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Absorption Coefficient in Periodic InAs/GaAs Nanostructures

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Abstract. Periodic nanostructure manufacture has been proposed as a procedure for obtaining new materials with tunable physical properties, such as the photon absorption coefficient. In this work we have theoretically investigated this quantity in ordered InAs/GaAs cubic quantum dot systems. We solved the Schrödinger equation associated with these structures, using a set of $13 \times 13 \times 13$ plane waves at 12,167 equally spaced points of the Q space. We focused on the transitions between minibands arising from the conduction band. We took into account the different effective masses in each material. We included the effects of the strain by taking a conduction band offset of 0.5 eV, corresponding to strained InAs in GaAs.

1. Introduction

During the last few decades, investigations into one-dimensional superlattices have led to interesting applications in optoelectronics [1][2]. Two- and three-dimensional regimented nanostructures would also make available new applications because of the possibility of creating artificial crystalline structures with tunable properties. Therefore, technological efforts have been made to obtain this kind of material.

The physics of two- and three-dimensional periodic nanostructures is not yet well understood. Some works [3][4] have tried to gain an insight into the miniband structure arising from coupling between regimented quantum dots. They used a simple modeling of the systems and obtained some interesting results. Furthermore, other researchers [5] have studied quantization in two-dimensional structures consisting of arrays of crossed quantum wires, and also expect promising physical phenomena.

In this work we present a study of regimented three-dimensional quantum dot arrays. We evaluate the absorption coefficient for optical transitions between states in minibands arising from the conduction bands of InAs/GaAs. Finally we draw our conclusions and suggest future applications of these systems.

2. Theoretical Formalism

We proposed to study the optical absorption coefficient in regimented cubic quantum dot arrays. The quantum dot material is InAs embedded in a GaAs matrix. We included the effects of the strain in the conduction band offset and in the effective masses using the $k\cdot p$ approach of Bir-Pikus [6]. Our investigation focused on cubic quantum dots with an interdot separation equal to the side length of the cube. We took three different cases: array #1 is made up of 3 nm side length cubic quantum dots; array
#2 has quantum dots of 4 nm side length; and array #3 is formed by quantum dots of 5 nm side length. The array alignment is in the [100] direction. The period of the structure is hereafter called “supercell”.

We solved the Schrödinger equation of the system using the plane wave method. Because of the periodicity of the system, the wave functions satisfy the Bloch theorem:

\[ \Psi_{q,n}(\vec{r}) = \eta_{q,n}(\vec{r})e^{iq \cdot r} \] (1)

where \( \vec{q} \) is the wave vector associated with the supercell size and \( \eta_{q,n}(\vec{r}) \) is a function with the same periodicity as the supercell. Since each \( \vec{q} \) is related to several eigenenergies, the subindex \( n \) stands for each of the energy minibands arising from the quantization. It is useful to define a \( Q \)-space to locate each of the eigenstates of the system in the same way as the \( K \)-space is conceived for regular crystalline systems.

3. Miniband Structure

The solution of the Schrödinger equation provides a miniband structure for electrons related not only to the materials used but also to the geometry of the array. Figure 1 shows a part of the miniband structure of array #2. The existence of an electronic energy gap of about 63 meV is noticeable between the lowest energy miniband (from point M in the lowest to point X in the second). Taking into account that optical transitions are vertical in \( Q \)-space, the optical energy gap is about 150 meV (transitions at the X point). This could lead to interesting applications in far-infrared optoelectronics.

![Figure 1. Ten lowest energy minibands of the miniband structure of array #2. These are states arising from energy quantization in the bulk conduction band. The reference of energies is taken at the minimum of the bulk conduction band of InAs.](image)

4. Absorption Coefficient

In order to understand the optical behavior of the system, we carried out calculations of the absorption coefficient for transitions within the miniband structure arising from states in the conduction band. Starting from Fermi’s Golden Rule, we developed the theoretical expression of the absorption coefficient in regimented nanostructures:
\[ \alpha(h\omega_{op}) = \sum_{n_i} \sum_{n_f > n_i} \frac{w_{n_i \rightarrow n_f}(h\omega_{op})}{V} \]  

(2)

where \( w_{n_i \rightarrow n_f}(h\omega_{op}) \) is the absorption probability for transitions going from the \( n_i \) to the \( n_f \) minibands, \( h\omega_{op} \) is the photon energy and \( V \) is the volume of the periodic nanostructure. \( w_{n_i \rightarrow n_f}(h\omega_{op}) \) is obtained from the following expression [7]:

\[ w_{n_i \rightarrow n_f}(h\omega_{op}) = \frac{\hbar^2 \pi |\mathbf{e}|^2}{n_c c_{light} \varepsilon_0 \epsilon_0 \omega_{op}^2} \times \]

\[ \times \left\{ f(E_{n_i}) \int_{0}^{2\pi} \left[ \eta^*_{\mathbf{q},n_i}(r) \mathbf{\nabla} \cdot \mathbf{\eta}_{\mathbf{q},n_f}(r) \right] \delta(E_{n_i} - E_{n_f} - h\omega_{op}) \rho_Q dq \right\} \]  

(3)

\( |\mathbf{e}| \) is the absolute value of the electron charge, \( n_c \) is the mean refraction index in the system, \( c_{light} \) is the speed of light in vacuum, \( \varepsilon_0 \) is the vacuum dielectric constant, \( m_0 \) is the electron rest mass, \( \omega_{op} \) is the photon frequency, \( f(E) \) is the Fermi-Dirac statistic, \( \hat{\xi} \) is the polarization of the potential vector of the photon and \( \rho_Q \) is the density of states in the \( Q \)-space (\( \frac{V}{8\pi^2} \) for the system studied in this paper).

For a given array with a miniband structure, equation (3) provides a result depending on light polarization (\( \hat{\xi} \)) and the position of the Fermi level (in \( f(E) \)). In order to increase the absorption, it is desirable to place the Fermi level between the two lowest minibands. Nevertheless, our calculations indicate that this implies very high levels of doping, and it could lead to undesired effects because of impurities. Therefore, we placed the Fermi level just at the bottom of the bulk conduction band in InAs. This might be related to a medium or high level of doping, maybe close to those doping results reported elsewhere [8].

![Figure 2. Absorption coefficient for the arrays studied for light polarization in [100].](image)
The absorption coefficients for arrays #1, #2 and #3 are shown in figure 2 for light polarization in the [100] direction. The results correspond to optical transitions between the ten lowest energy minibands. We observed the existence of thresholds for photon absorption determined by the miniband structure of the system. For the cases studied, these thresholds are about energies corresponding to far infrared (~200 meV), thus making it possible to propose these systems for use in sensor applications. For the arrays studied, the results provide a greater absorption coefficient for larger dots and greater interdot separations. The reason for this behavior might be the lower width of the lowest energy miniband when decreasing the dot coupling with neighbors, providing an almost constant energy level spread about 20-30 meV and enhancing the absorption for a certain photon energy. On the other hand, array #1 has the lowest energy miniband spread, about 100 meV (see figure 1), and therefore there are many photon energies able to pump carriers from the first to the second miniband, thus decreasing the absorption at the threshold.

A feature of these systems that could be useful for optoelectronic applications is the possibility of removing the carriers after photon absorption through the second miniband of the structure. Carrier transport along the minibands is possible, in contrast with photon absorption by single impurities or single dots. Thus, these systems could be useful for manufacturing QDIPs [9].

In our investigation we used three different arrays, but theoretical investigations could throw light on the influence of dot size and shape or interdot separations in the absorption coefficient, and therefore suggest new periodic nanostructures fitting the desired absorption coefficient profile.

Further, we believe that this type of structure could play an important role in designing intermediate band solar cells. It would be important to achieve the regimentation in order to obtain the miniband structure and to investigate the implications of using different materials in the dot and matrix to find the absorption thresholds of interest for these applications [8].

5. Conclusions
We have investigated the miniband structure formation arising from states of the conduction band in quantum dot arrays of several sizes. Quantum dots are made of InAs embedded in a matrix of GaAs. We took into consideration the stress in the structure, and calculated the absorption coefficient for three different array structures. The results suggest the existence of absorption thresholds at energies close to the optical band gap between the first and second minibands of the structure.

To summarize, we have shown that periodic semiconductor nanostructures could be an interesting topic in optoelectronics, and future studies may clarify their capabilities to develop new applications in this field. We have also suggested future technological applications for them as far-infrared sensors and proposed future theoretical investigations.

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