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A Theoretical investigation on the dimensions and annealing effects of InAs/GaAs quantum dots for device applications at high bit-rate optical transmission window of 1.3-1.55 μm

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Abstract. In this paper, we present theoretical model and computations for tuning the photoluminescence (PL) emission of InAs/GaAs quantum dots at 1.3 -1.55 μm by optimizing its height and base dimensions through quantum mechanical concepts. Simulation on the annealing induced compositional change in the QDs was carried out using Fick's diffusion model. Results from our computation illustrated that lower base size of 10 nm and larger height QDs of 5.1 nm can be effectively utilized for extending the PL emission to longer wavelengths with minimal blue-shift on annealing. This highlights the potential of our model and computation to assist in precisely engineering the optical properties of QD materials for specific device applications.

Introduction

Self-assembled InAs/GaAs quantum dots (QDs) are considered essential candidates for fibre optical communication devices such as photodetectors and lasers [1-3]. Last decade witnessed the growth and design of these QD devices in the high bit rate optical transmission window of 1.3-1.55 μm [4-8]. The major difficulty which arises during the growth of QDs is the dot size inhomogeneity and generation of non-radiative recombination centers as defects, which limits the device performance. The device efficiency can be improved by post growth thermal annealing which is well known for QD size homogenization and reduction of structural defects [9-10]. However, other than this, annealing also causes interdiffusion of gallium and out-diffusion of indium from the QDs. This leads to blueshift of the ground state (GS) photoluminescence (PL) peak away from the 1.3 -1.55 μm regime and thus impedes the design plan of these QD devices for high bit rate optical communication.

With this in view, the aim of this paper is to interpret theoretically the QD height and base dimensions which can exhibit longer wavelength PL emission at the optical transmission window as explained before and the blue-shift of the same on annealing. Here we have used quantum mechanical models and concepts to compute the transition energy state of the QD for different dimensions. Fick's diffusion model is used to study the In/Ga interdiffusion mechanism in QDs which alters the energy levels and cause shift in the GS PL peak.

Theoretical model

Quantized energy states of quantum wells and dots

The confinement energy of the carriers (electron and holes) for a finite rectangular quantum well is given by [11]

$$E(n^2) = \frac{2P^2}{(P+1)^2}\left[\left(\frac{n\pi}{2}\right)^2 - \frac{1}{3(P+1)^3}\left(\frac{n\pi}{2}\right)^4 - \frac{27P-8}{180(P+1)^6}\left(\frac{n\pi}{2}\right)^6 - \cdots\right]\times\left[\frac{\hbar^2}{mL^2}\right] \quad (1)$$

where n^2 is given by

$$n^2 = \sum n_j^2,\ j = 1,2,3 \quad (2)$$

P is the well strength parameter which depends on the potential depth V_0 with the following relation

$$P = \frac{\sqrt{2mV_0}}{\hbar}\frac{L}{2} \tag{3}$$

where L is the size of the well and m is the effective mass of electrons and holes taken for the computation. For an infinitely deep potential well ($P \to \infty$) equation (1) reduces to well known result for quantum wells

$$\lim_{P\to\infty} E(n^2) = \frac{\pi^2\hbar^2}{2mL^2}n^2 \tag{4}$$

Hence, for finite QD dimensions, the quantized energy states is given by

$$E_{nQD} = E(n_x^2) + E(n_y^2) +$$

$$\left[\frac{2P_h^2}{(P_h+1)^2} \times \left[\left(\frac{n_z\pi}{2}\right) - \frac{1}{3(P_h+1)^3}\left(\frac{n_z\pi}{2}\right)^4 - \frac{27P_h-8}{180(P_h+1)^6}\left(\frac{n_z\pi}{2}\right)^6 - \cdots\right] \times \left(\frac{\hbar^2}{mb^2}\right)\right] \tag{5}$$

where we have taken square base dimension of the QD of size L with height b and P_h given by

$$P_h = \frac{\sqrt{2mV_0}}{\hbar}\frac{b}{2} \tag{6}$$

For 3D infinite potential box ($P \to \infty, P_h \to \infty$), equation (5) reduces to

$$\lim_{\substack{P\to\infty \\ P_h\to\infty}} E_{nQD} = \frac{\pi^2\hbar^2}{2m}\left[\left(\frac{n_x^2+n_y^2}{L^2}\right) + \left(\frac{n_z^2}{b^2}\right)\right] \tag{7}$$

Annealing induced interdiffusion in quantum dots

The In/Ga interdiffusion in QDs is modeled by Fick's second equation

$$\frac{\partial C(x,t)}{\partial t} = D\nabla^2 C(x,t) \tag{8}$$

where C is the mole fraction of In and D is the diffusion constant of InAs in the QD heterostructure. Here, we have assumed that the QD is purely composed of InAs and hence C=1 for asgrown QDs.
Arrhenius-type temperature dependence of the diffusion coefficient is taken to account for the variation with annealing temperature T [12].

$$D = D_0 \exp\left(-\frac{E_a}{KT}\right) \tag{9}$$

where E_a is the activation energy and D_0 is the maximum diffusion coefficient at infinite temperature.
The position-dependent bulk band gap after interdiffusion is obtained from the following empirical relation involving indium content x in $In_xGa_{1-x}As$ [13]

$$E_g = 1.519 - 1.584x + 0.475x^2 \tag{10}$$

The GS PL peak energy of the QD is calculated by

$$E_{PL} = E_{nQDe} + E_g + E_{nQDh} \tag{11}$$

where E_{nQDe} and E_{nQDh} are the quantized energy states of electron and holes respectively.

Computation and Simulation results

Minimum dispersion and low loss of signals at 1.3 and 1.55 μm wavelength are effectively utilized by optical sources which are applicable for gigabit ethernet links offering efficient fiber coupling and communication. Hence it is of much interest to extend the wavelength of QDs past 1.3 μm so as to bring the advantages of the QDs to telecommunication application. In this section, we present calculations for minimum QD dimensions at which the GS PL peak is extended beyond 1.3 µm wavelength.

Here, we have chosen minimum QD dimensions since higher QD coverage or larger dimensions leads to the nucleation of large sized ripened QDs which undergo strain relaxation through the formation of V-shaped structural defects [14]. The result of our calculations is depicted in Fig.1 where the 1.3 µm wavelength is shown by the dark line for ease of understanding by the reader. It is seen that for all fixed base size of QD, the GS PL peak can be extended to longer wavelength with increase in QD height. For lower base size of the QD i.e 5 nm, the same cannot reach the telecommunication window region, even though the QD height is increased to a larger extent. It cannot be extended beyond 0.85 µm wavelength. However, as the size of the QD base is increased to 10 nm, the GS PL peak of the QDs can be tuned to 1.3 µm for QD height of 5.1 nm. Further increase in QD base size to 15, 20 and 25 nm can extend the same to 1.3 µm at shorter QD heights of 4.1, 3.9 and 3.8 nm respectively.

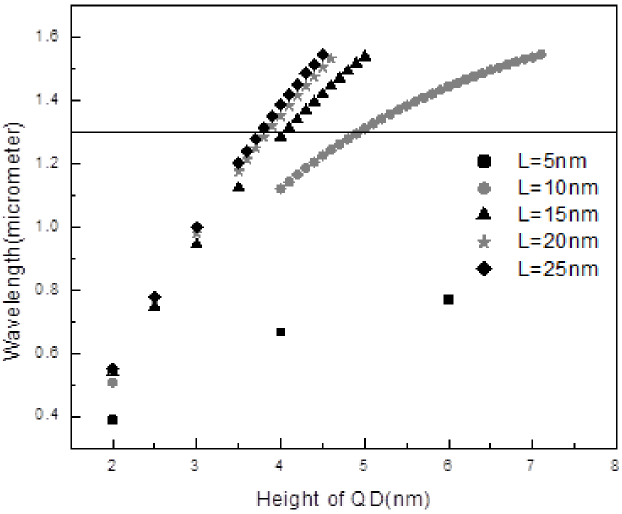

Fig. 1. Computations of the GS PL peak for different height and base dimensions of QDs

We also computed the changes in the GS PL peak at different annealing temperatures for these aforesaid QD dimensions. Fig. 2 shows our computational results of the same. It is seen that for all these QDs, the GS PL peak blueshift is minimum at 650°C annealing temperature with slight change from the asgrown PL peak. Pronounced blueshift is noticed with further increase in annealing temperature. However, amongst these QDs, least GS PL peak blue-shift is observed for QD having lower base size of 10 nm with 5.1 nm height as seen from Fig.2. It also depicts that the GS PL peak of this QD is above the 1.3 µm wavelength (as shown by dotted line) even at 700°C annealing temperature. Changing the base size further from 15 to 25 nm causes larger blueshifts and thus tunes the same below the 1.3 µm wavelength region at the same annealing temperature.

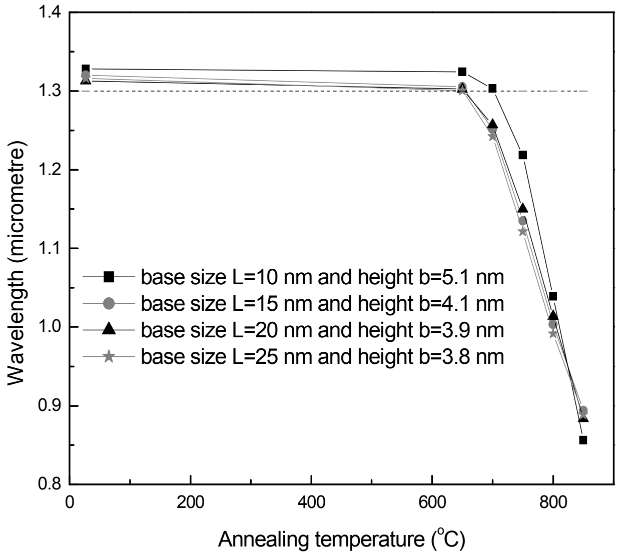

Fig. 2. Effect of annealing temperature on the GS PL peak of quantum dots for different height and base dimensions

Previous experiments have showed that the annealing causes reduction of non-radiative recombination centers at around 700-750°C which improves performance of QD devices [9-10]. Thus to bring the high performance QDs to operate at the telecommunication window, the height of the QDs should be increased so as to tune the PL emission at longer wavelengths such that the blue-shift in the PL peak even at 750°C is above the 1.3 µm wavelength. We have calculated the dimensions for this type of application, which is plotted in Fig. 3. Here also more prominent blueshift can be seen for larger QD bases i.e 15 – 25 nm.

The degree of GS PL peak blueshift at each annealing temperature is plotted in Fig.4. The blueshift is minimum for QDs having smaller base size and larger height (L=10nm, b=5.1 nm) for annealing upto 750°C. This suggests that the rate of indium out-diffusion from the QD is more along the axis or in the growth direction of the QD than the lateral direction. Hence for larger QD height having greater distance from the QD central core to the top and bottom interface, out-diffusion of indium and hence the blueshift is suppressed. However, as the temperature is increased to 800°C and above, In/Ga inter-diffusion increases rapidly in all direction, which causes significant increase in blueshift of the GS PL peak. At 850°C the blueshift even crosses the blueshift of the QDs having larger bases and lower heights i.e QDs having dimensions: L=15nm b=4.1 nm, L=20 nm b=3.9 nm and L=25 nm b=3.8nm.

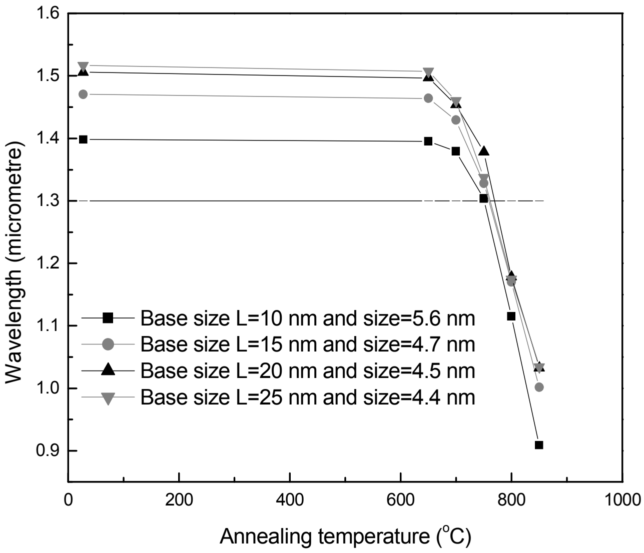

Fig. 3. QD height and base dimensions for tuning PL emission at longer wavelengths and prevent GS PL peak blueshift below 1.3 μm even at 750°C annealing temperature

Conclusion

In summary, our studies shed light on the QD height and base dimensions which can tune the PL emission in the telecommunication window of 1.3-1.55 μm. Blue-shift in the GS PL peak of the QDs on annealing has also been calculated. These modeling and computations will address the need for a valuable design tool for molecular beam epitaxial growers of QD based devices for infrared detector applications. Our computation revealed that QDs tuned at 1.3 μm with lower base size and larger height (L=10 nm. B=5.1 nm) have minimum blue-shift in the GS PL peak, the property which can be well exploited as superior performance devices in optical communication.

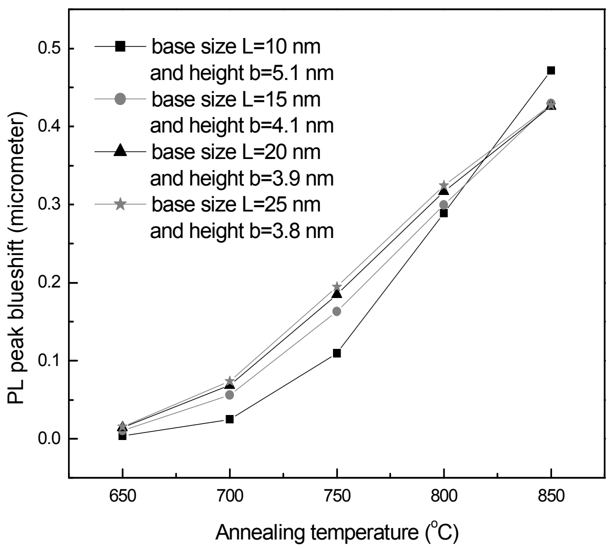

Fig. 4. Degree of GS PL peak blueshift at each annealing temperature as compared to the asgrown QD

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