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Effect of Asymmetric Well Quantum Dots-in-a-well Infrared Photodetectors on Density of States Using NEGF Formalism

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Abstract

Local Density of State (LDOS) and hence Density of State (DOS) at different energy levels of asymmetric conical shaped InAs/InGaAs quantum dots-in-a-well (DWELL) infrared photo-detector has been calculated through Non-Equilibrium Green’s Function (NEGF) approach to explain the tri-band operation. Method of finite difference is used to solve the kinetic equation of Green’s function and Self-energy is calculated in a recursive manner. Monotonic red shift of spectral response with incremental quantum well width is observed in terms of energy level difference, which is found in good agreement with previously reported experimental data, and the wavelengths corresponding to the peaks of responsivity is estimated from the DOS profile. Relative effect of changing the bottom quantum well width on ground and other higher state energy levels are also reported.

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1. Introduction

With three-dimensional confinement for electrons in the quantum-dot structure, quantum-dot infrared photodetectors (QDIPs) have become a zone of interest for theoretical and experimental studies in recent years. As the epitaxial growth of the III-V semiconductor quantum dot structures has reached maturity, devices now have superior performance characteristics compared to mercury cadmium telluride (MCT) photodetectors because the MCT’s epitaxial growth problems limit the manufacturing yield of large area focal plane arrays. Compared to quantum well infrared photodetectors (QWIPs), QDIPs have additional degrees of confinement, leading to major advantages such as: QDIPs are sensitive to normal-incidence IR
radiation, which is forbidden in n-type QWIPs due to polarization selection rules; QDIPs exhibit comparatively long effective carrier lifetimes (~100s of picoseconds), which has been confirmed by both theory and experiment, and QDIPs exhibit low dark current[^1][^2]. Ideally, QDIPs should show improved performance characteristics such as high responsivity, high detectivity, and high operating temperatures.

The Quantum Dot in a Well (DWELL) detectors, in which the active region consists of InAs quantum dots embedded in an InGaAs quantum well, represent a hybrid between a conventional quantum well infrared photodetector (QWIP) and a quantum dot infrared photodetector (QDIP). Like QDIPs, the DWELL detectors display normal incidence operation without gratings or opto-couplers, while demonstrating reproducible “dial-in recipes” for control over the operating wavelength, like QWIPs[^1]. Moreover, the DWELL detectors also have demonstrated bias-tunability and multi-color operation in the mid wave infrared (MWIR, 3–5 μm), long wave infrared (LWIR, 8–12 μm) and very long wave infrared (VLWIR, >14 μm) regimes. Photodetectors operating in the mid-infrared have many applications in medical and environmental sensing, thermal imaging, night vision cameras, and missile tracking and recognition, mine detection and remote-sensing.

In this paper, the Local Density of State (LDOS) and hence the DOS of the asymmetric DWELL QDIP are obtained using the NEGF method. The responsivity of the DWELL can be understood from the information provided by the DOS. A numerical technique based on the method of finite differences is used to solve the kinetic equation of Green’s function. Self-energy is calculated in a recursive manner. The estimated energy levels obtained by this approach are compared with the experimentally measured responsivity of the asymmetric DWELL QDIP and a monotonic red shift of the Energy level difference (which indicates monotonic red shift of spectral response) with gradual increase of Quantum Well width is theoretically verified.

2. Theoretical Modeling of DWELL QDIP Structure

The DWELL detector grown by MBE, reported in Ref [1], consists of a ten-period active region of 6nm In_{0.15}Ga_{0.85}As, 2.4 ML of InAs, 6 nm In_{0.15}Ga_{0.85}As, and 50 nm GaAs, as shown in Fig. 1(a). The quantum dots are placed in the In_{0.15}Ga_{0.85}As quantum well which is in turn surrounded by the GaAs region. The quantum dots are situated in the upper half of the quantum well and have a conical shape whose base dimension is of 11 nm and height is of 6nm. The QD material InAs is deposited over the substrate and due to the lattice mismatch between deposited material and substrate, the strain is built up gradually. After a critical thickness (2.4 ML) is reached, the two-dimensional growth changes into a three-dimensional one and dislocation free QD islands begin to grow.

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[^1]: Reference 1
[^2]: Reference 2

Figure 1: (a) Cross-section schematic of a 10 layer InAs/InGaAs quantum dot in a well detector, (b) Schematic of the cross section along cylinder axis of the device used for the theoretical model.
For numerical analysis we have modeled the DWELL device as shown in Fig 1(b). 60% of the band gap difference between InAs and GaAs is counted as the conduction band offset.\textsuperscript{4,5} The band offsets calculated are 477 meV between InAs and In\textsubscript{0.15}Ga\textsubscript{0.85}As and 93 meV between In\textsubscript{0.15}Ga\textsubscript{0.85}As and GaAs. The conduction band edge of the In\textsubscript{0.15}Ga\textsubscript{0.85}As is selected as reference energy level. A linear interpolation between two binary values is used to calculate the effective masses in the different materials. The effective masses used for GaAs, InAs and In\textsubscript{0.15}Ga\textsubscript{0.85}As are 0.067, 0.027 and 0.061 (in terms of electron mass) respectively.

For analysis, the device is thought of consisting of array of identical cylinders, where each cylinder contains one quantum dot. To calculate Hamiltonian of the device, a cross section along the cylinder axis is taken and disintegrated into a large number of equally spaced grids. The finite difference method is used to solve the differential equation governing Green’s function. The retarded Green’s function of the system is defined as\textsuperscript{6}

\[
\left( E - H_{op} - \Sigma'(E) \right) G'(x, x'; y, y') = \delta(x - x')\delta(y - y') \quad (1)
\]

Here $E$ is the total energy of electron, $\Sigma'$ is the self energy and $H_{op}$, the Hamiltonian operator of the system, is given by\textsuperscript{7}

\[
H_{op} = -\nabla \cdot \left( \frac{\hbar^2}{2m(x, y)} \right) \nabla + V(x, y) \quad (2)
\]

Here $V(x,y)$ is the potential energy seen by the electron and $m(x,y)$ is the effective mass. The diagonal elements of spectral function is given by

\[
\text{diag}(A(x, y; E)) = -2 \text{Im}[G'(x, x'; E)] \quad (3)
\]

The density of states, which is the number of states per unit energy per unit volume, is given by

\[
N(E) = \frac{1}{2\pi} \text{Tr}[A(x, y; E)] \quad (4)
\]

3. Numerical Calculation

The quantum dot photodetectors under our analysis have an estimated dot density of $5 \times 10^{10} \text{cm}^{-2}$, and the average spacing between two adjacent dots is about 60nm.\textsuperscript{2} Due to this relatively large distance, in our simplified model of the quantum dot photo-detector, the neighboring dots are assumed to be vertically and laterally decoupled, and a quantum dot is modeled so as to be surrounded by semi-infinite contact composed of InGaAs and GaAs layer, and InAs wetting layer. The contact can be thought of being a continuation of cylinder radius and the quantum dot exists at the center of the cylinder.

Modeling quantum dot photo-detectors in such a way gives the benefit of exploiting the property of translational invariance of the contact. The Hamiltonian matrix for the device, which is tridiagonal and Hermitian, is formed by finite difference method and is given by\textsuperscript{8}

\[
H_{op} = \begin{pmatrix}
\alpha_{s1} & \beta_1 & 0 & \cdots & 0 \\
\beta_1 & \alpha_{s2} & \beta_2 & \cdots & \\
0 & \beta_2 & \alpha_{s3} & \beta_3 & \\
\vdots & \ddots & \ddots & \ddots & \beta_{s_{N-1}} \\
0 & \cdots & \cdots & \beta_{s_{N-1}} & \alpha_{s(N)}
\end{pmatrix} \quad (5)
\]
Here,

\[
\alpha_{\nu(i)} = \begin{bmatrix}
    U_{x1} + 2tx_{(i)} + 2ty_{1} & -ty_{1} & 0 & \cdots & 0 \\
    -ty_{1} & U_{x2} + 2tx_{(i)} + 2ty_{2} & -ty_{2} & 0 & \cdots \\
    \vdots & \vdots & \ddots & \ddots & \ddots \\
    0 & \cdots & \cdots & -ty_{(N_{y}-1)} & U_{x(N_{y})} + 2tx_{(i)} + 2ty_{(N_{y})}
\end{bmatrix}
\]

and \( \beta_{(i)} = \begin{bmatrix}
    -tx_{x_{1}} & 0 & \cdots & 0 \\
    0 & -tx_{x_{2}} & \cdots & \vdots \\
    \vdots & \vdots & \ddots & \ddots \\
    0 & \cdots & \cdots & -tx_{x_{N_{x}}}
\end{bmatrix} \)

The self energy term is

\[
\Sigma' = \begin{bmatrix}
    \tau g, \tau^* & 0 & \cdots & 0 \\
    0 & 0 & \cdots & 0 \\
    \vdots & \vdots & \ddots & \ddots \\
    0 & \cdots & \cdots & \tau g, \tau^*
\end{bmatrix}
\]  

\( \text{tx} \) is the coupling energy between adjacent grid points along x direction, and is given by \[9\],

\[
\text{tx} = \frac{\hbar^2}{2m^*a^2} \]  

g_c is the retarded green’s function of a unit cell of the contact, and is solved from the recursive relation \[7\],

\[
g^{-1}_c = ((E + i\eta)I - H_c - \tau g^* e^{\tau}) \]  

4. Results and Discussion

The reported structure in Ref [2] has three color response with peaks at wavelengths of 5, 11, and 25\(\mu\)m. The corresponding energy transitions \( \Delta E \) due to photon absorption at these wavelengths are \( \sim 250, 113 \) and \( \sim 50 \) meV. Our calculated DOS for DWELL structure with bottom quantum well of 6nm (symmetric DWELL structure) is shown in Fig. 2(a). From the calculated DOS, we get E0, E1, E2, E3 (corresponding to each abrupt rise in DOS profile) as -270.3meV, -28meV, 64meV, and 112meV and results in E1 – E0, E2 – E1 and E3 – E2 as 242.3, 92 and 48meV and thus explaining the tri-band operation satisfactorily.

The experimentally measured spectral response of the asymmetric DWELL with increasing bottom well width shows a monotonic red shift \[2\]. This result can be intuitively expected because increasing Quantum Well width means decreasing the confinement for electron and hence the neighboring energy levels comes closer, thus leading to smaller wavelength of photon absorption.

A rigorous theoretical analysis of DOS for various Well width structure yields the same expected result. From fig 2(b), we see, the width of Quantum Well hardly has any prominent effect on the position of ground state energy, though it significantly changes other levels, causing a monotonic shift of DOS towards lower energy level with gradually increasing Well width. An interesting observation is that, the higher energy levels are getting closer to ground state at a rate faster than lower energy level, thus reducing the relative distance between any two energy levels we consider for transition. The corresponding energy levels and their differences are shown (in meV) in the table 1.

It is a point of interest to see how different sites of the device contribute to different energy states. Figure 3 (a) shows the potential profile for the DWELL model with 6 nm bottom half Quantum Well.
From fig 3 (b), we see, at the ground level (E= -278meV), energy state is provided solely by the quantum dot. From figure 3(c), we can see, at the first continuum energy level (E= -15meV), the density of state is concentrated at wetting layer of InAs. Figure 3 (d) reveals that, at second continuum energy level (E= 77meV), the energy states resides prominently at InGaAs Quantum Well sites.

![Graph](image)

Figure 2: (a) Calculated DOS of the DWELL structure (b) : Effect of Changing bottom half Quantum Well width on DOS

| Well Width | E0          | E1          | E2          |
|------------|-------------|-------------|-------------|
| 3nm Well   | -270.3      | -23         | 79          |
| 4nm Well   | -270.3      | -26         | 74          |
| 6nm Well   | -270.3      | -28         | 64          |

5. Conclusion

In this paper, the Density of States of the InAs / InGaAs DWELL structure is determined through the formalism of Green’s function method. Inspite of several approximation and assumption to make the model as simple as possible to reduce computational cost, the energy levels, corresponding to sharp rise of the DOS profile, have closely matched to the expected value of energy state in order to explain the three color operation of DWELL. Furthermore, the effect of asymmetry in the dimension of Quantum well over the spectral response of the DWELL device found experimentally is strongly supported by the theoretical analysis performed in this paper.

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Figure 3. (a): Potential profile of simplified model of the device with symmetric Quantum Well (b): Local Density of State at ground level (c)LDOS at E=-15meV (d) LDOSat E=77meV

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