# Photon Absorption in Regimented Quantum Dot Arrays

A. Luque Rodríguez, S. Rodríguez-Bolívar, and F.M. Gómez-Campos*
Departamento de Electrónica y Tecnología de los Computadores. Facultad de Ciencias. Universidad de Granada, 18071 Granada, Spain. +34 958 241 577
e-mail: fmgomez@ugr.es

***Abstract*— A study of the intraband absorption coefficient in cuboid InAs quantum dot periodic nanostructures embedded in GaAs is presented. The miniband structure of electron states in the conduction band is related to the shape of the quantum dots. The effect of strain is also taken into account in the simulations through a previous 8x8 k•p calculation. We analyze the influence on the absorption coefficient on the miniband structure of the systems.**

***Quantum dots, 3D superlattices, optical absorption***

## I. INTRODUCTION

Research on regimented arrays of quantum dots is an interesting topic due to the possibilities of controlled modifications of optical, electronic and thermoelectric properties of semiconductor materials [1]. Applications in optoelectronic and other electronic devices have been theoretically proposed [1-4] due to their easy tuning properties by means of controlling size, shape, and density of quantum dots.

Arrays of quantum dots are systems that take advantage of those properties to elaborate new materials by making supracrystals, where quantum dots play the role of ordinary atoms in common crystalline materials. In these new systems the electronics states form a miniband structure, labeled by a new parameter, $\vec{q}$. Then a new Q-space arises, and miniband energies would be represented into that space equivalently to the regular dispersion relations $E(\vec{q})$ in crystals.

With the advent of supracrystals the range of applications of quantum dots can be widely extended. An important requirement needed for avoiding an undesirable degradation of these properties is to achieve a good ordered structure in the system. The Stranski-Krastanov method is the most used technique to grow quantum dots, but this is not the most appropriate technique for achieving regimentation because of their random nature. However recently a few papers have been published where ordered nanostructures are developed and characterized, showing excellent agreement between experimental results and theoretical predictions [5-6].

Manufacturing InAs quantum dots in GaAs is a highly developed technique, even to obtain regimented structures [7]. It has been achieved to stack about 20 layers of quantum dots, and hence, it could be a good candidate to carry out an investigation in this topic.

In this paper we analyze the influence of the shapes of the InAs quantum dots in GaAs in an infinite, regular supracrystal. First we present the theoretical framework and the simulations remarks. Then we present and discuss the results obtained. Finally we draw the main conclusions.

## II. SIMULATION OF ARRAYS OF QUANTUM DOTS

We have studied an infinite and regular supracrystal made of a GaAs matrix in which InAs quantum dots are embedded. For the sake of simplicity we have assigned cuboid geometries to the quantum dots.

To simulate the system we have set up a supercell that is repeated periodically in the space in an ordered arrangement. Fig.1 shows the different supercells considered.

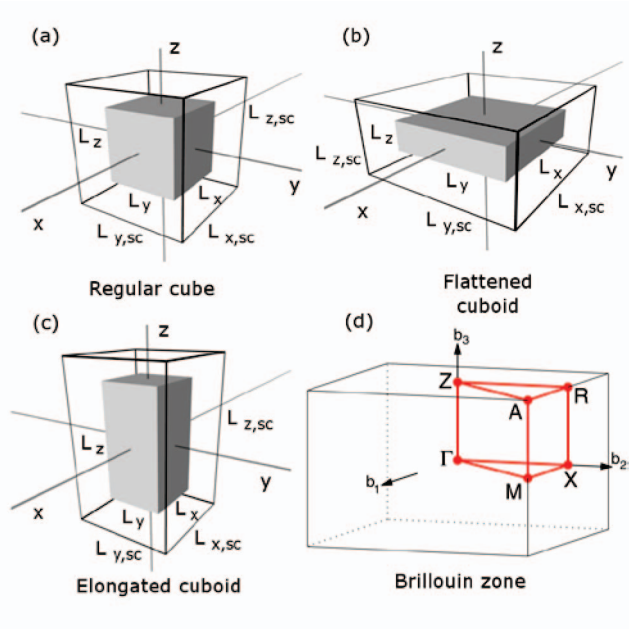

Figure 1. (a), (b) and (c): Supercells for the three studied cases. (d) Q-space of the system and points of interest.

Then we have carried out our investigation within the Effective Mass Aproach (EMA) to solve the Schrödinger equation of the system [4]. This framework could help to gain an insight into the physical behavior of these systems, at least from a qualitative point of view. Previous papers have shown close relations of EMA with more complex frameworks even in the nanometer scale [8], suggesting that EMA could be an useful way of approaching complex nanostructure systems. Corrections could be incorporated later in order to improve the accuracy of the results.

The quantum dots are modeled by means of a potential $V(\vec{r})$, this being zero inside the dots (InAs) and 0.5007eV outside the dots (GaAs), in accordance with previous estimations for the conduction band offset in strained InAs/GaAs [4]. Further, different effective masses were considered inside the dots and in the matrix. We used $m_{InAs} = 0.023m_0$ (obtained from the Pikus-Bir 8×8 k•p Hamiltonian) and $m_{GaAs} = 0.063m_0$ [4].

Considering the periodicity of the system, the Bloch-Floquet theorem provides the structure of the solutions:

$$\Psi_{\vec{q},n}(\vec{r}) = \eta_{\vec{q},n}(\vec{r})e^{i\vec{q}\cdot\vec{r}} \qquad (1)$$

In this manner, the wavefunction is written as the product of a plane wave and a function with the periodicity of the supercell (the period of the structure, depicted in Fig. 1), $\vec{q}$ is the wave vector related to the supercell periodicity, and $\eta_{\vec{q},n}(\vec{r})$ is a $\vec{q}$-dependent function with the same period of potential ($n$ is the miniband quantum number). The range of variation of $\vec{q}$ defines the so-called Q-space, equivalent to the K-space for regular crystals [4][9] but related to the periodicity of the supracrystal.

Introducing the wavefunction in the Schrödinger equation, this is written as:

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

where $m(\vec{r})$ is the position-dependent effective mass.

Due to the periodicity of the system we have solved Eq. (2) using the plane wave approach [10] because of its inherent advantages. In this case, the cuboid geometries studied in this paper allowed us to obtain an analytic expression for the hamiltonian matrix obtained from Eq. (2) by projections of the basis states. To expand the envelope function, we used the basis

$$\psi_{\vec{q},n_x,n_y,n_z}(\vec{r}) = e^{2\pi i\left(\frac{n_x}{L_{x,sc}}x+\frac{n_y}{L_{y,sc}}y+\frac{n_z}{L_{z,sc}}z\right)}e^{i\vec{q}\cdot\vec{r}} \qquad (3)$$

for $n_x$, $n_y$ and $n_z$ ranging from -6 to 6 to guarantee the convergence of the solution in the range of energies studied [11]. $L_{x,sc}$, $L_{y,sc}$ and $L_{z,sc}$ are the lengths of the supercell in each of the directions. Finally the problem was solved by diagonalization.

To calculate the photon absorption, we used the following theoretical expression of the absorption coefficient in regimented nanostructures [4]:

$$\alpha(\hbar\omega_{op}) = \sum_{n_i}\sum_{n_f>n_i}\frac{w_{n_i\to n_f}(\hbar\omega_{op})}{V} \qquad (4)$$

where $w_{n_i\to n_f}(\hbar\omega_{op})$ is the absorption probability for transitions going from the $n_i$ to the $n_f$ minibands, $\hbar\omega_{op}$ is the photon energy and $V$ is the volume of the periodic nanostructure. $w_{n_i\to n_f}(\hbar\omega_{op})$ is evaluated as follows:

$$w_{n_i\to n_f}(\hbar\omega_{op}) = \frac{\hbar^2\pi|e|^2}{n_r c_{light}\varepsilon_0 m_0^2\omega_{op}}\times \int_{Q-space} f(E_{n_i})\left[1-f(E_{n_f})\right]\times \left|\hat{\xi}\cdot\int_{\text{supercell}}\eta^*_{\vec{q},n_f}(\vec{r})\nabla\eta_{\vec{q},n_i}(r)d\vec{r}\right|^2\times \delta(E_{n_f}-E_{n_i}-\hbar\omega_{op})\rho_Q d\vec{q} \qquad (5)$$

where $|e|$ is the absolute value of the electron charge, $n_r$ is the mean refraction index in the system, $c_{light}$ is the speed of light in vacuum, $\varepsilon_0$ is the vacuum dielectric constant, $\omega_{op}$ 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.

## III. RESULTS

In Figure 2 the four lowest minibands of regimented quantum dot systems are depicted for several cuboid dot

shapes. They all correspond to 250 $nm^3$ quantum dots. By setting up the same volume along this study, we would be able

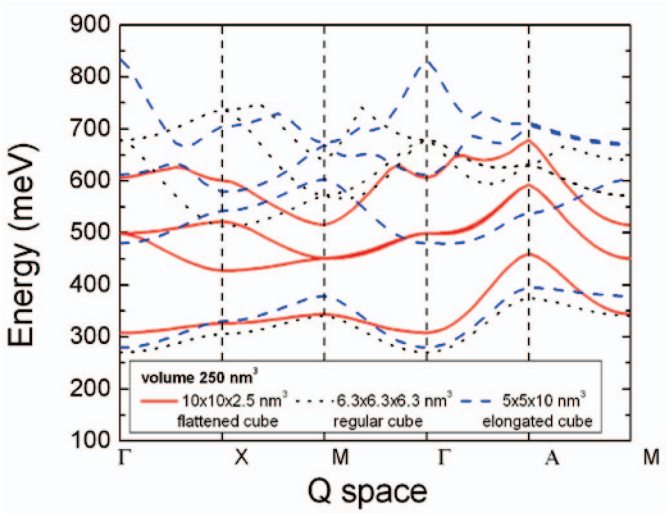


Figure 2. Minibands for the three analyzed samples: flattened cuboids (solid lines), regular cubes (dotted lines) and elongated cuboids (dashed lines).

to discuss the effect of shapes on the optical absorption coefficient.

Quantum dot lengths are indicated in the legend in Fig. 2. They correspond to the three different cases shown in Fig. 1: regular cubes; flattened cubes, in which the length of one of the dimensions is a quarter than those of the long ones; and elongated cubes, with a side twice longer than the others. The flattened cuboid could be considered as a rough approximation to lens shaped quantum dots, while the elongated cuboid would correspond to pillar-shaped quantum dot or nanorod.

The separation between neighbouring dots has been kept at 3 nm along X, Y and Z direction for every case. With this value we obtain a noticeable interaction between dots, and therefore the states form an energy miniband. The corresponding points in the Q-space are also depicted in Fig. 1.

It is clear that a band gap between first and second miniband appears in Fig. 2 for all the cases. The location of the first miniband is practically the same for the three samples with their minima located around the gamma point. However the upper minibands are strongly influenced by the shape of the quantum dot. Furthermore in this figure it is clear that the typical degeneration obtained in a regular cube is broken in the other two cases because of their geometry.

Figures 3 and 4 show the computed absorption coefficient for the three previous studied samples for light polarization in (1,0,0) and (1,1,1) directions. When light polarization is in the (1,0,0) direction the allowed transitions for the absorption lead to a well-defined threshold value for each shape: about 12,42 μm (0.1 eV) for flattened cuboids, about 6,21 μm (0.2 eV) for regular cubes, and about 4,97 μm (0.25 eV) for elongated cuboids. This behavior could be analyzed in terms of the transitions between the minibands shown in Fig. 2: from X to M points in the Q-space the minibands are almost parallel, favoring a particular photon energy that could be related with that threshold (optical transitions are vertical in this representation). Paying attention to transitions along that direction clearly show that the energy of the absorbed photon would be approximately the same for regular cubes and elongated cuboids, both being about 200 meV. The energy for the absorbed photon in the flattened cuboid case is about 100 meV. This is noticed in Fig. 3, where the absorption threshold takes place for greater wavelengths in flattened cuboids. This relation shows the importance of transitions along the X-M direction, revealing the relevance of the states in the boundaries of the Brioullin zone in the Q-space.

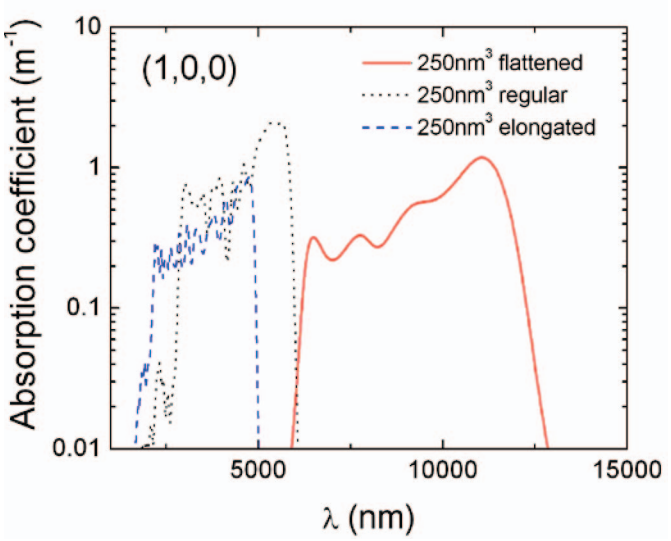


Figure 3. Absorption coefficient for three different samples for light polarization in the (1,0,0) direction. Fermi energy was placed at the midgap of the quantum dot. Samples with 250 $nm^3$ and three different shapes were used to analyze the effect of changes in the shape.

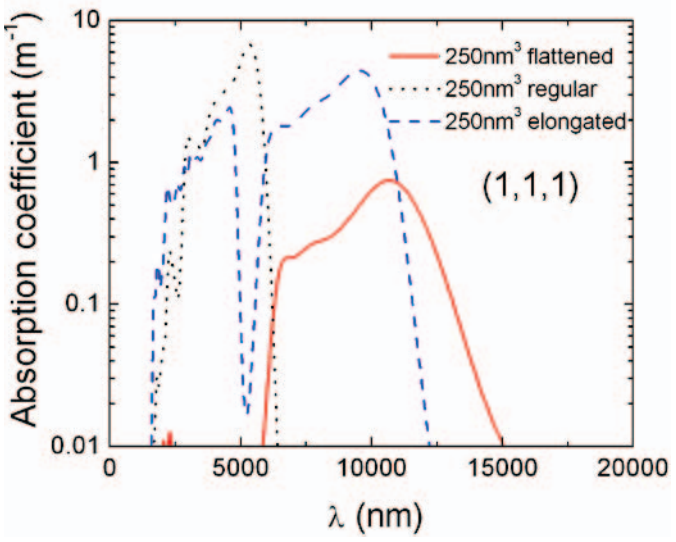


Figure 4. Absorption coefficient for three different samples for light polarization in the (1,1,1) direction. Fermi energy was placed at the midgap of

the quantum dot. Samples with 250 $nm^3$ and three different shapes were used to analyze the effect of changes in the shape.

In regards to Fig. 4 it is noticeable that light polarization may also influence in these thresholds. Flattened cuboids shift the threshold to higher wavelengths, but elongated cuboids show a dramatic change in the absorption profile. The cause for this change might be the existence of selection rules applying for these regimented systems, blocking absorptions between the lowest energy minibands for (1,0,0) that are allowed when light polarization is along (1,1,1). The z-component in the light polarization, in combination with the asymmetries and degenerations of elongated quantum dots in the z-direction, could be the cause of this behavior.

## IV. Conclusions

We have calculated the absorption coefficient in arrays of 250 $nm^3$ InAs quantum dots embedded in GaAs and found thresholds in the photon absorption coefficient at about 12,42 μm, 6,21 μm and 4,97 μm for flattened, regular and elongated cuboids respectively. We also have investigated the dependence of threshold with light polarization, finding interesting changes for elongated cuboids. These thresholds are in the far infrared region of the electromagnetic spectrum and could be used to develop detectors.

Studies about the existence of thresholds in the absorption coefficient for other quantum dot volumes and its dependence with light polarization are underway.


## Acknowledgment

This work was carried out within the framework of research project TEC2010-16211, supported by the Spanish Ministerio de Ciencia e Innovación.


## References


[1] T. L. Lazarenkova, and A.A. Balandin. “Miniband formation in a quantum dot crystal”, Journal of Applied Physics, 89, 5509 (2001).

[2] C.W. Jiang, and M.A. Green. “Silicon quantum dot superlattices: Modeling of energy bands, densities of states, and mobilities for silicon tandem solar cell applications”, Journal of Applied Physics, 99, 114902 (2006).

[3] F. M. Gómez-Campos, S. Rodríguez-Bolívar, et al. “Bandgap calculation in Si quantum dot arrays using a genetic algorithm”, Physica E: Low-dimensional Systems and Nanostructures, 41, 1712 (2009)

[4] S. Rodríguez-Bolívar, F. M. Gómez-Campos, et al. “Miniband structure and photon absorption in regimented quantum dot systems”, Journal of Applied Physics, 109, 074303 (2011)

[5] V. B. Verma, N. L. Dias, et al., “Bandstructure Engineering With a 2-D Patterned Quantum Well Superlattice”, IEEE Journal of Quantum Electronics, 47, 417 (2011).

[6] V. B. Verma, V. C. Elarde, J. J. Coleman, “An Analytical Model for the Ordered Nanopore Array Diode Laser”, IEEE Journal of Quantum Electronics, 45, 10 (2009)

[7] J. S. Wang, S. H. Yu, Y. R. Lin, H. H. Lin, C. S. Yang, T. T. Chen, Y. F. Chen, G. W. Shu, J. L. Shen, R. S. Hsiao, J. F. Chen, J. Y. Chi, “Optical and structural properties of vertically stacked and electronically coupled quantum dots in InAs/GaAs multilayer structures”, Nanotechnology, 18, 015401 (2007)

[8] S. Rodríguez-Bolívar, F. M. Gómez-Campos, J. E. Carceller, “An atomistic-based correction of the effective-mass approach for investigating quantum dots”, 104, 104309 (2008)

[9] F. M. Gómez-Campos, S. Rodríguez-Bolívar, A. Luque-Rodríguez, J. A. López-Villanueva, J. E. Carceller, “Intraband photon absorption in edge-defined nanowire superlattices for optoelectronic applications“,Journal of Applied Physics, 108, 124307 (2010)

[10] Y. Ngo, S. F. Yoon, W. J. Fan, “Effects of size and shape on electronic states of quantum dots“Physical Review B, 74, 245331 (2006)

[11] S. Rodríguez-Bolívar, F. M. Gómez-Campos, A. Luque-Rodríguez, J. A. López-Villanueva, J. E. Carceller, IEEE-NANO 2009, 9th IEEE Conference on Nanotechnology, 707, (2009)