Theoretical Study on Controllability of Quantum State Energy in an InGaAs/GaAs Quantum Dot Buried in InGaAs

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We theoretically studied the relationship between quantum energy states and structural parameters of an InGaAs/GaAs quantum dot (QD) buried in strained InGaAs, emitting at 1.1 to 1.4 μm. The crystal distortion of the buried QD structure in three dimensions was computed based on the three-dimensional finite element method. Under the computed strain fields, the Schrödinger equation was solved to obtain wavefunctions and eigenenergies. By calculating the dependence on structural parameters, we investigated the controllable range of the ground state energy and the energy separation between the ground state and the first excited state. We found that the energy separation exhibited a maximum value as a function of QD composition, enabling us to identify the composition of the QD structure. The effects of the burying layer composition and QD diameter were also investigated to expand the controllable range of the state energy. We also showed that the wavefunction symmetry was improved by burying the QD in the InGaAs layer. Our results will be useful in developing advanced devices for optical telecommunications and quantum information technology.

Keywords: Quantum Dot, Energy State, InGaAs, Simulation, Symmetry.

1. INTRODUCTION

Many researchers have been investigating the use of self-assembled semiconductor quantum dots (QDs) as an essential material in next-generation photonic devices due to their high optical quality.1-2 There has been great progress in the development of QD devices for optical telecommunication applications, for example, semiconductor laser diodes (LDs),3-4 semiconductor optical amplifiers (SOAs),5,6 and photodetectors7 these technologies are expected to become suitable for practical applications in the near future. Recently, QDs have also shown potential as the main medium for generating and operating qubits in solid-state quantum information devices.8-9 To satisfy the demand for such QD devices, various fabrication techniques have been developed.10-11 One of the most widely adopted structures is InGaAs/GaAs QDs buried in strained InGaAs; this structure realized the first 1.3-μm continuous-wave lasing,12 the record low threshold current density,13 and high-bit-rate stable direct modulation of laser emission.14

To further develop QD devices, precise control of the quantum energy states is very important, because the energy structure dominates the performance of QD optical devices. For instance, the ground-state emission energy should match the wavelength employed in present optical fiber networks. The carrier lifetime of a QD, which depends on the separation between quantum energy states, determines not only the maximum speed and power of the device but also the preservation time of quantum information (qubits). In addition, it has been reported that symmetry of the wavefunction in a QD state is critical for generating quantum-entangled photon pairs.15 (The well-known Stranski-Krastanov-type QD, however, has quite an asymmetric shape.) The QD structure may exhibit improved wavefunction symmetry when buried in a strained InGaAs layer. This is because the crystal lattice of the QD is expanded in the growth direction,16 and the strain just above the QD is smaller in the InGaAs layer than the strain in the GaAs layer above a conventional QD. These effects should reduce the quantum confinement in the growth direction, improving wavefunction symmetry.

In this paper, we theoretically describe how the quantum state energy depends on the structural parameters of a QD buried in InGaAs. Among the numerous structural parameters, we selected the QD composition, the QD diameter, and the composition of the InGaAs layer in which the QD is buried (the “burying layer”). Normally, the indium

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composition of the QD is not a controllable parameter due to mass transport at the growth surface. Nevertheless, the composition is very important since it directly affects the state energy as much as the QD diameter does. The diameter of the QD can be controlled with various growth conditions, such as the growth temperature, the amounts of sources, the substrate orientation, the types of precursors, and the addition of a surfactant. The composition of the burying layer is also a controllable parameter that dominates the height of the quantum confinement potential. Based on the three-dimensional finite element method, we first simulated the elastic strain distribution and then solved the Schrödinger equation using the strain-modified background potential. We investigated the controllable range of the ground-state energy and the energy separation between the ground state and the first excited state using realistic structural parameters.

2. CALCULATION MODEL

We assumed a dome-shaped InGaAs QD; the lower part was buried in an InGaAs layer and the rest was capped by a GaAs layer. The substrate was GaAs. Figure 1 shows a schematic diagram of the buried QD. To apply the three-dimensional finite element method, we regarded the structure as having continuous elasticity and divided it into cubes composed of six triangular pyramidal voxels. The length of each side of the cube was set to be 0.5 nm. In the calculation, because the indium composition was averaged in the voxels and the voxel boundaries were not, in general, aligned with the QD boundaries, the boundaries of the QD structure had a maximum uncertainty of 0.5 nm. We used the values of the material parameters at 300 K. First, we estimated the strain distribution in the structure so that the strain energy was minimized. Figure 1 shows, as an example, the \( z \)-direction strain distribution in one-fourth of the sheets sliced through the bottom, center, and top of the QD. After estimating the strain distribution, we calculated the strain-induced modification of the band gap and effective mass. Then, we solved the Schrödinger equation to obtain the wavefunctions and the eigenenergies of the electrons and holes. Figure 2 shows examples of the calculated electron wavefunctions in the ground state and the first excited states. The nodes of the first excited states exist in the \( x-y \) plane but not in \( z \) direction due to the relatively flat shape at the top of the QD. Because we assumed the QD structure to be symmetric in the \( x-y \) plane, the two excited states were degenerate.

We investigated the influence of the structural parameters of both the QD and the burying layer on the quantum state energies. We assumed a QD diameter of 20 nm, a QD height of 10.5 nm, a burying layer thickness of 6 nm, and a wetting layer thickness of 0.5 nm. These values were reported in the experiments in Ref. [18]. We assumed that the indium composition in the QD was the same as in the wetting layer. We used 0.15 as the standard indium composition of the InGaAs burying layer. Unless otherwise indicated, these parameters were used in the calculations described below.

3. RESULTS AND DISCUSSION

We investigated the influence of the QD composition on the emission wavelength of the ground-state exciton transition, \( \lambda_{g0} \), and the energy separation between the ground state and the first excited state, \( \Delta E_{12} \). The exact value of the QD composition was left unknown in many previously published studies. This was probably because the molecular component of the QD may not be the InAs, even when only indium and arsenic atoms are supplied during QD formation, due to mass transport at the growth surface. The composition of the nano-sized crystal buried in the matrix should be identified carefully. Most analytical methods described in the literature detect averaged information in the sample’s thickness direction. Recently, cross-sectional scanning tunneling microscopy revealed that the indium composition in QDs is not uniform but modulates in the (001) growth direction. However, the profile of the composition in the literature varies. In this simulation, we assumed a uniform QD composition since it gives the approximate general tendency of the relationship between the structure and the state energies. Since the emission energy gives direct information inside the...
Fig. 3. (a) Dependence on indium composition of QD on $\lambda_{gl}$ and $\Delta E_{12}$. (b) Direct strain in z-axis direction at the x–y plane for monolayers higher than the bottom of the QD. The origin of x is set at the center of QD.

quantum confinement potential, this simulation will be useful in estimating the QD composition.

Figure 3(a) shows $\lambda_{gl}$ and $\Delta E_{12}$ as a function of the indium composition of an In$_x$Ga$_{1-x}$As QD. Here, we compare the cases of a QD buried in InGaAs and a QD buried in GaAs. In both cases, $\lambda_{gl}$ increases as the QD indium composition increases. A variation of 0.5 in the indium composition corresponds to $\lambda_{gl}$ shifts of 0.24 $\mu$m and 0.22 $\mu$m for the QDs buried in InGaAs and GaAs, respectively. These figures suggest that an InAs ($x = 1$) QD buried in GaAs can realize 1.3-$\mu$m emission using the dimensions assumed here, i.e., a diameter of 20 nm and a height of 10.5 nm. We note that $\Delta E_{12}$ in both cases has maximum values at intermediate QD compositions. The value of $\Delta E_{12}$ is relatively insensitive to the QD composition around the maximum point. The maximum value is less than 80 meV, even for the QD buried in GaAs, which has a higher potential barrier than the QD buried in InGaAs. Also, we can see that the maximum points for the two burying layers occur at slightly different QD indium compositions, namely, at 0.68 for the QD buried in InGaAs and at 0.65 for the QD buried in GaAs.

Since the dependence of $\lambda_{gl}$ on the QD indium composition differs from that of $\Delta E_{12}$, we can assign an average QD composition by evaluating both $\lambda_{gl}$ and $\Delta E_{12}$. For example, the reported 1.3-$\mu$m emission of a QD buried in InGaAs having $\Delta E_{12}$ of 69 meV indicates a QD indium composition of 0.85.$^{26,29}$ Since we can evaluate the dimensions of the dot structure by electron microscopy and it is not difficult to analyze the indium composition of the burying layer, the combination of such an experimental evaluation and our computational estimation is effective in identifying the QD composition.

Let us discuss the reason why $\Delta E_{12}$ exhibits a maximum value at an intermediate QD indium composition. Since the continuous level is common throughout the surrounding structure, the quantum confinement potential gets deeper as the indium composition of the QD increases. At low indium composition, where the quantum confinement potential is shallow, the increased potential barrier height enlarges the state energy separation at the bottom of the potential. At high indium composition, we think that there are two reasons for the reduced separation between the ground state and the first excited state. One is the expansion of the strain field due to large lattice mismatch of the QD. As shown in Figure 1, lattice distortion is quite small at the center of the QD, where the actual bottom of the confinement potential is located, and there is a highly strained area around this area of small distortion. These high-strain fields expand slightly outwards as the indium composition increases, that is, as the lattice mismatch of the QD increases, as shown in Figure 3(b). Although this expansion is not large, it affects the actual size of the quantum confinement potential. The other reason is that the quantum confinement varies among sublevels. At high indium composition, the wavefunction of the low-order states is well-confined in the deep potential, but the envelope function of the high-order states still penetrates deep into the potential barriers. As a result, when the potential becomes even deeper, the enhancement of the quantum confinement is not effective for the low-order states in comparison with the higher-order states. In addition, a large number of energy states is allowed in the deep potential. These effects reduce the energy-state separation near the bottom of the confinement potential. For these reasons, the maximum value of $\Delta E_{12}$ in Figure 3(a) depends on the material surrounding the QD. Since the continuous energy level is higher for the QD buried in GaAs than for the QD buried in InGaAs, the reduction in energy separation occurs at a comparatively low indium composition for the QD buried in GaAs.

Next, we simulated how the indium composition of the burying layer affects the state energies of the QD buried in InGaAs. The composition, which can be controlled during QD growth, dominates not only the height of the quantum confinement potential but also the three-dimensional lattice distortion distribution. The indium composition of the burying layer is generally set to be less than 0.2, in order to produce optical devices operating at room temperature. Above this value, the optical properties of the QD are strongly affected by the large lattice distortion. For example, the emission efficiency degrades abruptly at high compositions. If we can overcome this drawback by burying QD in InGaAs, it should be possible to achieve high wavelength stability with respect to ambient temperature variations.$^{30}$ Figure 4 indicates the dependence of $\lambda_{gl}$ and $\Delta E_{12}$ on the indium composition of the burying layer.
QD compositions of 0.85 and 0.68 are compared. We see that the indium composition of the burying layer does not have a large effect on $\tau_{\text{gl}}$ and $\Delta E_{12}$. More specifically, a variation of 0.03 in the indium composition of the burying layer corresponds to a $\tau_{\text{gl}}$ change of about 0.01 $\mu$m and a $\Delta E_{12}$ change of about 2 meV. Therefore, it is clear that isolation of the energy states will not be affected much by controlling the indium composition of the burying layer. Since the differentials of both $\tau_{\text{gl}}$ and $\Delta E_{12}$ with respect to indium composition $x$ (that is, the slopes in Fig. 4) are almost independent of the QD composition (0.68 and 0.85), the indium composition of the burying layer can serve as a tuning parameter to make fine adjustments to the state energy.

We then simulated how the QD diameter affects the state energies of the QD buried in InGaAs. Various growth techniques have been developed to control the QD diameter, which is directly related to the state energy and the maximum spatial density. Until now, the size of a QD could be modulated not only in the growth direction but also in the same plane using a growth surface molding technique. QDs buried in InGaAs have been shown to be promising candidates to achieve both high fabrication density and long emission wavelength. We see from Figure 5 that the QD diameter is very useful to control $\tau_{\text{gl}}$ and $\Delta E_{12}$. Here, we again compare QD compositions of 0.85 and 0.68. A variation of 1 nm in diameter corresponds to a change of about 5.1 meV in $\Delta E_{12}$ at the QD composition of 0.85 and a change of about 4.7 meV in $\Delta E_{12}$ at the QD composition of 0.68. We can see that $\Delta E_{12}$ of almost 80 meV can be obtained by a QD buried in InGaAs with a diameter of 18 nm. When the QD composition is 0.85, the emission wavelength is reduced to 1.28 $\mu$m at a diameter of 18 nm. However, other structural parameters, such as the indium composition of the burying layer, can be adjusted to compensate for this small mismatch of $\tau_{\text{gl}}$. If we do not care about the emission wavelength, the QD buried in InGaAs exhibits equivalent energy-state isolation to the QD buried in GaAs.

Finally, we compared the wavefunction symmetry of the ground state electrons of the QD buried in InGaAs and the QD buried in GaAs (Fig. 6). Here, both QDs exhibit a $\Delta E_{12}$ of 78 meV (18-nm In$_{0.15}$Ga$_{0.85}$As QD buried in In$_{0.15}$Ga$_{0.85}$As and 20-nm In$_{0.8}$Ga$_{0.2}$As QD buried in GaAs). The shapes of the wavefunctions in the $x$–$z$ plane are compared since polarization control of a QD-based LD and a QD-based SOA relies on the symmetry in the $x$–$z$ plane. For quantum information devices, perfect symmetry is also desirable to generate entangled photon pairs in any direction. The QD shape is assumed to be symmetric in the $x$–$y$ plane in our calculation. In the simulated intensity plots at the top of Figure 6, there does not appear to be much difference between the QDs, but in the envelope plots at the bottom, we can clearly see that the wavefunction symmetry on the two axes is better for the QD buried in InGaAs than for the QD buried in GaAs. This is because the wavefunction of the QD buried in InGaAs shrinks in the $x$-axis direction and expands in the $z$-axis direction in comparison with the QD buried in GaAs. It should be possible to improve the symmetry further using a thick InGaAs burying layer. Figure 6 indicates that the QD buried in InGaAs is superior to the QD buried in GaAs in realizing symmetric wavefunctions with isolated energy states.

4. SUMMARY

We theoretically studied the controllability of quantum energy states in a quantum dot (QD) buried in InGaAs. We computed the crystal distortion in three dimensions and the eigenenergies of the QD based on the finite
element method. We simulated how the ground-state emission wavelength and the energy separation between the ground state and the first excited state depend on the QD indium composition, the indium composition of the burying layer, and the QD diameter. We demonstrated that the resulting dependencies can be used to estimate the composition of the QD structure. The QD buried in InGaAs was shown to be superior to the normal QD buried in GaAs in realizing symmetric wavefunctions with isolated energy states. This controllability will be helpful in advancing optical device development and future quantum information technology based on QD structures.

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References and Notes


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