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Polarizability of Exciton in Surface Quantum Well

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ABSTRACT: *Surface quantum wells are seeking considerable attention due to their asymmetrical nature of polarized interface and its consequences. Their results with and without external perturbations are expected to be remarkably different from their counterparts in symmetrical quantum wells. Effect of electric field on binding energies of light hole and heavy hole exciton in surface quantum well composed of vacuum/GaAs/$Ga_{1-x}Al_xAs$ are theoretically calculated as a function of well width and Al composition. Effect of image charges arising due to the mismatch of the dielectric constant at the vacuum/GaAs interface is considered. Stark shift and polarizability of exciton in this Surface Quantum well is also calculated for various strengths of electric field with different well width confinement as well as Al concentration. Our results show that: (1) exciton binding energy increases as the electric field applied along the growth axis increases; (2) stark shift in exciton energy decreases as electric field, Al composition and well width increase; and (3) polarizability of exciton decreases when the electric field increases, but increases when well width increases. Variation of our results with those for other symmetrical wells will provide a choice of the well for electric field applications.*

Keywords: Surface quantum well, electric field, exciton, binding energy, polarizability

1. INTRODUCTION

Theoretical and experimental investigations of excitons in low dimensional semiconductor system have attracted extensive attention, due to their potential applications in opto-electronic devices such as light emitting and laser diodes with polarized output.[1] A plenty of theoretical studies have been made to understand the effect of electric field on the binding energy of hydrogenic impurities in various low dimensional semiconductor systems in the past few years.[2–7] The exciton binding energy in Cylindrical quantum dot, Triangular quantum well, Rectangular quantum well and Coupled double quantum well have been investigated theoretically and experimentally by several authors.[8–13]

The response of exciton to the electric field in such confined systems has to be considered for the fabrication of spintronic and opto-electronic devices.[14,15] Monier et al. determined the oscillator strength of excitons as a function of well width in $In_xGa_{1-x}As/GaAs$ quantum wells under large electric field.[16] The influence of uniform electric field on binding energy of excitons in inhomogeneous quantum dot is analysed by Khamkhami et al.[17] The Stark shift and ground state energy of exciton bound to ionised donor in Spherical quantum dots are determined as a function of electric field and dot radius.[18] Wu and Xia studied the effect of electric field on exciton polarizability and binding energy in CdSe/ZnS nanocrystal quantum dots using the diagonalisation method.[19] Feddi et al. have determined the effect of electric field on polarizability of an exciton bound to an ionised donor in a spherical quantum dot by perturbative-variational method.[20]

Investigations on surface quantum wells (SQW) composed of a quantum well with infinite barrier on one side and finite barrier on another side, are of special interest due to the asymmetric nature that leads to: (1) the presence of localised resonant states above the finite single quantum barrier; and (2) the formation of image charges for electron and hole at the single infinite barrier/well interface with large dielectric constant mismatch, unlike the symmetrical quantum wells, where the image charge formation is at both interfaces.[21]

In our previous work, we have estimated the exciton binding energy in SQW formed by vacuum/$GaAs/Ga_xAl_{1-x}As$ considering with and without the image charge potentials for isotropic and anisotropic masses.[22] We observed that SQW shows certain differences in the behaviour of binding energy of excitons. It is of interest to extend our studies on excitons in such SQW under external perturbations especially the quantum confined Stark effect. In the present work, we have studied the effect of electric field in such a SQW composed of vacuum/$GaAs/Ga_xAl_{1-x}As$ with image charge potentials. The binding energies and polarizabilities of the excitons are calculated variationally as a function of well width as well as Al concentration for different strengths of electric field.

2. MODEL AND FORMULATION

SQW is considered as a nanostructure of well material GaAs with barrier $Ga_{1-x}Al_xAs$ on one side and vacuum on other side shown in Figure 1.[21]

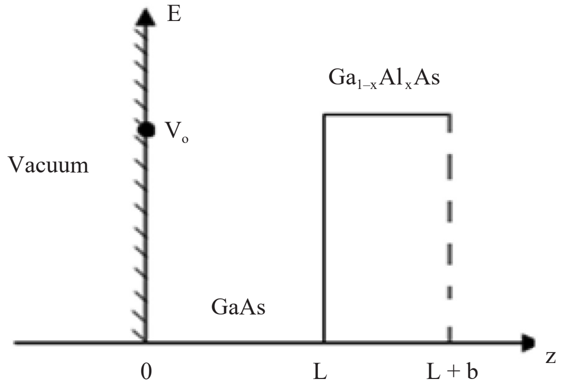

Figure1: SQW.

2.1 Well State and Ground State of Excitons

The electron states (without conduction band non-parabolicity), light hole states, heavy hole states and exciton states (with image charges and isotropic masses) are obtained using the theory of our previous work.[22]

2.2 Effect of Electric Field

The Hamiltonian of exciton in SQW with electric field along the growth axis is given by:

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_F \tag{1}$$

where $\mathcal{H}_0$ is unperturbed Hamiltonian dealt with in Section 2.2 of our previous work.[22]

The perturbation term for electric field along the growth axis is expressed as:[15]

$$\mathcal{H}_F = \eta\ (z_e - z_h) \tag{2}$$

where z_e and z_h are the z-coordinates of the electron and hole, η is the dimensionless measure of the electric field defined as $\eta = \frac{eFa^*}{R^*}$ with a* and R* as the effective Bohr radius and effective Rydberg respectively.

The trial wavefunction of excitons in the SQW with electric field is taken to be of the form:[20]

$$\psi = \psi_o\left[1+\eta b\left(z_e - z_h\right)+\eta^2 c\left(z_e - z_h\right)^2\right] \tag{3}$$

where ψ_o is the wavefunction for unperturbed Hamiltonian H_o used in our previous work.[22] Whereas, a in ψ_o, b and c are the variational parameters.

Exciton energy levels in the presence of electric field are calculated as:

$$E_{ex}\left(F \neq 0\right) = \min_{a,b,c} \frac{\left\langle \psi^* | \mathcal{H} | \psi \right\rangle}{\left\langle \psi^* | \psi \right\rangle} \tag{4}$$

For an applied electric field F, the Stark Shift on the exciton energy can be calculated as:[24]

$$\Delta E = E_{ex}\left(F \neq 0\right) - E_{ex}\left(F = 0\right) \tag{5}$$

The polarizability of the exciton is then determined from quadratic Stark effect as:[24]

$$\alpha = -\frac{\Delta E}{F^2} \tag{6}$$

Well state energies of electron, light hole and heavy hole are also affected by the presence of electric field, which are calculated as follows.

$$E_j\left(F \neq 0\right) = \mathrm{E_j}\left(\mathrm{F}=0\right) + \left\langle \psi_j^* | \eta z_j | \psi_j \right\rangle \tag{7}$$

where j = e or ih (i = l for light hole and i = h for heavy hole) and ψ_j is the wavefunction used in Section 2.1 of our previous work.[22]

The binding energy of the exciton in the presence of electric field is calculated as:

$$\mathrm{E_b}\left(\mathrm{F} \neq 0\right) = \mathrm{E_e}\left(\mathrm{F} \neq 0\right) + \mathrm{E_{ih}}\left(\mathrm{F} \neq 0\right) - E_{ex}\left(\mathrm{F} \neq 0\right) \tag{8}$$

3. RESULTS AND DISCUSSION

The parameters of the material used in the present work such as effective masses of light hole, heavy hole and electron; reduced masses of light hole and heavy hole exciton; dielectric constant for GaAs are given in Table 1. The energy gap difference ΔE_g between GaAs and $Ga_{1-x}Al_xAs$ is determined by the following expression:[23]

$$\Delta E_g = 1.155x\ 0.37x^2\ \text{eV} \tag{9}$$

The barrier height V_{oe} or the conduction band discontinuity is taken to be $0.65\Delta E_g$, hence the potential well height of the valence band V_{oh} is $0.35\Delta E_g$.[25] We have taken x = 0.3 for all calculations in the present work.

Table 1: Material parameters used in the calculations.

Parameters[23]	m_e^*	m_{hh}^*	m_{lh}^*	μ_{hh}^*	μ_{1h}^*	ε_0
GaAs	0.0665 m_0	0.34 m_0	0.94 m_0	0.05562 m_0	0.03895 m_0	13.2

Notes: m_0 is the free electron mass

Figures 2 and 3 display the variation of binding energy of lh and hh exciton as a function of well width for different electric fields. For a given electric field F, the exciton binding energy increases as the well width decreases, reaches a maximum at a certain well width (L = 8 nm for lh exciton and L = 6 nm for hh-exciton) and starts to decrease for further reduction of the well width. The Coulomb attraction energy is roughly proportional to 1/r, and the square well quantisation energy to $1/r^2$. Therefore, in most simplistic approximation, at sufficiently small values of r, one may ignore the Coulomb term which can lead to a maxima of excitonic binding energy with respect to reducing well widths. Moreover, when the well width L is reduced, the wave function of the exciton compressed in the well, leads to more binding, however the exciton wave function spread out into the surrounding interface after certain value of L. This causes the binding energy to be decreased as L is further reduced.[22,23]

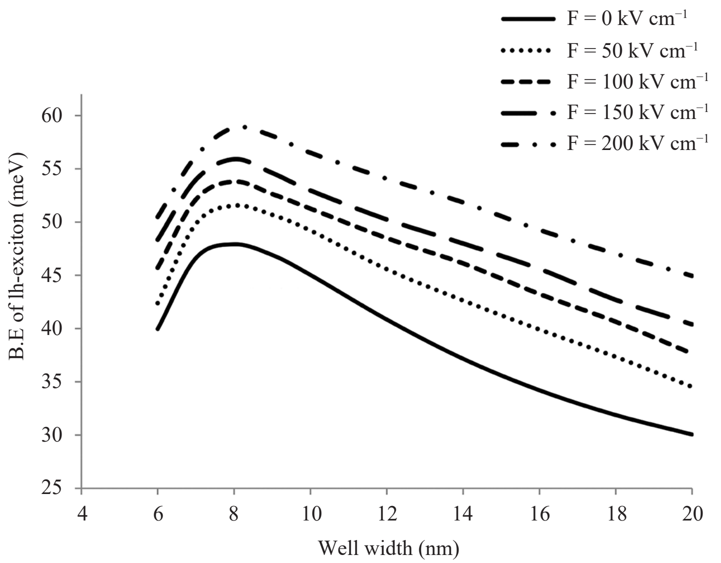

Figure 2: lh-exciton binding energy as a function of well width for different electric fields.

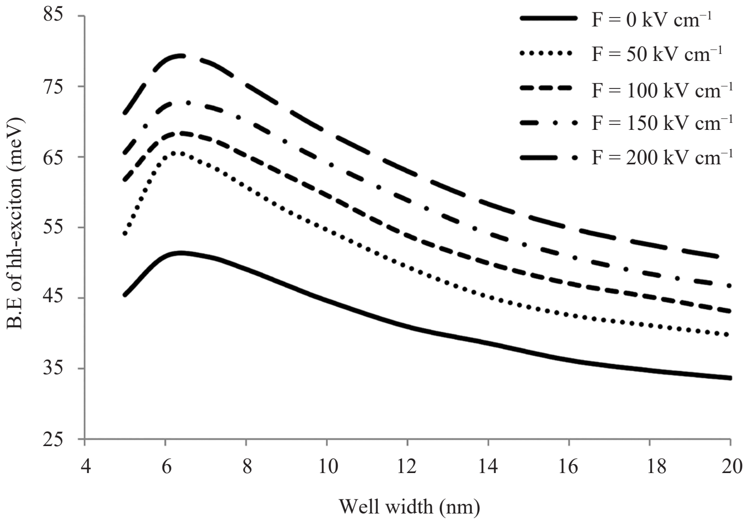

Figure 3: hh-exciton binding energy as a function of well width for different electric fields.

In symmetrical quantum wells, the applied electric field pulls the electron against the direction of electric field and hole along the direction of electric field. Hence, the exciton becomes more polarized and the exciton binding energy is reduced.[15] But in SQW, due to the asymmetric nature and large dielectric constant mismatch at the vacuum/GaAs interface, image charges are formed for the electron and the hole. A dead layer, free of excitons, is formed near the interface, due to the repulsion of charge carriers and their images. Hence unlike the symmetrical quantum wells, application of electric field cannot pull apart the electron and hole of the exciton since they will be repelled by their image charges at the interface. This contrary behaviour leads to the increased confinement of exciton and increase in the binding energy with increased applied electric field as shown in Figures 2 and 3. But this result is contrary to the results reported by other authors.[14,15,19]

Reason for this significant dissimilarity may also be due to: (1) the large reduction in the electron-hole kinetic energy as applied electric field increases; and (2) the competing effects of the confining potential, image potential and the potential resulting from the applied electric field that changes the optical properties significantly.[26] A detailed study of this mechanism can be undertaken as a future work for quantitative understanding. It is also observed that the binding energy of hh-exciton is greater than that of lh-exciton for a given applied electric field.[12]

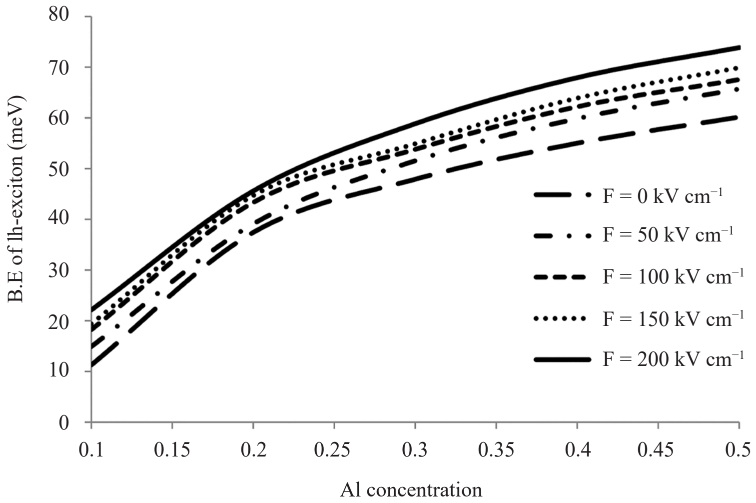

Figure 4: lh-exciton binding energy as a function of Al concentration for different electric fields.

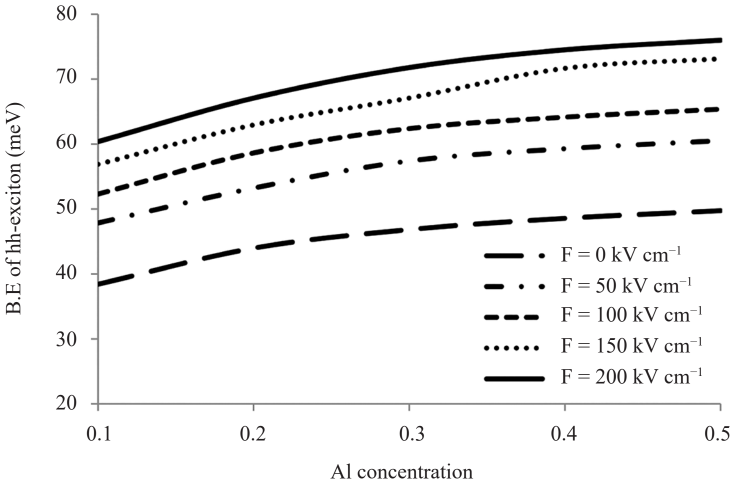

Figure 5: hh-exciton binding energy as a function of Al concentration for different electric fields.

We display in Figures 4 and 5 the variation of lh-exciton and hh-exciton binding energies, respectively, as a function of the Al concentration for different strengths of electric field with well width L = 9 nm. It is clear to see that binding energies increases with Al concentration, due to the raise in the barrier height of the quantum well. It should be noted that the choice of the concentration of Al, becomes important for device applications.

Figures 6 and 7 illustrate the Stark shift in lh-exciton and hh-exciton energy respectively as a function of electric field for different well widths. It is observed that the Stark shift decreases as the electric field increases, since the exciton energy shifts monotonically towards lower energy as the electric field increases due to the quantum-confined Stark effect. This behaviour is in good agreement with the results reported by Wu et al. and Dujardin et al.[19,24] It is also noted that the Stark effect on exciton energy with large well width is less than that with small well width and it shows nearly linear behaviour with electric field. The negative values of Stark shift indicate a red shift in the exciton energy in the presence of electric field.

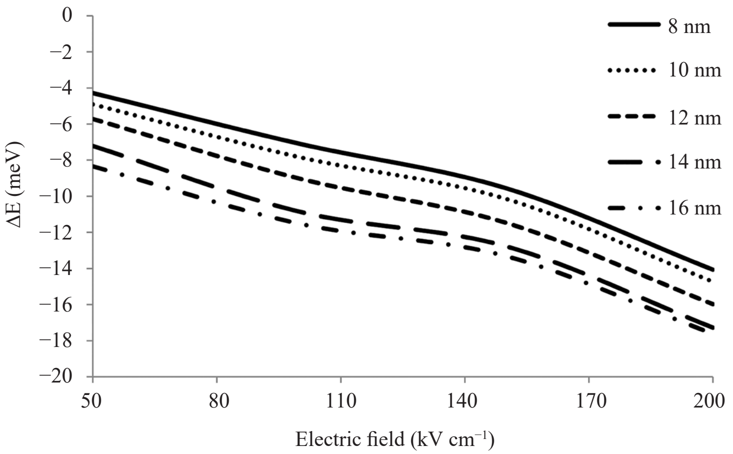

Figure 6: Stark shift in lh-exciton energy for different well widths.

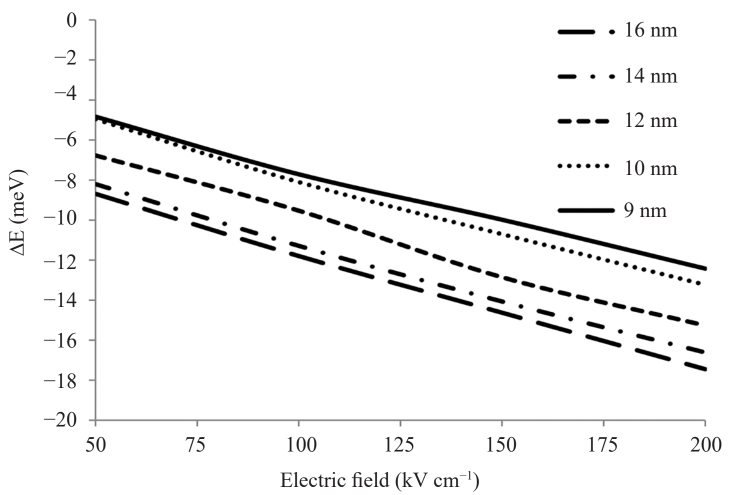

Figure 7: Stark shift in hh-exciton energy for different well widths.

Figures 8 and 9 show the Stark shift in lh and hh exciton energy as a function of Al concentration for different electric fields. Stark shift decreases monotonically with Al concentration up to x = 0.4, after which it remains constant for a given electric field. The reason for these variations may be due to the raise of the barrier height as the increase of the Al concentration.

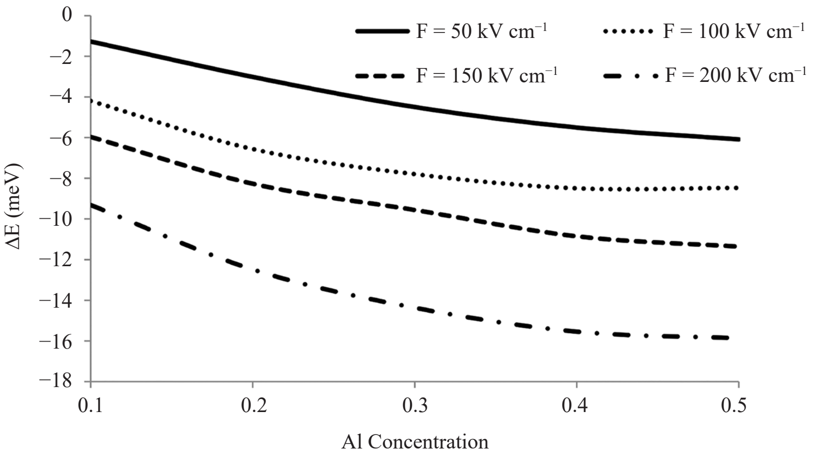

Figure 8: Stark shift in lh-exciton energy for various Al concentrations.

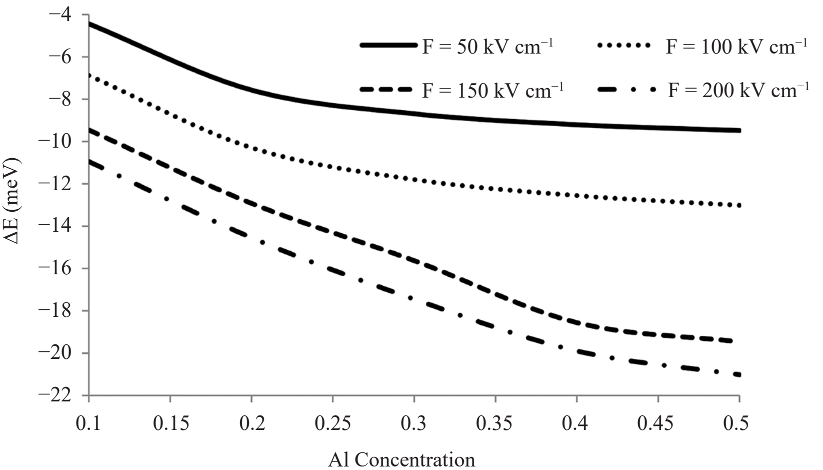

Figure 9: Stark shift in hh-exciton energy for various Al concentrations.

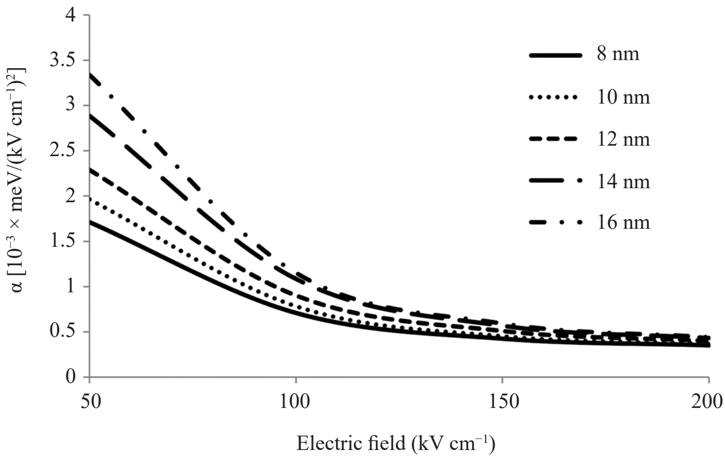

Figure 10: Polarizability of lh-exciton as a function of electric field for different well widths.

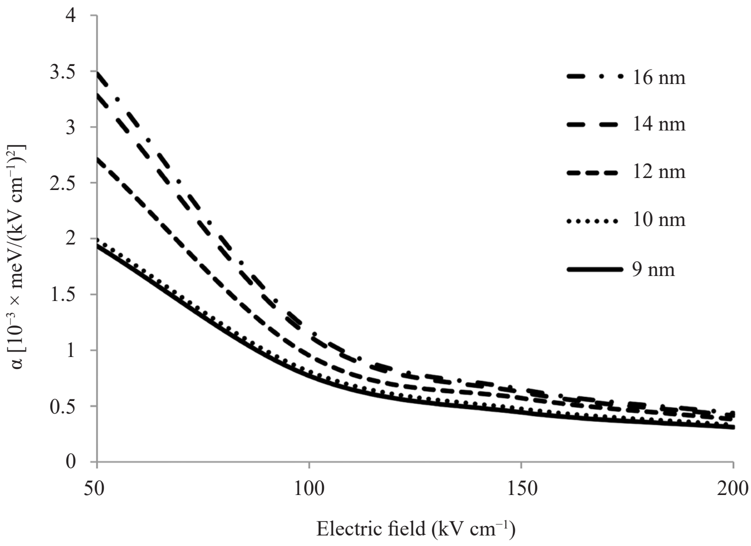

Figure 11: Polarizability of hh-exciton as a function of electric field for different well widths.

We show the variation of polarizability of lh-exciton and hh-exciton as a function of electric field for different well widths in Figures 10 and 11, respectively. The polarizability of both lh and hh-exciton strongly increases with the well width and gradually decreases with electric field increases up to F = 150 kV cm^{-1}, beyond which the polarizability remains unchanged.[19,24] This is consistent with our result shown in Figures 2 and 3 that the applied electric field reduces the kinetic energy of electron and hole, hence binding energy of the exciton increases with the electric field. Polarizability of the exciton is sensitive to the well width for lower strength of electric field and insensitive for higher strength of electric field. These observations may be of use in the choice of electric field and confinement for potential applications.

4. CONCLUSION

We have performed a theoretical investigation of the effect of electric field on binding energy of exciton, Stark shift in exciton energy and polarizability of exciton in SQW formed by vacuum/GaAs/Ga_xAl_{1-x} Al as a function of well width and Al concentration considering the effect of image charges. It is found that lh and hh-exciton binding energy increase with increase in electric field. Stark shift in excitonic energy shift towards higher energy as the electric field, well width and Al concentration decrease. The result also shows that the polarizability of the exciton decreases when the electric field increases, but increases with well width. Our attempt to study the quantum confined Stark effect in SQW showed that these behaviours in SQW vary with those in other symmetrical quantum wells due to their asymmetrical nature of polarized interface. Hence our results may provide an understanding on the choice of the well for electric field applications. The role of band bending due to the application of electric field, which is also expected to be of different nature in SQW, is not exclusively studied at present in our calculations and may be considered for future work.

5. ACKNOWLEDGEMENTS

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