Optical properties of dilute nitrogen GaInNAs quantum dots

Tomic, S

http://dx.doi.org/10.1063/1.2715096

<table>
<thead>
<tr>
<th><strong>Title</strong></th>
<th>Optical properties of dilute nitrogen GaInNAs quantum dots</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Authors</strong></td>
<td>Tomic, S</td>
</tr>
<tr>
<td><strong>Type</strong></td>
<td>Article</td>
</tr>
<tr>
<td><strong>URL</strong></td>
<td>This version is available at: <a href="http://usir.salford.ac.uk/18649/">http://usir.salford.ac.uk/18649/</a></td>
</tr>
<tr>
<td><strong>Published Date</strong></td>
<td>2007</td>
</tr>
</tbody>
</table>

USIR is a digital collection of the research output of the University of Salford. Where copyright permits, full text material held in the repository is made freely available online and can be read, downloaded and copied for non-commercial private study or research purposes. Please check the manuscript for any further copyright restrictions.

For more information, including our policy and submission procedure, please contact the Repository Team at: usir@salford.ac.uk.
Optical properties of dilute nitrogen GaInNAs quantum dots

Stanko Tomic

Computational Science and Engineering Department, CCLRC Daresbury Laboratory, Warrington, Cheshire WA4 4AD, United Kingdom

(Received 25 December 2006; accepted 15 February 2007; published online 21 March 2007)

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 InNAs QD. The optical characteristics at room temperature and 1.5 μm wavelength are discussed. © 2007 American Institute of Physics. [DOI: 10.1063/1.2715096]

It has been shown that in the conventional InAs/GaAs QD’s (Ref. 27) the optical matrix element initially increases with QD size as the electron and hole wave functions become more localized in k space, providing a better overlap with highly anisotropic (at larger k) bulk optical matrix element. The QD optical matrix element then reaches a maximum for some intermediate “critical” size, beyond which it decreases in larger dots. In larger dots the piezoelectric field produces significant potential “pockets” in the QD bottom corners, in which the whole ground state can be localized. In this case the overlap with the electron wave function is significantly reduced.

In dilute nitrogen QDs two additional phenomena need to be taken into consideration. First, the presence of nitrogen increases confinement of the QD electron wave functions compared to equivalent N-free structures. This means that the ground state electron wave function of the N-containing QD, of the same size as its N-free counterpart, is spread over a larger area in k space, overlapping the highly anisotropic (in k space) bulk optical matrix element, d_e(k). Moreover, it has been shown that the strong N-CB mixing reduces the bulk or quantum well optical matrix element at the band edge. In N-containing bulk, though, the significant decrease of |d_e(k)| occurs at smaller wave vector than in equivalent N-free material, when the electron’s kinetic energy approaches the energy gap which is also reduced in N-containing materials due to the BAC effect. Therefore, above analysis suggests the increased electron confinement effect in dilute N-containing QD implies: (i) a significantly reduced ground state optical matrix element in N-containing QDs of small to intermediate size, where confinement effects dominate over the piezoelectric field effect, (ii) a less steep initial increase of the optical matrix element as the QD size increases, due to a significant (~30%) admixture of the nitrogen character |ψ_N⟩ in the electron wave function, that provides a reduced sensitivity of the optical matrix element on the QD size, and (iii) the “critical” size of the N-containing QD, where the optical matrix element reaches its maximum, is larger than in the N-free QDs. Secondly, the presence of nitrogen reduces the lattice mismatch of the QD material relative to the GaAs matrix. Reduced lattice mismatch reduces strain, which in turn reduces the piezoelectric field in N-containing QD structures. Being more pronounced for larger QD’s, after a certain QD size, the amplified piezoelectric effect eventually dominates over the confinement.
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 \(a=h/D_b\), and truncation factor \(t=1-D_t/D_b\), where \(D_t\) and \(D_b\) 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 \(e\) 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 \(In_{0.02}As_{0.98}\). For \(Ga_{0.3}In_{0.7}N_{0.02}As_{0.98}\) QD grown at 450 °C, Nishikawa \(et\ al.\) \(11\) reported lateral dimension of the dot \(D_b=15\) nm, height \(h=5\) nm, \(9,11\) and PL emission 1.145 \(\mu\)m at \(T=10\) K. \(9\) It has been reported by Sopasen et al. \(8\) that the QD islands are generally bigger and of smaller density in \(In_{0.02}As_{0.98}\) samples than in the \(Ga_{0.3}In_{0.7}N_{0.02}As_{0.98}\) system. For the \(In_{0.02}As_{0.98}\) QD structures the optimal growth temperature is in the range below 420 °C, where its height is estimated to be \(h=6.7\) nm, \(8\) and we assume \(D_b=20\) nm. Having fixed the aspect ratio to \(a=1/3\) and \(D_b=15\) nm for \(Ga_{0.3}In_{0.7}N_{0.02}As_{0.98}\) QDs, we change the truncation factor to match the \(e\)-\(h\) transition wavelength with the measured one. In Fig. 1(a) the variation of the \(e\)-\(h\) 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 \(\sim 10\) 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 \(D_b=15\) 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 shape, is visible in Fig. 1(c). This also underlines a good uniformity of the ground state optical matrix elements. The variation in the optical matrix element is estimated to be between +18% and −12% of its average value of \(I_{100}\) =0.127. In the indium rich, and bigger, \(D_b=20\) nm, \(In_{0.02}As_{0.98}\) QDs the increased lattice mismatch produces a stronger piezoelectric field. At the same time, the increased In content moves the CB edge of the host material downwards on the absolute energy scale, further away from N resonant level, reducing the amount of N-band character in the \(e\) state (\(\langle s_N\rangle\sim 7\%)\), indicating a larger optical matrix elements in this QD system. This is indeed visible in Fig. 1(b), for a cylindrical QD where the piezoeffect is not so influential. Away from \(t=0\), the amplified piezofield has the maximal and minimal values. In Fig. 2(a) the variation of the optical matrix element with the QD shape in two QD material systems at two temperatures as in (a). Open triangles show the variation of the matrix element in \(In_{0.02}As_{0.98}\) when the piezofield is set to zero. (c) The ground state electron and hole charge density and evolution of its overlap with the QD shape change: (upper row) \(Ga_{0.3}In_{0.7}N_{0.02}As_{0.98}\) QDs and (lower row) \(In_{0.02}As_{0.98}\) QDs.

![FIG. 1. (Color online) (a) QD shape variation of the e0-h0 transition wavelength for \(Ga_{0.3}In_{0.7}N_{0.02}As_{0.98}\) (circle) and \(In_{0.02}As_{0.98}\) (squares) at two temperatures: \(T=300\) K (open) and \(T=10\) K (solid). Star presents experimentally observed transition energy as reported in Ref. 9. (b) Variation of the optical matrix element with the QD shape in two QD material systems at two temperatures as in (a). Open triangles show the variation of the matrix element in \(In_{0.02}As_{0.98}\) when the piezofield is set to zero. (c) The ground state electron and hole charge density and evolution of its overlap with the QD shape change: (upper row) \(Ga_{0.3}In_{0.7}N_{0.02}As_{0.98}\) QDs and (lower row) \(In_{0.02}As_{0.98}\) QDs.](image-url)
The optical matrix element variation with the QD size is presented for the three systems. For the Ga\textsubscript{0.3}In\textsubscript{0.7}N\textsubscript{0.02}As\textsubscript{0.98} and Ga\textsubscript{0.3}In\textsubscript{0.3}N\textsubscript{0.02}As\textsubscript{0.98} 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, ε0, confinement, and piezoelectric field, as described above. For intermediate QD sizes the InN\textsubscript{0.02}Ga\textsubscript{0.98} 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 ε0-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 ε0-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 provide good quantum confinement, which dominates the optical characteristics. At 1.5 μm and above, the GaInNAs QD material system in the design of QD devices operating at 1.5 μm and at RT.

![Graph](image_url)

**FIG. 2.** (Color online) (a) Variation of the fundamental optical transition wavelength vs QD size: Ga\textsubscript{0.3}In\textsubscript{0.7}N\textsubscript{0.02}As\textsubscript{0.98} (circle), Ga\textsubscript{0.3}In\textsubscript{0.7}N\textsubscript{0.02}As\textsubscript{0.96} (diamond), and InN\textsubscript{0.02}As\textsubscript{0.98} (squares) at T=300 K. (b) The optical matrix element dependence on the QD size for the three material systems as in (a). (Inset) Evolution of the 0 to 60 charge densities overlaps with the QD size in Ga\textsubscript{0.3}In\textsubscript{0.7}N\textsubscript{0.02}As\textsubscript{0.98} QD. (c) The optical matrix element dependence on the ground state transition wavelength for three material systems obtained from (a) and (b).

27The |â0|2 is reduced to 20% of its maximal value at kx=0.1 Å⁻¹ in Ga\textsubscript{0.3}In\textsubscript{0.7}N\textsubscript{0.02}As\textsubscript{0.98} vs kx=0.14 Å⁻¹ in Ga\textsubscript{0.3}In\textsubscript{0.7}As.0.