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Modeling of intraband absorption for quantum dot-in-well structures with low computational cost

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Abstract. Much effort has been committed to development of quantum-dot-based infrared photodetectors owing to their potential for normal-incidence absorption and low dark current. Quantum-dot-in-well structures offer additional advantages, such as better wavelength tunability and improved carrier collection. This system presents a challenge for modeling of electronic structure, as it requires solution for a complex system (quantum dot plus quantum well) with both discrete levels and the continuum energy spectrum. The Green’s function method, mostly used for such problems, has very high computational cost. Here we use the Finite Element Method to model intraband absorption spectra of quantum-dot-in-well structures within the effective mass approximation.

1. Introduction
Quantum dot infrared photodetectors (QDIPs) have attracted much interest in recent years [1-4], aiming to overcome the limits of HgCdTe and quantum well (QW) detectors. Due to the three-dimensional carrier confinement in the quantum dot (QD), these devices have potential advantages, such as sensitivity to normal incidence radiation and low dark current. Quantum-dot-in-well (DWELL) structures offer additional advantages, such as better control over operating wavelength and improved carrier collection. The DWELL devices rely on transitions between the bound states in the dot and the subbands in the surrounding QWs. The QD-based intersubband photodetector is a promising technology for the 3-12 µm wavelength region.

This system presents a challenge for modeling of the electronic structure, as it combines zero-dimensional QDs and 2-dimensional QWs with discrete and continuous energy spectra, respectively. The Green’s function method is the tool mostly used for such problems [5-6], but it has a very high computational cost. Here we use a simplified approach employing the Finite Element Method within the effective-mass approximation. We find that it has both low computational cost and good accuracy, thus allowing modeling of the intraband absorption spectra for a wide range of QD parameters.

2. Experimental details
We investigated a DWELL system, in which InAs dots are embedded asymmetrically in a GaAs well, surrounded by a thick Al₀.₁Ga₀.₉As barrier. A schematic diagram of the structure is shown in figure 1.
Result of the transmission electron microscopy (TEM) on the sample is shown in figure 2. The dots were found to have a truncated shape with height of 7 nm and width of 35 nm on average. The dot density was estimated as $3 \times 10^{10}$ cm$^{-2}$, corresponding to 60 nm of lateral separation between the dots.

3. Modeling

For all calculations, we employed the Finite Element Method using COMSOL Multiphysics commercial software. Strain effect was taken into account in the continuum-elasticity approximation using standard deformation potential theory. All material parameters were taken from reference [7].

Since the inter-dot distance is more than 50 nm both laterally and vertically, the interaction between the dots is negligible. Therefore, modeling for an isolated QD is a good approximation. We approximated the QW by a large flat quantum box. This allowed us to calculate the quasi-continuum energy spectrum and relevant wave function by solving directly the 3D effective mass problem.

The model includes layers of square boxes with different compositions as described in figure 1. We assumed a dot with truncated-cone shape, positioned in the middle of the thin In$_{0.15}$Ga$_{0.85}$As strain-reducing layer. The wetting layer is considered negligible, as it actually coincide with the strain-reducing layer. As illustrated in figure 2, the dot is positioned asymmetrically in the GaAs well.

Because of In diffusion, the In$_{1-x}$Ga$_x$As dot composition is expected instead of pure InAs. The dot composition was estimated prior to modeling of the intraband absorption spectra, assuming homogeneous composition in the dot. The transition energies between electron and hole levels were modeled for isolated dot using the conventional 8-band strain-dependent $k\cdot p$ Hamiltonian [8-9] and compared to the experimental photoluminescence (PL) data.

For the entire DWELL structure, we modeled the quasi-continuum spectrum of the subbands using only the one-band strain-dependent effective mass approximation. The energies and matrix elements of the transitions between the ground state (GS) of the dot and the excited states of the DWELL structure were determined. (Note that only the GS of the dot is normally occupied in such a device.) Finally, the intraband absorption spectra were simulated by superimposing the Gaussian broadening on the calculated transitions, to account for inhomogeneous distribution in the dot size and geometry.

4. Results and Discussions

The PL data in figure 3 show two distinct peaks at 0.99 eV and 1.04 eV. The low energy peak (PL 1) corresponds to the transition between the ground states of electrons and holes (D0-V0), while the higher energy peak (PL 2) is due to transition between their excited states (D1-V1). When compared to the PL data, the results of multi-band $k\cdot p$ model for isolated In$_{1-x}$Ga$_x$As QD in the GaAs matrix show that the percentage of Ga atoms in the dot is approximately 25-30% (figure 4).
Figure 3. Experimental PL spectra at 300 K.

Figure 4. Calculated transition energies (D1-V1 and D0-V0) for the In$_{1-x}$Ga$_x$As QD as a function of composition at 300 K. Dashed lines show energies of the experimental PL transitions.

We have modeled the optical spectra of the DWELL structures for a wide range of QD geometrical parameters. We found that the best agreement with experiment is achieved for the QD parameters very close to that obtained from the TEM data (figure 2). The modeled spectra for a DWELL with In$_{0.75}$Ga$_{0.25}$As QD using the experimentally deduced parameters are shown in figure 5. The vertical lines are individual transitions while the bold lines show the absorption spectra with superimposed Gaussian broadening of 5 meV. The results show expected strong absorption for $z$-polarized light as compared to the in-plane polarization. The normal-incidence experiments correspond to in-plane polarized light, figure 5(a). From modeling, the 1st and 2nd subbands are present in the well, with transitions to them in the ranges of 4.5-5.9 $\mu$m and 3.9-4.4 $\mu$m, respectively. Peaks below 3.9 $\mu$m correspond to bound-to-continuum transitions. Also from calculations, there are strong absorption peaks corresponding to the transitions between the ground and excited dot states (GS-ES), with peaks at around 6.7 $\mu$m, 7.3 $\mu$m and 8.5 $\mu$m.

Figure 5. Calculated zero-bias transitions at 77 K for polarizations along (a) x/y, and (b) z directions, respectively. Bold lines simulate absorption spectra with superimposed broadening of 5 meV.
Figure 6 shows the experimental photocurrent spectra at various bias voltages. Note that distortions around 4.3 \( \mu \text{m} \) and 5-7 \( \mu \text{m} \) are due to atmospheric absorption. Peak positions are in good agreement with modeling. At low positive bias, figure 6(a), peaks are observed at 3.5 \( \mu \text{m} \) (GS to continuum), 4.2 \( \mu \text{m} \) (GS to 2nd subband), and 5 \( \mu \text{m} \) (GS to 1st subband). At higher positive bias, peaks at around 6 \( \mu \text{m} \) and 7.5 \( \mu \text{m} \) emerge, which we associated with the GS-ES transitions. These transitions are also observed under negative bias, figure 6(b). The subband-related transitions are shifted towards longer wavelength in this case, due to applied electric field and asymmetric dot position in the well.

The photocurrent measurements were performed under normal incidence radiation. However, due to scattering, contribution from \( z \)-polarized component is likely. This is particularly important for the GS-ES transitions (e.g. at 6 \( \mu \text{m} \)), for which the \( z \)-polarized absorption is at least three orders of magnitude stronger than in-plane polarized one.

![Photocurrent spectra](image)

**Figure 6.** Photocurrent spectra obtained at 77 K under (a) positive bias, and (b) negative bias. Shaded bands at 4.3 \( \mu \text{m} \) and 5-7 \( \mu \text{m} \) show atmospheric absorption band.

### 5. Summary

Using a model with low computational cost, we explored electronic spectra of a DWELL structure for a wide range of QD geometrical parameters. Our results show good agreement with the experimental data. The model provides an efficient tool for design of the DWELL systems.

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