that both exciton binding energy and oscillator strength are enhanced in the DQW structure which has a smaller dielectric constant for the barrier than for the well. In addition, the existence of a stable room temperature exciton is predicted in a realistic DQW system. DQW can be said to be a very suitable material for optical devices which use the excitonic transition and operate at room temperature.

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