Photon Absorption in Periodically Regimented Nanostructures

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Abstract. Calculations based on the Effective Mass Approach of the miniband structure in the conduction band, joint density of states and photon absorption coefficient for InAs quantum dots embedded into a GaAs matrix are presented. In our investigation we kept the same volume for the quantum dots (250 nm $^3$) and the separation between quantum dots (3 nm) and changed the aspect ratio in order to determine its effects on the quantities. From the results we draw conclusions that could enlighten the physical processes about photon absorption in regimented nanostructures.

1. Introduction

From the first proposal of theoretical one-dimensional superlattices by L. Esaki and R. Tsu [1] to nowadays, electronics have witnessed revolutionary changes in experimental and theoretical fields, and many researchers in the world have contributed to perform what once was considered just a speculative model. In the recent years two- and three-dimensional regimented arrays of nanostructures has attracted great attention by experimental [2-3] and theoretical [4-7] groups. Therefore, prediction on the physics of such systems is needed to gain insight on how they would work.

In this work we present a study of the confinement and photon absorption by regimented arrays of quantum dots. We calculated the miniband structure, joint density of states (JDOS) and photon absorption for arrays of cuboid InAs quantum dots embedded into a GaAs matrix. For the sake of clarity we did this study for quantum dots having the same volume, but changing their shapes.

2. Theoretical Formalism

The theory for two or three-dimensional periodical arrays of quantum dots share common features with that of regular crystals. Schrödinger equation for these systems is:

$$\frac{-\hbar^2}{2} \nabla \left[ \frac{1}{m(\vec{r})} \nabla \right] \psi_{\phi,n}(\vec{r}) + V_{\text{strained}}(\vec{r}) \psi_{\phi,n}(\vec{r}) = E_n(\vec{q}) \psi_{\phi,n}(\vec{r})$$

(1)

where $m(\vec{r})$ is the space-dependent effective mass, $V_{\text{strained}}(\vec{r})$ is the band profile (from a single band approach) where strain could be considered, $\psi_{\phi,n}(\vec{r})$ is the carrier wave function and $E_n(\vec{q})$ the corresponding eigenvalue. According to Bloch-Floquet theorem, the above $\psi_{\phi,n}(\vec{r})$ has the following structure.
\[
\Psi_{q,\epsilon}(\vec{r}) = \eta_{q,\epsilon}(\vec{r}) e^{i\vec{q}\cdot\vec{r}} \tag{2}
\]

where \(\eta_{q,\epsilon}(\vec{r})\) is a function having the periodicity of the superlattice and \(e^{i\vec{q}\cdot\vec{r}}\) is a plane wave with a phase related to a \(\vec{q}\) vector of the superlattice reciprocal space, the so-called Q space. For a given \(\vec{q}\), the \(\eta_{q,\epsilon}(\vec{r})\) function was expanded using 2197 plane waves (13 in each direction) within the normalized plane wave approach and the resulting Hamiltonian was diagonalized to obtain both \(E_\epsilon(\vec{q})\) and \(\Psi_{q,\epsilon}(\vec{r})\). The absorption coefficient \(\alpha(\hbar\omega_\text{op})\) was evaluated using the method presented elsewhere [4] about photon absorption in periodic nanostructures.

We have done the study for quantum dots having three different shapes: flattened cuboids (\(L_x=10\) nm, \(L_y=10\) nm, \(L_z=2.5\) nm), regular cubes (\(L_x=6.3\) nm, \(L_y=6.3\) nm, \(L_z=6.3\) nm), and elongated cuboids (\(L_x=5\) nm, \(L_y=5\) nm, \(L_z=10\) nm). All of them have the same volume (250 nm\(^3\)) and the separation between neighbour quantum dots is 3 nm for every case. The dots were aligned along the X, Y and Z directions in a tetragonal crystal system. We used the notation for the relevant points in the Q space following the usual name given in the literature for tetragonal crystal systems [8].

3. Results

In this section we show the main results obtained from this study about miniband structure, JDOS and photon absorption.

3.1. Miniband structure and JDOS

Figure 1 shows the miniband structure belonging to the conduction band for the three samples. The lowest value of the first miniband is practically the same for the three cases. The width of the first miniband, i.e. the spreading in energy from the lowest to the highest value within a miniband, goes from 152 meV for the flattened cuboid down to 103 meV for the regular cube case. The miniband structure is crucial to understand the photon absorption process. It is observed how the quantum dot side lengths play a relevant role in the miniband profiles and the degeneracy of the bands.

![Miniband structures for quantum dot arrays with three dots having different shapes (sizes in the text).](image-url)
It is clearly shown that a gap between first and second miniband appears. Selection rules for photon absorption imply $\vec{q}$ vector conservation [4] and therefore the transitions for optical absorption are vertical in Figure 1. Similar gaps are found between higher minibands (for instance, between third and fourth minibands for the flattened cuboid), but the occupancy of these minibands are low and their contribution is negligible in the absorption process. The distance between the first and second miniband could give us an approximated idea about the absorption energies. Regular cube shows the higher vertical separation between first and second miniband ($\sim 0.25$ eV) while the lowest separations are for the flattened cuboid ($\sim 0.1$ eV).

In order to understand the whole photon absorption process, a rough approximation to approach this phenomenon is to consider transitions just between the first and second miniband, assuming a fully occupied first miniband and empty second miniband. Although this is a rough modelling of the problem, this would help us to study these structures in the first steps, and afterwards we shall show more accurate calculations. With this aim we calculated the JDOS for transitions between the first and second minibands and show it in Figure 2. One can identify an absorption threshold for elongated and flattened cuboids about 100 meV and about 200 meV for regular cubes. In the next section we show these values are relevant to understand the absorption coefficient.

![Figure 2. Joint density of States (JDOS) computed for transitions between the first and second minibands for the three studied cases.](image)

### 3.2. Absorption coefficient.

Finally, the absorption coefficient is computed taking into account the ten lowest energy minibands, a light polarized in (1,1,1) direction, and the occupancy factor for each miniband. The latter is a function of the Fermi level. In this work we placed it at the InAs midgap. However, since the calculations where done for a Fermi level far from the carrier states, a shift of $\Delta E$ in the position of the Fermi level just implies a change in the value of the absorption coefficient ($\sim \exp(\Delta E/kT)$) [9], thus the absorption coefficient profile is almost unaffected. In other words, the absorption could be more or less intense but the threshold and transmission energies would be the same. In Figure 3 the absorption coefficient for the three cases is depicted, where a threshold value is found for the absorption coefficient in agreement with those observed in the JDOS. This means that a simple model considering only the two first minibands and computing the JDOS helps to obtain the threshold energies.

Regarding to the absorption coefficient magnitude, a sample with a lower first miniband implies more proximity to the Fermi level, and hence higher occupied states and higher number of available transitions. This is the case of the regular cube and elongated cuboid (Figures 1b and 1c) which have their first miniband slightly lower than the flattened cuboid (Figure 1a), slightly reducing the absorption coefficient values.

It is worth to note the double peak that appears in the absorption coefficient for the elongated cuboid. The peak at low energies is due to transitions between the first and second miniband (Figure
c). The second peak is for transitions between the first miniband and the third and higher minibands. The gap between the second and third minibands (Fig. 1c) corresponds in the absorption coefficient with the deep valley between the two peaks.

![Absorption coefficient graph](graph.png)

**Figure 3.** Comparison between the absorption coefficients obtained for the three different shapes for an incident light polarized in (1,1,1).

### 4. Conclusions

The calculation of the miniband structure and photon absorption coefficient in regimented structures of InAs quantum dots in a matrix of GaAs has been presented. The quantum dot volume has been kept constant at 250 nm³ and three different shapes have been analyzed. The most important feature is the existence of a threshold in the absorption coefficient about photon energies lying in the far infrared region of the spectrum. The thresholds are closely related to the miniband structure and JDOS for transitions between the first and second miniband. According to these predicted features, these periodic systems might be of application in far infrared photon detectors.

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