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Análisis autosimilar de pozos cuánticos cuasirregulares delta dopados tipo n en GaAs
Selfsimilar analysis of n-type delta-doped quasiregular GaAs quantum wells

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Resumen

Se estudia la esctructura electrónica de pozos cuánticos delta dopados tipo n en GaAs, en el cual el sistema de multiples pozos es construido de acuerdo a la secuencia de Fibonacci. Los bloques *A* y *B* corresponden a pozos delta dopados con una densidad de impurezas n_{2DA} y n_{2DB}, y el mismo ancho de los pozos. La aproximación de Thomas-Fermi, el modesemi-empírico de enlace fuerte (tight-binding) sp^3s^* incluyendo el espín, el modelo de empalme de la función de Green y la matriz de transferencia fueron implementados para obtener el potencial de confinamiento, la estructura electrónica y la autosimilaridad del espectro. La fragmentación del espectro electrónico se presenta cada vez que los bloques *A* y *B* interaccionan, y aumenta a medida que la diferencia de impurezas entre *A* y *B* aumenta. La función de onda del primer estado de las bandas fragmentadas presenta características críticas, esto es, no es un estado localizado ni extendido, presenta características de autosimilaridad. Por lo tanto, las características cuasiregulares se conservan independientemente de la complejidad del sistema y pueden afectar el funcionamiento de los dispositivos basados a estas estructuras.

Palabras clave: Delta-dopado QWs, densidad de estados, Fibonacci, multicapas, fragmentación

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Abstract

We study the electronic structure of n-type delta-doped quantum wells in *GaAs* in which the multiple well system is built according to the Fibonacci sequence. The building blocks *A* and *B* correspond to delta-doped wells with impurities densities n_{2DA} and n_{2DB}, and the same well width. The Thomas-Fermi approximation, the semi-empirical sp^3s^* tight-binding model including spin, the Surface Green Function Matching method and the Transfer Matrix approach were implemented to obtain the confining potential, the electronic structure and the selfsimilarity of the spectrum. The fragmentation of the electronic spectra is observed whenever the building blocks *A* and *B* interact and it increases as the difference of impurities density between *A* and *B* increases as well. The wave function of the first state of the fragmented bands presents critical characteristics, this is, it is not a localized state nor a extended one as well as it has selfsimilar features. So, the quasiregular characteristics are preserved irrespective of the complexity of the system and can affect the performance of devices based on these structures.

Keywords: Delta-doped QWs; density if states, Fibonacci, multilayers, fragmentation

Introduction

It is well known that some features of the aperiodic order appear in different parts of nature. Aperiodic order or order without periodicity has emerged to properly describe an increasing number of complex systems. A typical example of order without periodicity is the sequence of Fibonacci numbers $F_n = 1, 1, 2, 3, 5, 8, ...$ or its symbolical analog constructed using two type of building blocks *A* and *B* as well as the successive application of the substitution rules $g(A) = AB$ and $g(B) = A$. The result is a set of letters (*A, AB, ABA, ABAAB,* etc.) perfectly ordered but not periodic. The Fibonacci numbers are peculiar since they appear from chemistry, biology to astrophysics [*Maciá, 2006, 397*]. From the technological stand point the aperiodic or quasiperiodic multilayer structures have attracted a lot of attention due to the peculiar characteristics of their electronic spectra: fragmentation, selfsimilarity, critical wave function and fractality [*Pérez, 2001, 3689*]. These characteristics are the results of interplay between the short-range and long-range effects in these systems. The most promising applications of quasiregular multilayers have been as electronic and optic filters, specifically their most spectacular result is in the field of non-linear optics with the generation of second and third harmonics [*Zhu, 1997, 843*].

It is important to mention that most of the mentioned studies have been performed using simple systems such as rectangular quantum wells. However, from the experimental stand point this is not a limitation and other quantum well systems like triangular, parabolic or delta-doped can be readily achieved. From a fundamental perspective the latter [*Wood, 1980, 383; Schubert, 1985, 608*] are ideal to test if the quasiregular characteristics are preserved irrespective of the complexity of the system.

In this work, we calculate the electronic spectra of delta-doped quantum well multilayers arranging according to the substitution rules of the Fibonacci sequence. The letter *A (B)* corresponds to delta-doped quantum well with impurity concentration n_{2DA} (n_{2DB}) and well width d_{wA} (d_{wB}). The study is performed within the framework of the semi-empirical sp^3s^* tight-binding method including spin, together with the Surface Green Function Matching Method as well as the Transfer Matrix model. The confining potential of the Fibonacci delta-doped quantum well system is modeled analytically by means of the Thomas-Fermi approximation. We find that irrespective of the complexity of the system the fragmentation, selfsimilar and critical characteristics of the electronic spectra are well preserved. However, some special conditions have to be fulfill in order to obtain the quasiregular characteristics: 1) certain degree of

interaction between the starting delta-doped quantum wells have to be warranty and 2) a higher impurity concentration ratio (n_{2DB}/n_{2DA}) improves the mentioned characteristics.

Method: To describe the potential profile of the delta-doped quantum wells we have used the Thoma-Fermi approximation, which provides us an analytical expression of the form [*Ioriatti,1990, 8340*]:

$$V^*(z) = -\frac{\alpha^2}{(\alpha|z-l|+z_0)^4}, \quad \text{.....(1)}$$

where $\alpha = 2/15\pi$ and $z_0 = (\alpha^3/\pi n_{2D}^{au})^{1/5}$. Here l and n_{2D} represent the location and impurity concentration of the delta-doped quantum well. We use this expression to build our quasiregular system choosing appropriately the location (l_A and l_B) and impurity concentration (n_{2DA} and n_{2DB}) of the starting blocks *A* and *B* as well as subsequently applying the substitution rules of the Fibonacci sequence, *g(A) = AB* and *g(B) = A*. To calculate the electronic structure, we use the semi-empirical sp^3s^* tight-binding aproximation including spin together with the Surface Green Function Matching Method (SGFM) and the Transfer Matrix approach [*Vogl, 1983, 365; Priester, 1988, 8519; García, 1992*]. Within these approximations it is straightforward to calculate the electronic spectra through the Green function and its relation to the Density of States [*García, 1992*]. Finally, the confining potential of the Fibonacci delta-doped quantum wells is taking into account through the modification of the diagonal parameters of the tight-binding hamiltonian following Graf and Vogl [*Graf, 1995, 4940*] and the generalization proposed by Vlaev and Gaggero-Sager [*Vlaev, 1998, 1142*].

Results and Discussion: In order to reduce the time of calculation we have taken the Density of States at the origin of the two-dimensional Brillouin zone, $k_x = k_y = 0$, and projected it to the central part of the inhomogeneous slab, this is at the middle of the Fibonacci delta-doped quantum well system. Under these conditions we refer to the Density of States (DOS) as Local Density of States (LDOS).

We find, through LDOS calculations, that in order to obtain fragmentation it is important that the delta-doped wells of the starting blocks, *A* and *B*, present significant interaction. This can be warranted reducing the width (d_{wA} and d_{wB}) of the starting blocks. We also obtained a higher

fragmentation as the ratio between impurity concentrations, n_{2DB}/n_{2DA}, increases, Fig. 1. Likewise, the fragmentation is enhanced for high generations *(g)*, Fig. 2. With this information at hand, we can investigate other peculiar characteristics of the quasiregular systems such as selfsimilarity and critical wave functions.

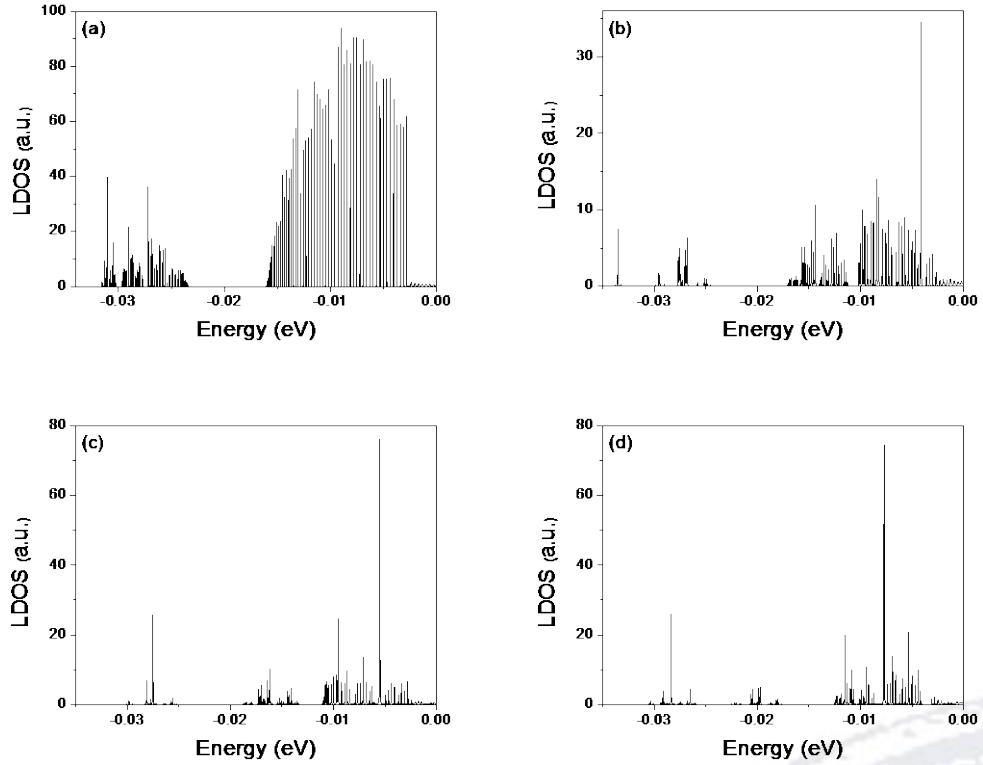
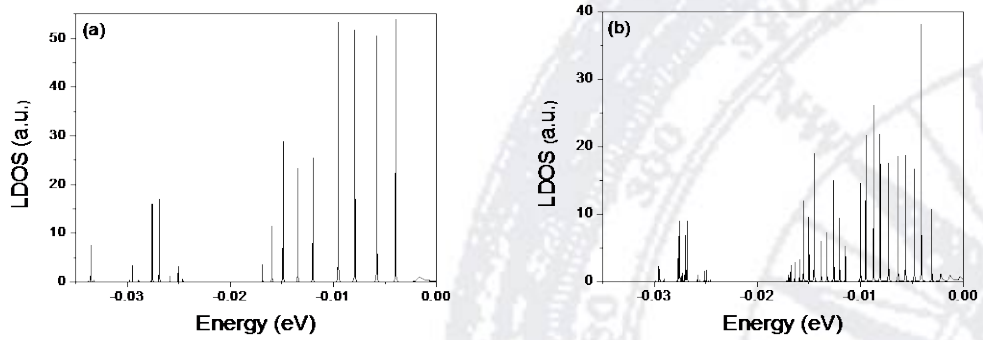


FIGURE 1: Local Density of States of Fibonacci delta-doped quantum wells for the set of parameters: $d_{wA}=d_{wB}=100$ MLs, g=10 and $n_{2DB}=3.0$ a) $n_{2DA}=3.1$, b) $n_{2DA}=3.5$, c) $n_{2DA}=4$, and d) $n_{2DA}=5$. The impurity concentrations come in unit of 10^{12} cm^{-2}.



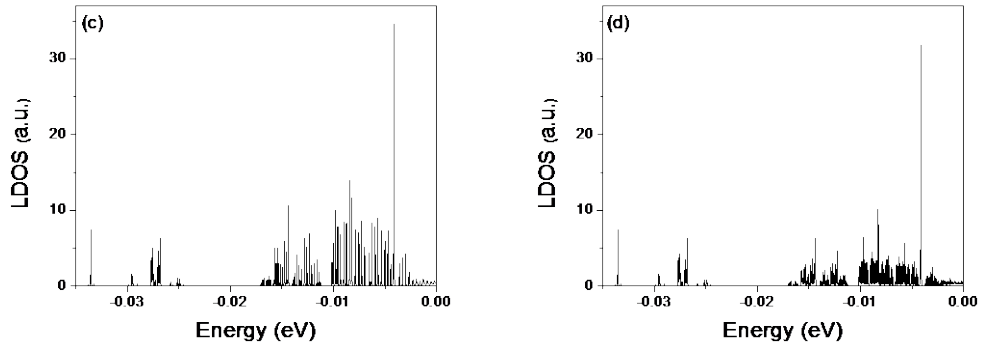
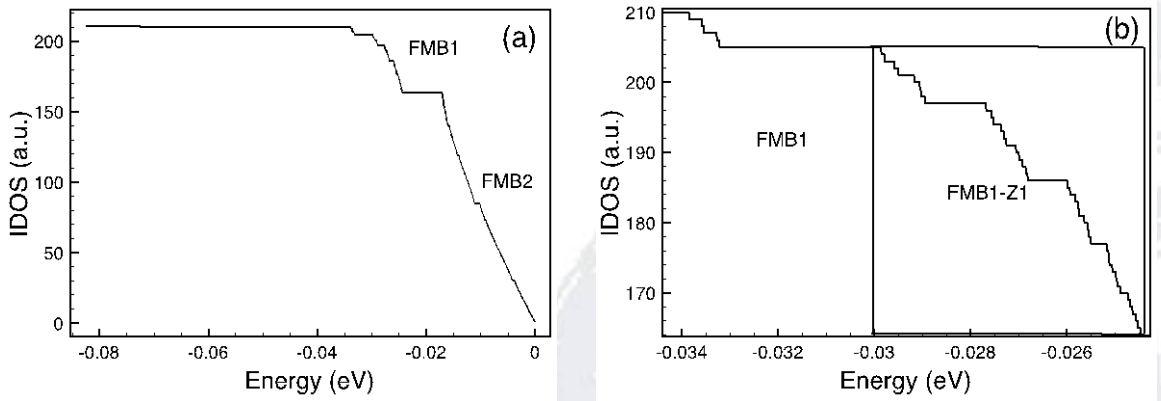


FIGURE 2: Local Density of States of Fibonacci delta-doped quantum wells for the set of parameters: n_{2dB}/n_{2DA}=3.5/3.0, $d_{wA}=d_{wB}$=100MLs, and a) g=6, b) g=8, c) g=10, and d) g=12. The impurity concentrations come in unit of 10^{12} cm^{-2}.

According to our computational possibilities, the best system to analyze the mentioned characteristics is a Fibonacci delta-doped quantum well system with $d_{wA} = d_{wB} = 100$ *MLs*, $n_{2DB}/n_{2DA} = 3.5/3.0$ and $g = 12$.

In Fig. 3 we show the Integrated Density of States (IDOS) of the mentioned system finding two fragmented bands FMB1 and FMB2, respectively. Taking amplifications of FMB1 successively, Fig. 3 (b), (c) and (d), we can appreciate the self-replicating character of the electronic spectrum.



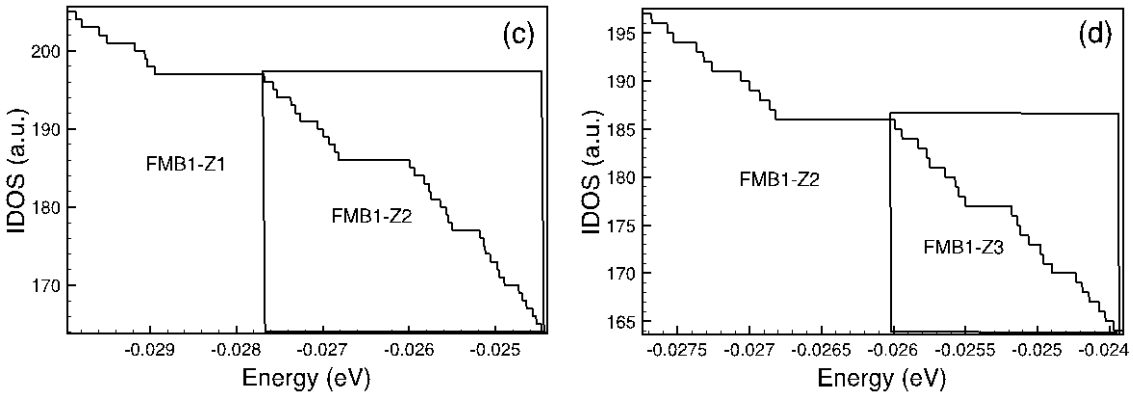


FIGURE 3. Integrated Density of States of Fibonacci delta-doped quantum wells for the set of parameters: n_{2DB}/n_{2DA} = *3.5/3.0,* $d_{wA} = d_{wB}$ = *100 MLs,* and g = 12.

The critical nature of the wave function is presented in Fig. 4. To obtain this result we have taken the spectral strength of the first state of FMB1 as well as its amplification, Fig. 4 (a) and (b), respectively.

Other useful characteristic in quasiregular systems is the fractal dimenison [*Pérez, 2001, 3689*]. This characteristic can be calculated through the box counting method [*Pérez, 2001, 3689*]. In our case, as a preliminar result, we have computed the fractal dimension for particular case, D(q=0). The Fibonacci delta-doped quantum well system used corresponds to the following parameters: d_{wA}=d_{wB}=100MLs and g=7, giving a value of D(q=0)=0.5895.

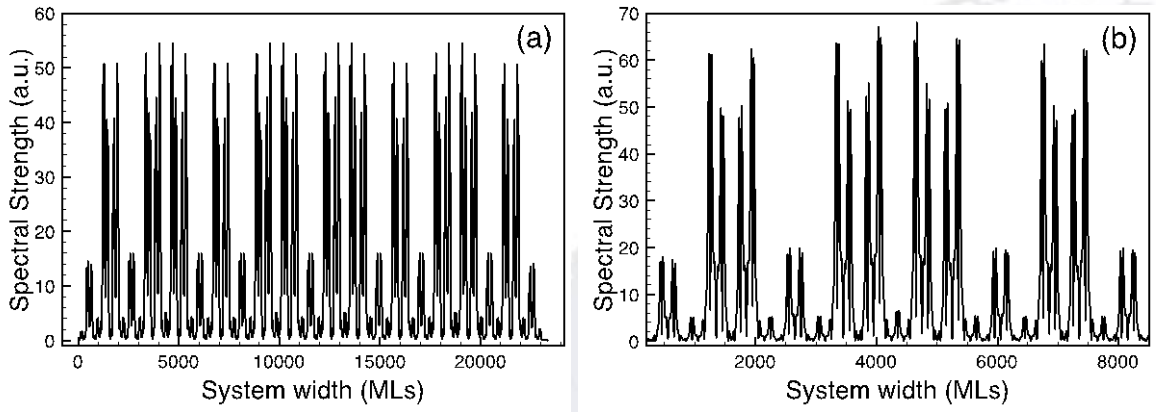


FIGURE 4. Spectral Strength of the first state of the fragmented band FMB1 of Fig. 3.

Conclusion: In summary, we find that the fragmentation, selfsimilar and critical nature of the electronic spectra of quasiregular quantum well systems are well preserved irrespective of the complexity of the system as well as of the theoretical model used to describe it. However, some

special conditions have to be fulfilled in order to obtain the mentioned characteristics. In particular, for delta-doped quasiregular structures building according to the Fibonacci sequence it is important that the starting blocks *A* and *B* sustain: 1) a certain degree of interaction, and 2) a considerable contrast between their impurity concentrations.

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