Sección Especial: VI Reunión Española de Optoelectrónica – Optoel'09

On the application of periodic quantum wire nanostructures in optical sensors

Sobre la aplicación de nanoestructuras periódicas de hilos cuánticos en sensores ópticos

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Recibido / Received: 16/09/2009. Versión revisada / Revised version: 18/11/2009. Aceptado / Accepted: 19/11/2009

ABSTRACT:

Las nanoestructuras periódicas han sido propuestas como materiales artificiales que muestran características únicas. Un ejemplo de este tipo de sistemas, obtenido experimentalmente, consiste en una matriz bidimensional de hilos cuánticos paralelos colocada sobre una matriz similar girada 90 grados. De tal manera, los cruces entre los hilos cuánticos se distribuyen en dos dimensiones, y pueden comportarse como una matriz ordenada de puntos cuánticos. Este sistema se espera que muestre una estructura de bandas particular, dando lugar a interesantes interacciones con la luz que podrían ser útiles para el desarrollo de generaciones futuras de sensores ópticos.

Key words: Periodic Nanostructure, Quantum Wire, Superlattices, Miniband Structure, Absorption Coefficient, Silicon.

RESUMEN:

Periodic nanostructures have been proposed as artificial materials showing unique features. An example of this kind of systems, obtained experimentally, consists on a two-dimensional parallel quantum wire array placed on a similar array turned 90 degrees. In such a way, the crossings of the quantum wires are arranged in two dimensions, and could behave as a quantum dot ordered array. This system is expected to show a particular band structure giving rise to interesting interactions with light that could be useful for development of future generations of optical sensors.

Palabras clave: Nanostructura Periódica, Hilo Cuántico, Superredes, Estructura de Minibandas, Coeficiente de Absorción, Silicio.

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1. Introduction

Because of the interesting possibility of tuning the physical properties of matter, periodic nanostructures have been proposed as materials with unique features for applications in electronics and optoelectronics [1,2]. In the same manner than band structure appears in regular solid state crystals, the periodicity of the electrostatic potential profile in such systems give rise to the appearance of a miniband structure within conduction and valence bands [1-3], having bandgaps and effective masses closely related to the nanostructure geometry instead of being uniquely determined by atomic elements and their spatial arrangements as regular crystals.

Electrically, they usually exhibit high effective masses, thus may not being useful for most applications related to carrier transport. Nevertheless, this is an issue in exploration [4]. Optically, they open interesting fields of application not only by the availability tune of their optical properties, but also for the possibility of turning indirect bandgap materials into systems with increased optical absorption coefficients. This is especially striking for developing new silicon applications in optoelectronics, i. e. optical sensors. Since silicon technology is hugely developed nowadays, exploring its application in optoelectronics has been an interesting field of investigation, since its indirect bandgap have relegated it during decades to a second level of importance in optoelectronics.

Nevertheless, periodic nanostructure physics investigation is an interesting issue further than silicon. In particular, III-V materials have also been proposed for manufacturing these systems [3,4].

In this work we investigate the optical absorption coefficient of one of these periodic nanostructures made of silicon and silicon dioxide for intraband transitions (i.e. the initial and final state come from the bulk conduction band). The nanostructure is composed by two parallel silicon quantum wire arrays placed in such a manner that a two-dimensional connection point array is observed. These connection points behave somewhat like ordered quantum dot arrays [3,4], and the implications of this fact are manifested in the absorption coefficient.

This communication is organized as follows: in section 2 we describe the periodic nanostructure in detail; in section 3 we summarize the way we modelled the system to study it theoretically; section 4 gathers the main results achieved in this investigation; and finally we draw the main conclusions in section 5.

2. Description of the periodic nanostructure

The nanostructure under study is depicted in Fig. 1. It could be basically described as two quantum wire periodic arrays rotated 90 degrees and placed one of the top of the latter. Both arrays are embedded into another material having a greater band gap, in such a way that carriers would be confined in the wire structure. The procedure of fabrication of these nanostructures has been reported previously [5]. Regarding its physical behaviour, previous works [3,4] have suggested that these structures could behave both as quantum dots, confining the carriers in the crossings of the wires, and also as quantum wires, by interconnecting adjacent crossings. Further, and probably the most interesting feature of such systems, is the dispersion relation arising from the periodic repetition of the same structure in the space. This leads to behaviour similar to regular crystals, but being possible to tune its properties by changing sizes and materials. In this manner, interaction with light could be controlled, being possible to obtain interesting absorption coefficients. In particular, it is possible to achieve photon absorption by interband transitions.

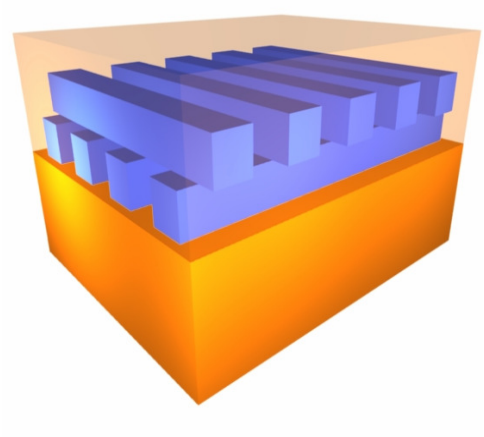

Fig. 1. Studied system. It is plotted in blue a section of the silicon quantum wire arrays. In orange (both solid and with transparency) is represented the silicon dioxide capping layer.

3. Modelling the system

Regarding the composition of the system, we studied the case where the quantum wire array is made of silicon, meanwhile the capping material is silicon dioxide. There are two main reasons why we studied this system: first of all, many efforts are currently devoted to use silicon technology for most of optoelectronics applications because the wide existing knowledge about silicon manufacturing, thus trying to overcome the drawbacks of bulk silicon indirect gap. Secondly, the described structure has been demonstrated to be possible to fabricate (although not using silicon dioxide as barrier but air) [5].

Our purpose is to study the band structure arising from electrons in this system. We used a conduction band offset between the wires and capping material equal to 3.25 eV. We modelled square-section quantum wire arrays having 2 nm side length, and 2 nm separation between them. The geometry of the system is depicted in Fig. 1.

In our study we considered the ellipsoidal anisotropy and nonparabolicity of the silicon conduction band [6]. The procedure used in this work to consider nonparabolicity and anisotropy of the conduction band has been described in detail elsewhere [6,7]. These effects are especially important when modelling nanostructures, where the single effective mass approach falls down. Further, the connection with more complex approaches, such as atomistic modelling can be estimated [8]. However, the effective mass approach provides a simpler framework to obtain a first physical insight on the systems under study, and it is especially useful when trying to obtain macroscopic magnitudes such as the absorption coefficient. Qualitative behaviours could be also predicted, and after that, more accurate theoretical results might be obtained in future calculations using more complex frameworks.

The miniband structure was obtained by solving the Schrödinger equation of the system:

$$T\psi(\vec{r}) + V(\vec{r})\psi(\vec{r}) = E\psi(\vec{r}), \qquad (1)$$

T being the kinetic energy operator (having the nonparabolicity and anisotropy into account), $V(\vec{r})$ being the electrostatic potential (considering the conduction band offset arising from the heterostructure), E the eigenenergies and $\psi(\vec{r})$ the electron envelope functions. It is worth to note that the T operator was included in the calculation having into account the existence of different energy levels for each valley because of the ellipsoid orientation.

In order to solve the problem, we considered that periodic systems fulfil the Bloch theorem:

$$\psi(\vec{r}) = e^{i(q_x x + q_y y)}\eta(\vec{r}), \qquad (2)$$

where $\eta(\vec{r})$ is a function with the periodicity of the cell, and q_x and q_y are quantum numbers arising from the periodicity in X and Y directions (see Fig. 2 for the cell of the periodic structure). Equivalently to regular crystal formalism, Bloch theorem in these systems provides a Q-space similar to regular K-space. The two-dimensional periodicity of this mesh gives rise to a two-dimensional Q-space.

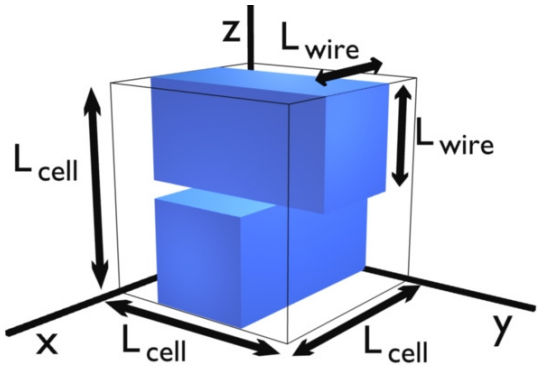

Fig. 2. Cell of the periodic nanostructure. Its repetition in the x and y direction provides the studied system of Fig. 1. In the z direction there is no repetition. Capping layers above and below the cell are modelled as hard barriers.

Having in consideration the periodicity of $\eta(\vec{r})$, it is possible to expand this function in Fourier series. As a result, we obtain the band structure of the nanostructure. Therefore, it is necessary to clarify which would be the period of the structure. In Fig. 2 we depicted the cell providing the whole system by two-dimensional repetition in the *XY* plane.

4. Results

We investigated the band structure of the described system. As an example, in Fig. 3 we plot the seven lowest energy minibands from electronic states in valleys having x-oriented ellipsoids of the periodic nanostructure using L_{wire}=2 nm and L_{cell}=4 nm. This is just a part of the dispersion relation $E(\vec{q})$ of the system. It is worth to notice that the system will have minibands up to 3.25 eV, where the continuum spectrum has its minimum energy because of the capping layer. Nevertheless, they would be almost totally empty, except the lowest ones, i.e. those represented in Fig. 3. Besides the electronic states located in the *x*-oriented ellipsoids, there are states in the *y* and *z*-oriented ones providing additional minibands with particular features. Minibands arising from combination of electronic states in different ellipsoids have been considered having negligible effects.

It is interesting to notice in Fig. 3 the existence of direct bandgaps in the structure (thus reinforcing photon absorption). Further, the low amplitude of the minibands would not noticeably favour transitions from top to bottom of minibands, since the whole miniband would be almost equally populated and similar photon energies would be required for transitions.

Finally, the most important photon absorption may be found about 100 meV because the bandgap between first and second minibands.

Regarding the absorption coefficient, we evaluated it under several conditions:

- Fermi level corresponding to pure silicon. Light polarization in the *x* direction.
- Fermi level corresponding to pure silicon. Light polarization in the *z* direction.
- Fermi level corresponding to moderate doped silicon. Light polarization in the *x* direction.
- Fermi level corresponding to moderate doped silicon. Light polarization in the *z* direction.

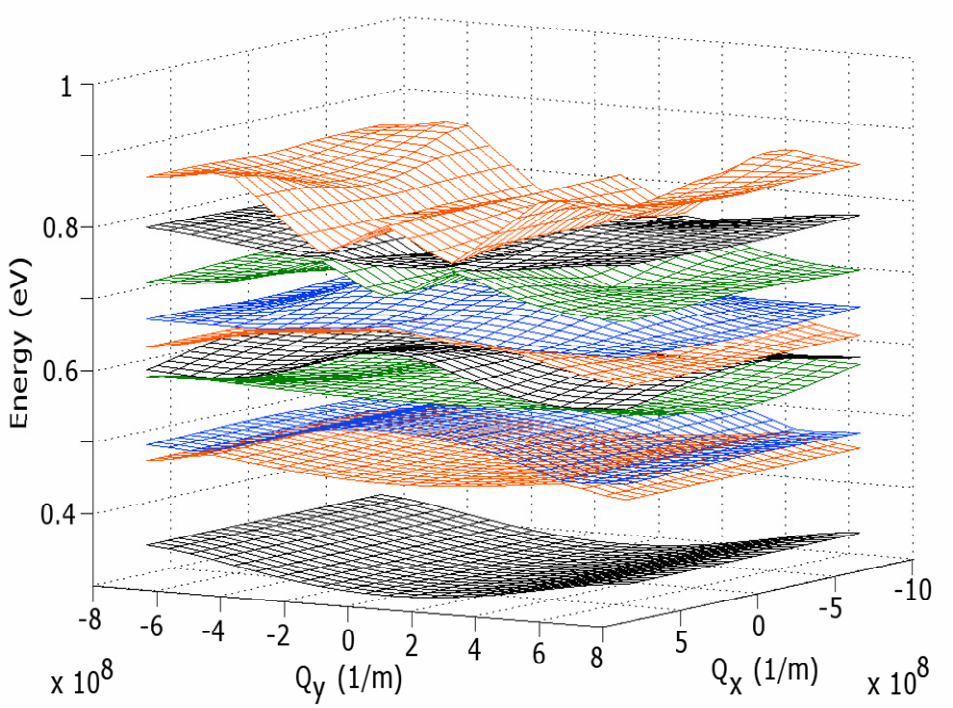

Fig. 3. Miniband structure arising from electronic states in valleys with *x*-oriented ellipsoids. The reference in energies is placed in the bottom of the bulk silicon conduction band.

The influence of the Fermi level would be relevant for populating the lowest energy minibands. The absorption coefficient should be low when the Fermi level is placed far from the miniband structure (i.e. few electrons in the minibands), and it is expected to be higher when the population of those minibands is increased.

With this idea in mind, we used two different positions of the Fermi level: we placed it in the energy corresponding to the middle of the bulk bandgap to simulate pure silicon and, in order to simulate doped silicon, the Fermi level was placed 200 meV below the bottom of the bulk conduction band (this corresponds to moderate doping).

In regards to light polarization, the different features of *z*-oriented ellipsoid minibands could lead to different absorption coefficient for polarization parallel to the confinement direction in comparison with *x* or *y* light polarizations. In consequence we investigated *x* and *z* polarizations to see this effect.

For the sake of simplicity, we considered absorption between the ten lowest energy minibands. Using this criterion, the probability of occupation of states in the highest miniband of this system is around 10^{-6} times lower than the lowest energy miniband. In this manner, absorption by carriers in upper minibands may be negligible.

Figures 4 and 5 represent the results obtained after this study. At a first glance it is noticeable the similitude between the respective (a) and (b) graphs. This fact has an easy explanation, since Figs. 4 and 5 represent the absorption coefficient for two different Fermi level positions. The closer the Fermi level to the conduction band, the higher population in the bands and, in consequence, the higher absorption coefficient. Not relevant changes in the shape of the curves are expected, but only a change in the values. Thus, our results suggest that the coefficient is increased more than 10^6 times by means of semiconductor doping.

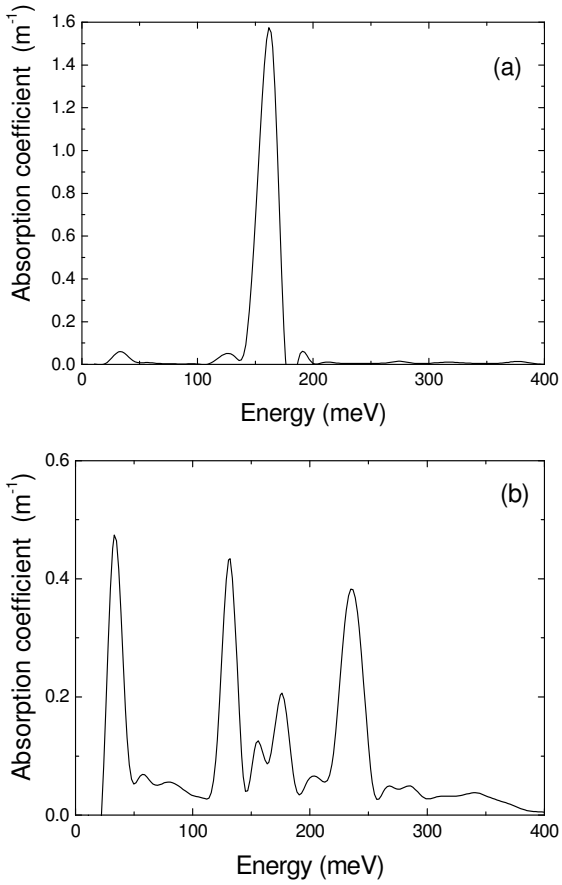

Fig. 4. Optical absorption coefficients vs. photon energy for (a) pure silicon and light polarization in the *x* direction and (b) pure silicon and light polarization in the *z* direction.

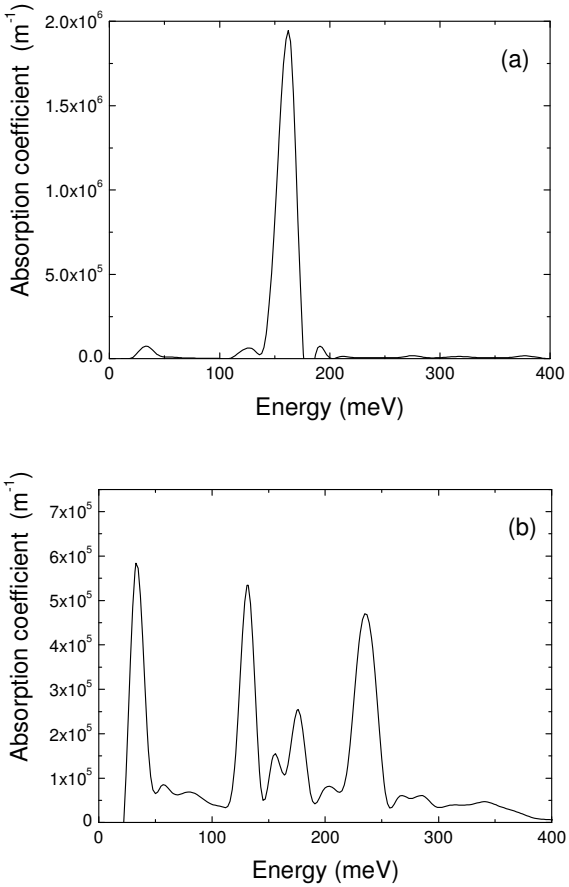

Fig. 5. Optical absorption coefficients vs. photon energy for (a) doped silicon and light polarization in the *x* direction and (b) doped silicon and light polarization in the *z* direction.

Comparing (a) and (b) curves, we observe a well defined absorption at energies around 160-170 meV in the (a) plots, meanwhile the (b) plots show several peaks in the absorption coefficient. This suggests a possible use of these structures for far-infrared light detection for x polarized beams (a). Further, the absorption peak seems to correspond with the energy gap between the lowest one and the second miniband of the structure, thus being possible in principle to scale the system for obtaining absorptions at other photon energies.

After our analysis, light polarized in the z direction (b) seems to be absorbed in a not so selective way, since several peaks are observed. This fact could be explored in more detail in order to know what kind of applications could provide the studied structure.

Both (a) and (b) have approximately the same threshold for absorption. The reader can observe how the absorption starts above a certain photon energy about 10-20 meV. We believe that this is caused by the miniband structure provided by valleys with z-oriented ellipsoids. Electrons in such valleys give rise to a miniband structure with very low energy bandgaps. Although Figs. 4(b) and 5(b) clearly show an absorption coefficient having a peak at this energy, Figs. 4(a) and 5(a) have an almost negligible peak around it. Therefore, the results show that certain miniband structure features would be apparent for certain light polarizations, whereas changing the polarization would reveal more clearly other characteristics firstly hidden. In particular, (b) plots slightly show the peak arising from the 160-170 meV x-oriented ellipsoids bandgap.

5. Conclusions

In this work we have studied the physics of light interaction with a certain periodic silicon-based nanostructure. Firstly, we have calculated the miniband structure of the system, observing energy gaps in the same manner than regular semiconductor crystals. After that, we have analyzed the absorption coefficient, suggesting that moderate doping could provide high values of it. Further, for certain light polarization it would be possible to reveal the existence of those bandgaps in the miniband structure, thus opening new trends in the search of novel silicon-based optoelectronic sensors.

Acknowledgements

This work has been sponsored by project TEC2007-66812, supported by the Spanish Secretaría de Estado de Universidades e Investigación, Ministerio de Educación y Ciencia.

