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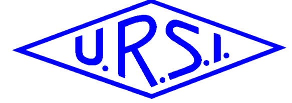

Exciton Binding Energy in $Ge_{1-x}Sn_x$ Quantum Wells: Fractional Dimensional and k.p Calculations

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Abstract

Exciton binding energies in GeSn QW with Ge (SiGeSn) barrier are calculated by fractional dimensional analysis and compared with multiband **k.p** calculation. The importance of the study in designing QCSE modulators is pointed out.

1. Introduction

Si or Group IV Photonics is a current research topic of immense application potential [1]. Its development in fullest form may lead to true electronics-photonics integration on Si platform using standard VLSI/ULSI technology. The main bottleneck in achieving the coveted goal lies in the indirect nature of band gap of Si and SiGe alloys. Efficient light emitters and high speed modulators cannot therefore be realized by using these materials.

During the past one or two decades $Ge_{1-x}Sn_x$ alloy has been demanding intense attention from workers engaged in the development of Si or Group IV Photonics [2]. The alloy can be grown on virtual substrates on Si platform. Under suitable strain and with Sn concentration x > 0.06 for unstrained condition, the alloy shows direct gap nature with Γ conduction band valley lying lower than indirect L valleys. A significantly high electron mobility has been predicted for GeSn alloy [3]. An optically pumped laser using the alloy has been reported [4].Photodetectors [5], heterophototransistors [6] having GeSn as active layer are studied and fabricated. Growth of the direct gap alloy layer, and its application as electronic and optoelectronic devices have been reviewed by Wirth et al [2].

It is well known that excitons, the electron-hole pair bound by Coulomb interaction, show interesting physical phenomena. Application of an external electric field to a Quantum Well (QW) leads to Quantum Confined Stark Effect [7], which is utilized to produce light modulators for fibre optic communication, as well as photodetectors. Unfortunately however, so far there are only a few reports on the excitonic properties in GeSn quantum nanostructures [8, 9].

In the present work, we make an attempt to estimate the values of excitonic binding energy in both unstrained and strained direct gap GeSn QWs. We first find out the composition of barrier layers, usually $Ge_{1-p-q}Si_pSn_q$ layers, that leads to direct gap type I QW in GeSn. The usual method of model solid theory [10, 11] is used for this purpose. After determining the proper compositions for the well and barrier layers, we calculate the binding energy of 1s excitons in the well. Instead of using sophisticated methods [9, 12], we first rely on a simple but accurate method based on fractional dimensional analysis (hereafter abbreviated as α-D). In this method, which has been employed by a number of workers for QWs, SLs, QWRs, and QDs [13-15], the fractional dimension α represents the nature of confinement. For example α = 3 stands for bulk (3 dimensional:3D) , α = 2 for purely 2D, and 2<α< 3 cover QWs of finite width. Since there are no experimental data, we then calculate the binding energy by using more accurate multiband **k.p** perturbation theory [9] and compare the results obtained by the two methods. The high binding energy is alluring to study further the absorption in electric field and design an Electro Absorption Modulator suitable at mid infrared wavelengths.

In the following, we first introduce briefly the fractional dimensional space and the method to calculate the dimensional parameter α for finite QW and give the expression for binding energy. Next we give the compositions of the well and barrier layers. The calculated values of binding energies are then presented and compared with **k.p** calculations.

2. Theory

The exciton bound state energies and wave functions can be calculated as a function of spatial dimension α which describes the degree of anisotropy of the electron-hole interaction. To express α, a pertinent dimensionless parameter, β is chosen as

$$\beta = \langle\frac{|z_e - z_h|}{a_0}\rangle = \int_{-\infty}^{+\infty} dz_e dz_h \frac{|z_e - z_h|}{a_0} \left|f_p^e(z_e)\right|^2 \left|f_q^h(z_h)\right|^2 \qquad (1)$$

β expresses the average electron-hole distance in the quantum confinement direction which has been considered along z direction.

$f_p^e(z_e)$ and $f_q^h(z_h)$ are the envelope functions of electron and hole respectively corresponding to the pth (qth) electron (hole) quantum level and a_0 is the three dimensional effective Bohr radius.

The fractional dimension α may be related to β by $\alpha = 3 - \exp(-\beta)$

To obtain better result, Christol et al [14] used β as the reduced value of the quantum well width, d as $\beta = d/2a_0$, where d is the thickness of the QW and a_0 is the 3D effective Bohr radius.

Considering one dimensional motion of a particle of effective mass $m*$ in a quantum well of depth V and well width d, the bound state energy, E of the particle can be determined using the well transcendental equation as follows

$$k_w d = n\pi - 2\sin^{-1}\left[r/\sqrt{r^2+s^2}\right] \quad (2)$$

where $r = k_w/m_w^*$, $s = k_b/m_b^*$, $k_w = \sqrt{2m_w^* E}/\hbar$, and $k_b = \sqrt{2m_b^*(V-E)}/\hbar$; m_w^* and m_b^* are the effective masses of the particle in the well and in the barrier respectively.

For finite quantum well when the spreading of envelope function into the barrier has been taken into consideration, the dimensionless pertinent parameter (β) will have the form $\beta = d^*/2a_0^*$, where $d^* = (2/k_b) + d$, and

$$a_0^* = \frac{\varepsilon}{\varepsilon_0}\frac{m_0}{\mu^*}a_H \quad (3)$$

μ^* is the mean value of the three dimensional reduced mass of exciton and is given by

$$\frac{1}{\mu^*} = \frac{1}{m_e^*} + \gamma_1^* \quad (4)$$

The mean values of electron effective mass and valence band parameters can be defined as

$$m_e^* = \beta_e m_{ew}^* + (1-\beta_e)m_{eb}^* \quad (5)$$

and

$$\gamma_1^* = \beta_h\gamma_{1w} + (1-\beta_h)\gamma_{1b} \quad (6)$$

Here two weighting parameters β_e and β_h are considered to account for the effective mass mismatch between the well and barrier material.

$$\beta_e = d/(2/k_{be} + d) \quad (7)$$

and

$$\beta_h = d/(2/k_{bh} + d) \quad (8)$$

According to the proposed model of Christol et al [14] , the binding energy of a confined exciton for finite quantum well is given by

$$E_b = \frac{E_0^*}{\left[1 - \frac{1}{2}e^{-d^*/2a_0^*}\right]^2} \quad (9)$$

where E_0^* is the mean value of the effective Rydberg energy for the three dimensional exciton.

In a two dimensional system, the heavy hole and light hole subbands split due to strong anisotropy and the in plane effective masses are taken as [16]

$$m_{hh} = \frac{m_0}{\gamma_1 + \gamma_2} \quad \textit{and} \quad m_{lh} = \frac{m_0}{\gamma_1 - \gamma_2}$$

The essential features of the multiband **k.p** calculation have been described in [9]. For strained layers the band line ups are calculated using model solid theory [10, 11] and deformation potential constants. Non parabolicity effects are considered. For pseudomorphic structures, the subband energies and envelope functions are calculated by using effective mass theory and axial approximation [17]

3. Results and Discussions

First, we explore the design space for heterostructures, in particular, lattice matched strained and strain-free GeSn QWs and GeSiSn barrier. We examine the specific cases in which the band offsets between wells and barriers are type I [11, 18]. The values of parameters used in our calculation are taken from [8, 18]

We have calculated compositions of $Ge_{1-x}Sn_x$ well and $Ge_{1-p-q}Si_pSn_q$ barrier for type I band alignment for both unstrained and strained conditions. For example, with 1.99 % strain, the values of x, p and q are, respectively, 0.04, 0.45 and 0.05. The band offsets are ΔE_c = 0.91 eV and ΔE_v = 0.22 eV. The values of dimensional parameter and exciton binding energies have also been calculated for a few relaxed and strained configurations.
We present in detail, however, the results for GeSn QW with Ge barrier, for the sake of comparison with k.p calculations. The values of α for relaxed (x=0.10, p/q= 0.35/0.20), tensile (x=0.08, p/q= 0.34/0.19) and compressive (x= 0.11, p/q= 0.36/0.20) strains are presented in Fig. 1. The curves show the same trend as exhibited in the work by Christol et al [14] for GaAs/GaAlAs QWs. The curves show an initial decrease, a minimum and then an increase with increasing well width. This trend is also exhibited by unstrained QWs.
With the values of dimensional parameter, the binding energies for 1s excitons can be calculated. We have obtained such values for transition between first electron subband (e1) and first heavy hole subband (hh1). The plots of binding energy versus well width for e1-hh1 transitions for relaxed, tensile and compressively strained QWs are shown in Fig. 2.

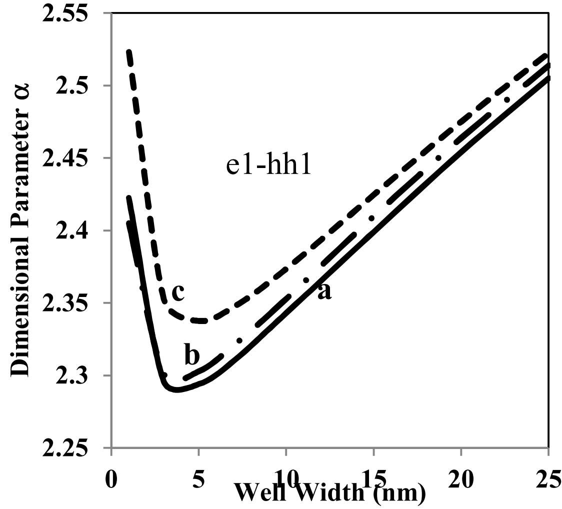

Figure 1: Dimensional parameter vs. well width for relaxed (a), compressively strained (b) and tensile strained (c) GeSn QWs. See text for compositions in well and barrier for each case.

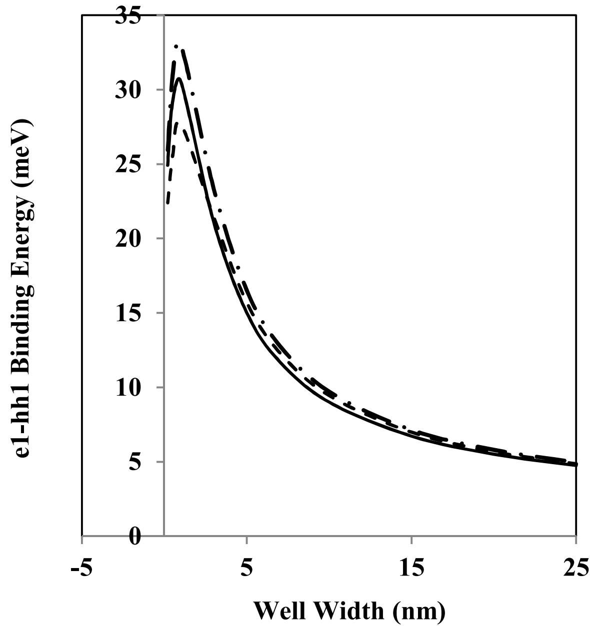

Figure 2: Binding energy of 1s exciton versus well width. Solid, dash-dotted, and dashed lines correspond to relaxed, compressively strained and tensile strained QW.

The plots in Fig. 2 show the same nature of variation as exhibited by GaAs QWs [14]. The binding energy first increases, reaches a maximum and then decreases. For very low and very high values of well width, the values tend towards bulk values as expected. The maximum corresponds to the situation when both electrons and holes are maximally confined in the QW.

We have also obtained the values of dimensional parameters and binding energies for e1-lh1 transitions for three cases: relaxed, and under compressive and tensile strains. The nature of the curves are similar to the trends shown in Figs. 1 and 2.

Since there are no experimental data on binding energy for excitons in GeSn QWs, we examine our results obtained by αD analysis in the light of results from more accurate k.p method. Fig. 3 gives representative plots of exciton binding energies for both e1-hh1 and e1-lh1, corresponding Bohr radii and oscillator strengths for a fixed value of well width of 10 nm and for different Sn compositions.

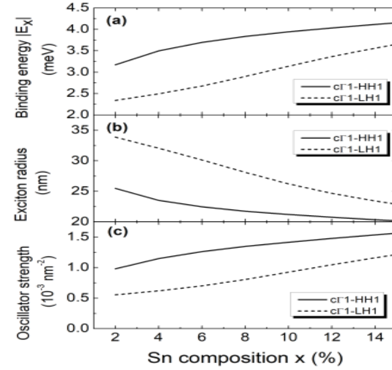

Figure 3: Exciton binding energy and Bohr radius of GeSn/Ge QWs calculated by **k.p** theory

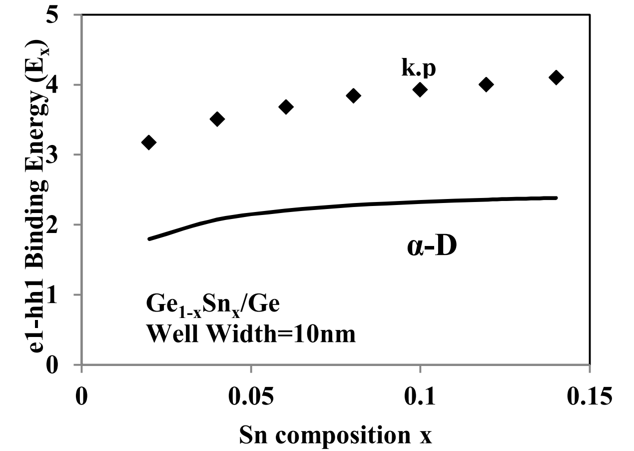

Figure 4. Comparison of binding energies for e1-hh1 transition obtained by k.p method and α-D analysis.

Fig. 4 shows the comparison for e1-hh1 transition. The agreement for GeSn QW is, unfortunately, not as much satisfactory as for GaAs QWs obtained earlier. It is clearly indicated that k.p theory yields higher values for the binding energy. We have also compared the α-D values with k.p values for e1-lh1 transition also. Again, the k.p values are higher. The difference may be attributed to the uncertainties in parameter values and various approximations involved in α-D analysis.

The plots indicate that under compressive strain and with proper compositions in the well and barrier, a binding energy as high as 32 meV for hh exciton, higher than in III-V compound semiconductor based QWs, can be obtained in GeSn QWs. The value for GeSn/GeSiSn

system is 27 meV. Larger exciton binding energy is associated with stronger QCSE. It is now of interest to study the absorption and recombination processes in GeSn QWs with and without applied fields to explore the potential of photonic devices exploiting excitonic effects.

4. Conclusions

We have calculated the binding energy of excitons in direct band GeSn QWs with Ge (GeSiSn) barriers giving rise to type I heterostructure. Value as large as 32(27) meV has been found for hh excitons. The findings are likely to encourage develop photonic devices based on excitonic effects at mid IR using Si substrate.

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