ELECTRONIC STRUCTURE OF A 2D ARRAY OF QUANTUM DOTS

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ABSTRACT

In this work we study the electronic structure of a 2D array of quantum dots within the tight binding approximation. The confining potential is emulated by a modulation in the hopping parameters of the system, which can be changed from weak to strong coupling between the dots. The obtained electronic structure shows arising of flat bands when the antidot region is increased. Such a behaviour points out the presence of discret energy levels of single dots, that should be present in the case of isolated quantum dots.

INTRODUCTION

The current development of crystal growth techniques have allowed the fabrication of two dimensional nanostructure arrays, and even lattices, such as quantum dots (QD) lattices, which constitutes a new generation of artificial structured materials with controlable electronic and optical properties [1][2]. Lee *et al.* has shown that it is possible to tune the size, orientation and the number of QDs in the basis of the QD crystal unit cell. This is achieved by means of epitaxially self-assembling of QDs on a coherently strained layer [1]. A good understanding on the transport and optical properties of this new systems is necessary to make their possible applications in quantum effect devices a reality. The electronic structure of QD lattices has been found using a variety of methods, for example augmented plane wave calculations (APW) [4] and envelope function approximation [3], where QDs are depicted shematically. As in *real crystals*, coupling between artificial atoms (QDs) leads to formation of minibands due to the splitting of discrete energy levels of single dots, generating an *artificial crystal*.

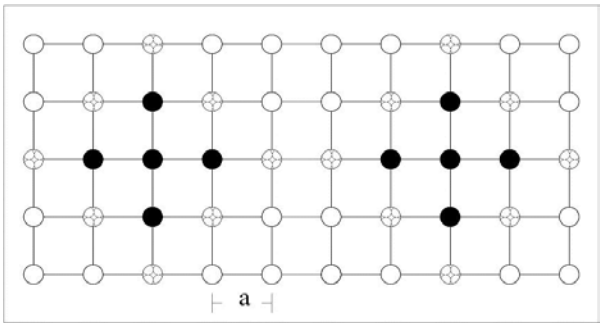


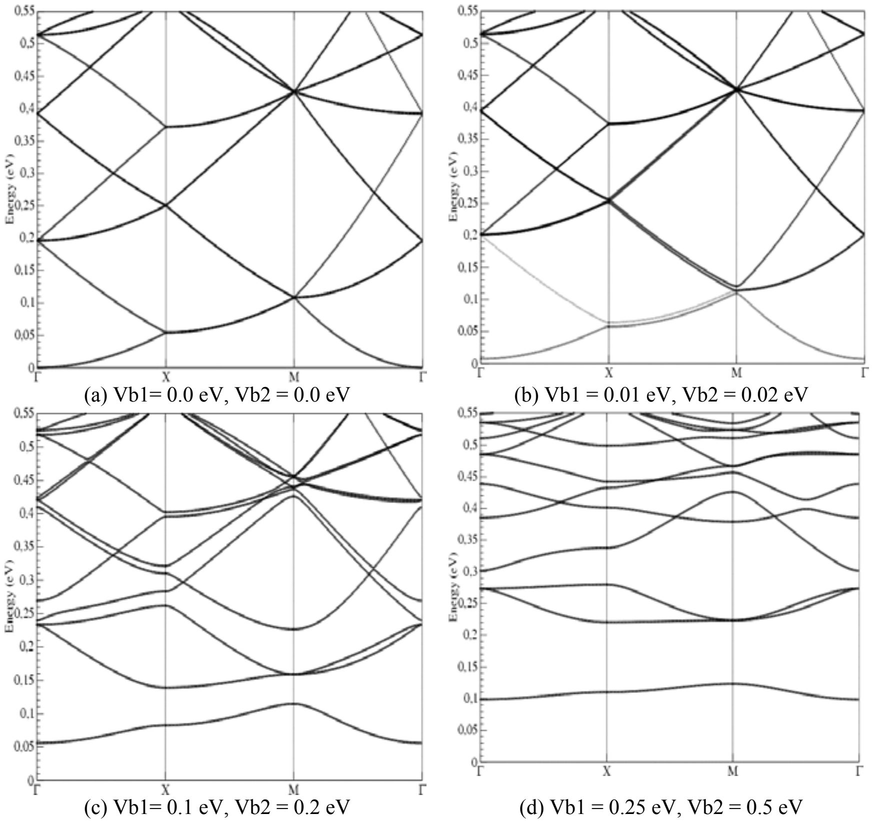
Figure No.1 : Two unit cells with 25 sites each one. The QD lattice parameter is 5a

Or s

In this work we simulate a 2D QD square lattice by means of a tight binding model and we make a qualitative study on the dependence of band structure with both the dot size and the strenght of the confining potential. In the next section we sketch the model employed. In section 3 the obtained results for QD lattices with 25 and 81 sites per unit cell are shown. Finally, our conclusion is given in section 4.

MODEL

We use a model proposed by Neto and Schulz [5] where the QD lattice is modeled by a square host lattice of s-like orbitals, which has a periodic modulation in the hopping parameters. The site self energy and the hopping parameters for the host lattice are choosen to get the GaAs effective mass of the conduction band bottom, m*=0.067mo. This is done throughout the relation [6]: $V^{j,j+1}_{ii} = \hbar^2/m^*a^2$ where $V^{j,j+1}_{ii}$ is the hopping parameter, m* is the effective mass and a=20 Amg is the host lattice parameter.



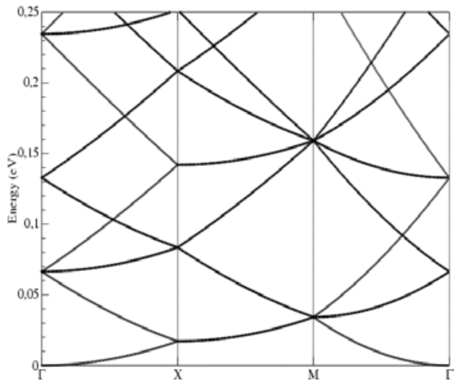
(a) Vb1= 0.0 eV, Vb2 = 0.0 eV (b) Vb1 = 0.01 eV, Vb2 = 0.02 eV

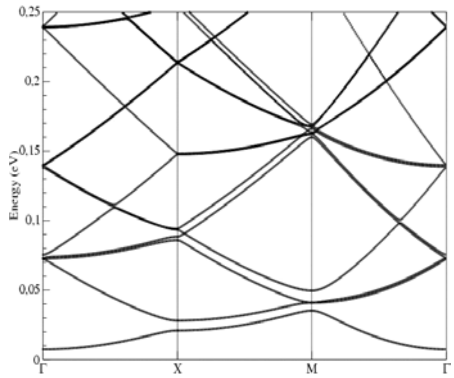
(c) Vb1= 0.1 eV, Vb2 = 0.2 eV (d) Vb1 = 0.25 eV, Vb2 = 0.5 eV

Figure No. 2: QD lattice band structure, unit cell: 5x5

In this case $V^{j,j+1}_{ii}$ relates two nearest neighbor sites in the same row of the unit cell. The values for the hopping parameter and the site self energy are: $V^{j,j+1}_{ii}$ = 0.142 eV and ⌫=0.568 eV respectivelly ($V^{j,j+1}_{ii}$=⌫/4). In order to emulate the QDs, the hopping parameters are changed for certain sites in the unit cell. In figure (1) we show two unit cells with 25 sites each one; sites marked and black ones have a hopping parameter lesser than that of the host lattice (white sites). In this way, when the unit cell is moved to whole space, we have a QD laticce formed by the white sites (dot region) surrounded by marked and black sites which form the antidot region.

The modulation strenght is related with the site barrier height. For white sites (dot region) the barrier height is zero, while for marked and black sites the barrier heights are V_{b1} and V_{b2} respectivelly. Then the hopping parameters in terms of barrier height are: V'= (⌧-V_{b1})/4 and V''= (⌧-V_{b2})/4 for marked and black sites respectivelly. Note that for $V_{b1}=V_{b2}=0$ we return to the host lattice case, where there is not modulation in the hopping parameters.





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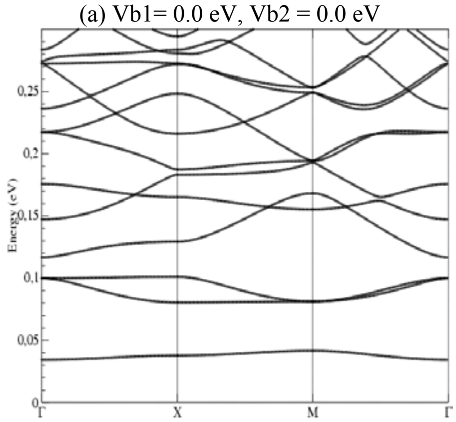

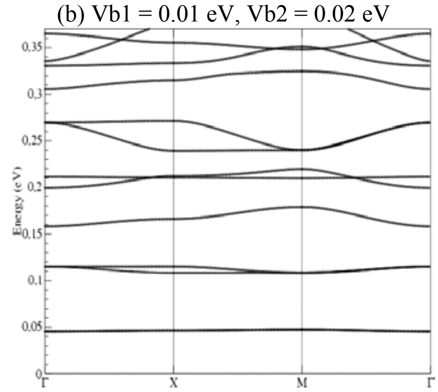

(c) Vb1= 0.1 eV, Vb2 = 0.2 eV (d) Vb1 = 0.25 eV, Vb2 = 0.5 eV

Figure No. 3: QD lattice band structure, unit cell: 9x9

RESULTS

We generate QD lattices with different sizes of unit cell using the same geometry (marked sites forming a rhombus) and calculate their band structure for several modulations i.e. barrier heights. The results are shown in figure (2) for 5x5 unit cell, and in figure (3) for 9x9 unit cell. The employed barrier heights are also shown. Comparing figures (2) and (3) we can observe that the band structure is a function of the modulation as the unit cell size; this is explained in terms of the number of sites belonging to the antidot region since, as the unit cell grows, the antidot region take up a greater space in the unit cell compared with the dot region. In general the quantity:

$$N_{rel} = \frac{whitesites}{blacksites}$$

will be a measure of coupling between the dots. For the 5x5 unit cell $N_{rel} = 2.4$ and for 9x9 unit cell $N_{rel}=1.6$. This means that QD are less interacting for big unit cells, actually it is displayed by the flat bands in the electronic structure of 9x9 unit cell lattice compared with that of 5x5 unit cell lattice, fig (3).

We have calculated the band structure for $V_{b1}=V_{b2}=\infty$, in such case the QDs are uncoupled, and the band structure shows the discrete energy levels of single dots; our result display a good agreement with the analytical values found for a infinite circular potential well, which ratio is equivalent to that of the dot region.

CONCLUSION

The coupling between the dots leads to formation of minibands. The behaviour of band structure shows the possibility of tailor the electronic properties of QD lattices by the change in the unit cell size and the strength of the modulation. The energy gaps are of the order of a few meV as is usual for nanostructures; then in a real device, the transitions between this minibands will require absortion of FIR radiation.

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