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Optical properties of dilute nitrogen GaInNAs quantum dots

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The authors present a theoretical study of the ground state optical transition matrix element in quantum dots (QDs) with a dilute amount of nitrogen. They have investigated the interplay between the nitrogen to the conduction band mixing and piezoelectric field on the optical matrix element. With a reduced amount of indium and an increased amount of nitrogen in the QD, the optical matrix element becomes on the average larger and less sensitive to the variation of both the QD shape and size than is the case of an InAs QD. The optical characteristics at room temperature and 1.5 μm wavelength are discussed. © 2007 American Institute of Physics. [DOI: 10.1063/1.2715096]

Optical properties of dilute nitrogen GaInNAs quantum dots

The GaInNAs semiconductor quantum dots (QDs) with dilute amount of nitrogen substitutional impurities are promising candidates for the active region in the next generation of optoelectronic devices.1–5 It has been found that replacing a small amount of the group V element by nitrogen in a III-V compound reduces the energy gap and increases the electron effective mass, a trend that is quite opposite to the most common III-V compounds, thus offering an alternative route to band structure engineering and improved optoelectronic properties.7 Recent advances in growth techniques facilitate the fabrication of self-assembled QDs with a very small amount (less than 5%) of nitrogen substitutional impurities in the QD region or in the capping layer.8–18 With appropriate tailoring of the QD morphology, this opens the possibility of GaAs-based optoelectronic devices emitting at 1.55 μm and beyond.

The aim of this letter is to identify the factors determining the optical properties of ideal dilute nitrogen QD, its dependence on the QD shape, and size as well as on the interplay between the nitrogen to conduction band mixing and piezoelectric field. In our analysis we ignore any nitrogen atoms spatial inhomogeneity inside the QD.

The strong interaction between the N resonant states and the conduction band edge means that the conventional eight-band k·p method cannot be applied directly to (Ga,In-)NAs and related heterostructures. Improved agreement was found between electron in-plane effective mass as predicted by the band-anitcrossing (BAC) model and that observed experimentally when there are no cluster states nearby in energy, with which the GaNAs conduction band (CB) edge can interact. Thus the electronic structure and optical properties are calculated below by extending the conventional eight-band k·p Hamiltonian to a ten-band model, where additional two spin degenerate N-related bands on the average represent the influence of the nitrogen. Full details of the calculations are given in Ref. 25. From non-self-consistent wave functions, we calculate the dimensionless scaled optical matrix element, \[ I_{yy} = \frac{1}{\hbar m_e P_s^2} |M_{ij}|^2, \]

where \( I_{yy} \) is the interband momentum matrix element of the QD material.
effect. The reduced piezoelectric field in N-containing QDs is less able to stretch or even to confine the hole ground state wave function in piezopotential pockets. This explains why the decrease of the optical matrix element is less abrupt and occurs for larger overall critical QD sizes in N-containing than in N-free QDs. Overall, this analysis suggests that nitrogen (a) reduces the ground state optical matrix element, when compared to the same size N-free QD, and (b) reduces the sensitivity of the optical matrix element on the QD size, providing more flexibility in device design.

To proceed with our analysis of more realistic QD structures, we consider the truncated cone QD shape. The QD size and shape can be described by three independent parameters; the QD height $h$, the aspect ratio $\alpha=h/D_h$, and truncation factor $t=1-D_t/D_h$, where $D_h$ and $D_t$ are diameters of the truncated cone at the base and at the truncation height, respectively. For a full cone we have $t=1$, while $t=0$ for a QD cylinder.

We first investigated the influence of the QD shape on the ground state transition energy and on the magnitude of the optical matrix element for $\hat{e}_x$ light polarization. To identify the influence of the In content on the electronic and optical characteristics we considered two QD materials with the same N content: Ga$_{0.3}$In$_{0.7}$N$_{0.02}$As$_{0.98}$ and In$_{N_{0.02}}$As$_{0.98}$. For Ga$_{0.3}$In$_{0.7}$N$_{0.02}$As$_{0.98}$ QD grown at 450 °C, Nishikawa et al. reported lateral dimension of the dot $D_h=15$ nm, height $h=5$ nm, and PL emission 1.145 $\mu$m at $T=10$ K. It has been reported by Sopasen et al. that the QD islands are generally bigger and of smaller density in In$_{N_{0.02}}$As$_{0.98}$ samples than in the Ga$_{0.3}$In$_{0.7}$N$_{0.02}$As$_{0.98}$ system. For the In$_{N_{0.02}}$As$_{0.98}$ QDs the structural overlap growth temperature is in the range below 420 °C, where its height is estimated to be $h=6.7$ nm, and we assume $D_h=20$ nm. Having fixed the aspect ratio to $\alpha=1/3$ and $D_h=15$ nm for Ga$_{0.3}$In$_{0.7}$N$_{0.02}$As$_{0.98}$ QDs, we change the truncation factor to match the $e_0$-$h_0$ transition wavelength with the measured one. In Fig. 1(a) the variation of the $e_0$-$h_0$ transition wavelength with truncation factor $t$ is presented for both material systems at low temperature and room temperature (RT). For Ga$_{0.3}$In$_{0.7}$N$_{0.02}$As$_{0.98}$ QDs, under the assumptions above, we deduce that the most likely value is $t=0.8$. From the variation of the $t$ factor we estimate that QD shape inhomogeneity might introduce ~10 meV line broadening in both material systems considered. In Fig. 1(b) we present the variation of the optical matrix elements with QD shape. Due to a reduced strain in $D_h=15$ nm Ga$_{0.3}$In$_{0.7}$N$_{0.02}$As$_{0.98}$ QDs the effect of the piezoelectric field is significantly reduced. A larger electron-hole overlap in this system, regardless of the QD size, but a more important question would be to estimate which material will exhibit better optical characteristics at the required wavelength, for instance, 1.3 or 1.5 $\mu$m.

To address this question, we proceed with the analysis of the ground state emission wavelength and optical matrix element dependence on the QD size. To identify the relative role of nitrogen in that context we extend the analysis to three material systems: Ga$_{0.3}$In$_{0.7}$N$_{0.04}$As$_{0.96}$, Ga$_{0.3}$In$_{0.7}$N$_{0.02}$As$_{0.98}$, and In$_{N_{0.02}}$As$_{0.98}$. We assume the same QD shape, keeping constant the truncation factor $t=0.8$ and the aspect ratio $\alpha=1/3$, and varying the cone base diameter in the range $D_b\in(10,30)$ nm. The 1.5 $\mu$m wavelength is achievable in all three material systems, Fig. 2, although with different QD sizes: $D_b=28.2$ nm for (In$_{N}$) ($T=0.01%$, $D_b=19.2$ nm for (In$_{N}$) ($T=70%$, $D_b=16.5$ nm for (In$_{N}$) ($T=100%$, $2%$).
The optical matrix element variation with the QD size is presented for the three systems. For the Ga0.3In0.7N0.04As0.96 and Ga0.3In0.7N0.02As0.98 QDs the optical matrix element is very similar over the whole range of the QD sizes considered. The regions where it is slightly larger in one material than in another are mainly determined by the interplay of the amount of nitrogen character [SN] in the ground state electron wave function, e0, confinement, and piezoelectric field, as described above. For intermediate QD sizes the In0.02Ga0.98 QD’s optical matrix element is significantly (up to 40%) smaller than in the other two systems. This is mainly due to a larger piezoeffect that reduces the e0-h0 overlap. Combining the results from Figs. 2(a) and 2(b) and using the QD size as a parameter, we deduce the variation of the optical matrix element versus wavelength of the e0-h0 transition. At 1.3 μm all three materials exhibit very similar optical characteristics. In this region the small QD size in all three cases provides good quantum confinement, which dominates the optical characteristics. At 1.5 μm and above, the Ga0.3In0.7N0.04As0.96 QDs are clearly the best candidate. Even though larger QD sizes are required than in In0.02As0.98 material for the same wavelength, the reduced piezoelectric field due reduced In and increased N content has less ability to deteriorate optical characteristics. This is another confirmation that an appropriate combination of N and reduced amounts of In can offer better material candidates for the dilute-N QD’s RT-optical characteristics than pure InAs:N material.8

In summary, we have presented a theoretical analysis of the optical characteristics of the ideal dilute nitrogen GaInNAs/GaAs QDs. At RT it is estimated that all material systems considered can exhibit emission wavelength of 1.5 μm and above. We conclude that (a) increased amount of N character in e0 and reduced piezoelectric filed in the QD can provide a better uniformity of the optical matrix element when the QD shape varies, and (b) with a reduced amount of In and increased amount of N (x ~ 4%) the same or better optical characteristics can be achieved at 1.3 and 1.5 μm than with the InAs:N QD material system. Our analysis shows advantages of Ga0.3In0.7N0.04As0.96 over equivalent InAs:N QD material system in the design of QDs operating at 1.5 μm and at RT.

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28The [CH], is reduced to 20% of its maximal value at $k_T \approx 1 \text{ Å}^{-1}$ in Ga0.3In0.7N0.04As0.96 vs $k_T \approx 1.4 \text{ Å}^{-1}$ in Ga0.3In0.7N0.02As0.98.