

## SEMICONDUCTORS OF CRYSTALLINE ALLOYS IN SUPERLATTICES

### SUPER-REDES SEMICONDUTORAS EM LIGAS CRISTALINAS

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**Abstract:** This work analyzes, from the effects related to the processes of transportation of carrier and the changes in the electronic structure of semiconductor materials due to the presence of defects and disorders in the alloys crystalline superlattice. These defects are located in specific areas of the material and either interact or remain inert. In general, they are described by local wave functions. The study of superlattices of semiconductor crystal considers important parameters such as disorder effects in crystals and the alternate periodic growth of the layer of two semiconductors with different gaps and minigaps energies. The quantum mechanical calculations are applied for determining the physical properties of the semiconductors crystals. This study encompasses the effects of defects and the crystalline disorders evaluation by quantum mechanics. Further, the presence of the defects in the periodic, quasiperiodic and disordered arrangements is discussed. The theoretical approach is used to understand the mechanism and the results of experimental techniques in which are characterized the current and optic transportation of a semiconductor crystal.

**Keywords:** Defects; Superlattices; Semiconductors; Quantum Mechanics.

**Resumo:** Este trabalho analisa a partir dos efeitos relacionados com os processos de transporte de portador e as mudanças na estrutura dos materiais semicondutores eletrônicos devido à presença de defeitos e desordens na super-rede de ligas cristalina. Estes defeitos estão localizados em áreas específicas do material e podem interagir permanentemente. Em geral, eles são descritos por funções de onda locais. O estudo de superredes de cristal semicondutor considera parâmetros importantes, tais como os efeitos da desordem em cristais e o crescimento periódico alternativo da camada de dois semicondutores com diferentes espaçamentos e minigaps de energias. Os cálculos de mecânica quântica são aplicadas para a determinação das propriedades físicas dos cristais semicondutores. Este estudo abrange os efeitos de defeitos e a avaliação de perturbação na estrutura cristalina via mecânica quântica. Além disso, discute-se a presença dos defeitos nos arranjos periódicos, quasiperiódicos e desordenados. A abordagem teórica é utilizada para compreender o mecanismo e os resultados das técnicas experimentais em que se caracterizam o transporte de corrente e de uma óptica de cristais de semicondutores.

**Palavras-chave:** Defeitos; Super-redes; Semicondutores; Mecânica Quântica.

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## 1 INTRODUCTION

The solid structures and especially the composition of the alloys are always investigated by the scientific field, and to refer the properties solids and heterostructures formed. Scientists over time is the strong tool use quantum mechanics to understand and make appropriate interpretations of the properties observed in these materials, the knowledge of these properties contribute to the technological development in the area of communications, data processing and in various electronics (Bastard,1986). It is well known that the electricity-conducting materials are also good thermal conductors (copper). Properties such as electrical resistivity and thermal conductivity can be qualitatively explained by the classical theory. However, when going for a quantitative analysis of the same does not occur. The values obtained for various macroscopic parameters such as the resistivity and heat capacity are not explained by the classical theory, when it involves significant variations with temperature. Temperature affects the properties of electronic systems in a number of fundamental ways. The most fundamental of properties is the energy band gap,  $E_g$ , which is affected by temperature according to the Varshni Equation, described by equation (1):

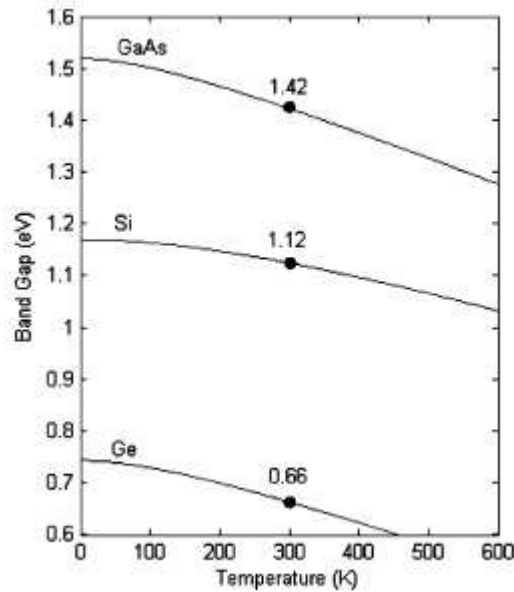
$$E_g(T) = E_g(0) - \frac{\alpha_E T^2}{T + \beta_E} \quad (1)$$

where  $E_g$  is the band gap energy at absolute zero on the Kelvin scale in the given material, and  $\alpha_E$  and  $\beta_E$  constants. Table 1 provides these constants for three material structures.

**Table 1.** Varshni equation constants for GaAs, Si, and Ge.

<b>Material</b>	$E_g(0)(eV)$	$\alpha_E(eV/K)$	$\beta_E(K)$
<b>GaAs</b>	1,519	$5,41 \cdot 10^{-4}$	204
<b>Si</b>	1,170	$4,73 \cdot 10^{-4}$	636
<b>Ge</b>	0,7437	$4,77 \cdot 10^{-4}$	235

Table 1 and (1) are used to generate Figure 1, which shows how the band gaps of the three materials decrease as temperature increases (the labeled points are the band gap of each material at room temperature).



**Figure 1.** Energy band gap temperature dependence of GaAs, Si, and Ge.

The structural defects in solids are an imperfection or we can say, the atoms are not fully organized in regular periodic arrangement in the crystal. Crystals typically are not perfect, and contain various imperfections or defects that affect many of its physical and mechanical properties.

However, compositions which comprise the structures of metallic materials are profoundly affected by the presence of crystalline defects and certain characteristics are often intentionally modified by the introduction of controlled amounts of defects. However, the defects allow to control the electrical behavior and / or of the optical semiconductor materials and structures. These semiconductor materials have great applicability in industrial field. And the defects contained in the semiconductor stems essentially from the wrong defect and / or the wrong concentration and / or in the wrong position in the structures formed in semiconductor materials.

It is important to note that some defects are formed in the semiconductor and point defect mainly depends on the vapor pressure of the components of the material composition. It is clear that the symmetrical dependence of a Schottky type AB type compound semiconductor. And, for the other types of defects such dependence is obtained in a similar way, but we know that some researchers have studied which can be seen in the literature (Bajaj, 2001).

The semiconductor heterostructures obtained by joining different materials have been investigated intensively because of their unique properties that are not observed in homogeneous. It was possible to artificially create structures such as quantum wells, quantum wires, quantum dots and super-networks, having a great technological impact, with applications in the development of new electronic and optical devices. These systems the exchange interaction between magnetic ions located and carrying the conduction and valence bands produces a Zeeman extremely large when compared with the conventional semiconductor. In the super-semi magnetic semiconductor networks, these effects are evidenced by the degeneracy of the spin in its unit cell. Soon, the heterostructures represent a practical one-dimensional confinement potential. In most cases, the special properties of the semiconductor heterostructures are due to the behavior of charge carriers (electrons and holes) in the potential containment previously designed (Cingolani; Ploog, 1991).

The present work is to analyze, from approaches developed, the physical model with strong concepts of quantum mechanics. This model, enabling discussion and understanding of

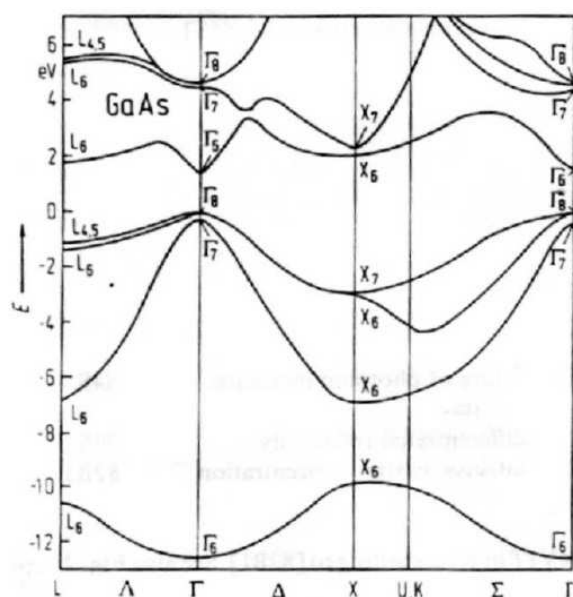
some fluctuations of energy, which causes the appearance of valence bands, suffer degeneration of disorder in semiconductor heterostructures.

## 2 DEVELOPMENT IN THEORY

### 2.1 INITIAL CONSIDERATION

Crystalline materials are constantly being investigated by scientists, particularly those materials with the formation of semiconductor heterostructures. It is necessary to understand the operation of semiconductor materials with and without the presence of impurities, it is crucial to know their electronic structures (Adenilson ; Francesco, 2004). I.e., it is extremely important to the understanding of the energy levels of these materials, and how they are affected by the presence of other atoms. This requires the application of quantum mechanics to describe the behavior of electrons as the free-electron theory, the effect of temperature on the Fermi distribution, density of state, the wave equation in a periodic potential, etc. Therefore, to understand the physical properties of metals, it is important to use the model of the Theory of Free Electron. This model tells us that the more weakly bound electrons of the constituents move freely through the crystal volume. The valence electrons of the atoms become conduction electrons and the forces between the conduction electrons and the ionic cores and the potential energy are negligible in the free electron model.

Use or composition of the material to be applied, it is necessary to study the behavior of such heterostructures and if the atoms are not isolated, the interaction forces between them are significant. The electrons in crystals are grouped into energy bands separated by energy regions for which no orbital electrons. These energy gaps or band gaps are known as forbidden zones (gap), resulting from the interaction of the waves of the conduction electrons with ions of the crystal (Lourenço et al., 2004). In the study of semiconductor super-networks, the calculations are made in the dispersion relation, applying the Kronig-Penney model for one-dimensional periodic potential (approximated by rectangular wells). Figure 2 shows the band structure of the GaAs semiconductor, which is representative of most semiconductor alloys formed from semiconductor materials that have the crystalline structure of the "zinc-blend", as is the case of the AlGaAs (Weisbuch et al., 1981).



**Figure 2.** Band structure of the GaAs semiconductor characteristic of crystal structure of type "zinc-blend".

The valence bands are degenerate at the point  $\Gamma$ . Confinement effects, such as, for example, quantum wells, raise this degeneracy. Close to  $\vec{k} = 0$  the hole states have different curvatures as can be seen in Figure 1. The difference in the curvature of these states is known as the effective mass tensor  $m^*$  in equation (1), represented by a 3x3 matrix  $m_{ij}$ . The effects of crystalline potential are expressed in the effective mass tensor that influences the dynamics of Bloch electrons. The effective mass tensor and its inverse are symmetric,

$$\left(\frac{1}{m^*}\right)_{ij} = \frac{1}{\hbar^2} \left(\frac{\partial^2 \mathcal{E}(\vec{k})}{\partial k_i \partial k_j}\right) \quad (2)$$

where  $m^*$  is the effective mass of charge carriers in the crystal lattice) causes the effective masses of holes occupying such states are different. Here, we use a simple notation ( $k$  instead of  $\mathcal{E}(k)$  or  $\vec{k}$ ) suitable for 1D, or for an isotropic energy dispersion in 3D. The isotropic energy means that  $\mathcal{E}$  is dependent only on  $k = |\vec{k}|$ . In the most general case, the effective mass is defined as a tensor but we won't go there. Note also that we are concerned with a non-relativistic only. It is helpful to check the above definition is reasonable for a free electron. In this case,

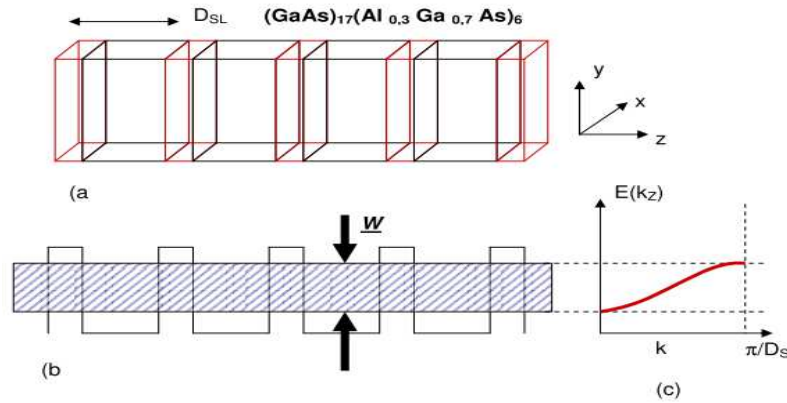
$$\mathcal{E}(k) = \frac{\hbar^2 k^2}{2m_e} \quad (3)$$

where for clarity often used  $m$  to mean  $m_e$ , the electron mass (Mesrine et al., 1997). Here, we are taking only the kinetic part, since the rest energy part,  $m_e c^2$  is just a constant. The energy dispersion  $\mathcal{E}(k)$  of the electron in a crystal contains information about the quantum mechanical interaction between the "bare" electrons with the electronic of semiconductors crystal lattice. Due to this interaction, the electron might find itself a bit more difficult to move around or a bit easier to move around.

As we shall see later on, this concept of "how easily the electron moves around" is the concept of the mobility, which is an important concept and is related partly to the effective mass. Among the structural composition AlGaAs and GaAs substrates generate offsets targeting high density which may extend to regions of its surface active. The properties and performance based devices are greatly influenced by their structures which are linked to defects in epitaxial stress in the system of their energy levels.

## 2.2 ENERGY LEVELS

Semiconductors Superlattices consist in a grouping of layers of different semiconductor materials; for instance, *A* and *B*, which are periodically arranged for a superstructure such as *ABBA...ABAB...BAAB*.



**Figure 3.** Illustration of three superlattices schemes: a) Periodic superlattice formed by GaAs/AlGaAs; b) Potential profile and c) Dispersion of energy.

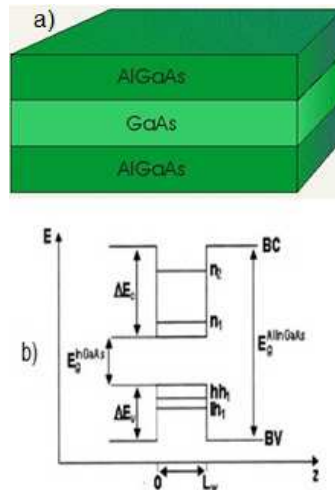
Figure 3 shows the propagations; i.e., without disorder characterizing the metallic behavior of sample. In the above figure,  $D_{SL}$  indicates the period of superlattices and  $W$  the width of miniband. The direction of growth of layers is seen in  $z$  direction. In characterizing electronic transportation in semiconductors heterostructures, it is usual to add the electronic effective mass and the microscopic effects of the crystalline net in the electron movement (Chen et al., 2004). The samples are formed of materials with different conduction bands, and therefore, the study of electronic transport in semiconductor heterostructures, a common practice is to incorporate electron effective mass in the microscopic effects of the crystal lattice in the movement of electrons.

In this case, for example of a structure formed by A and B, the effective electron masses has two  $m_A^*$  and  $m_B^*$ . In each, the wave function assumes the type Bloch  $e^{(ik_z z)} u_{k_z}(z)$  where the periodic  $u_{k_z}(z)$  is regarded the same in both materials and  $k_z^i (i = A, B)$  depends on the kinetic energy of the electron in each semiconductor layer.

The wave functions of the super-network are determined by the condition continuity between the wave functions of each specific material,  $\psi_A = \psi_B$  and the probability of the current density,  $\frac{1}{m_A^*} \frac{\partial \psi_A}{\partial z} = \frac{1}{m_B^*} \frac{\partial \psi_B}{\partial z}$ , interfaces between A and B, the structure of the semiconductor material.

### 2.3 QUANTUM WELL

Quantum well is a system comprised of two semiconductors materials with gaps of different energies. Figure 4 shows the construction of heterostructures leagues of AlGaAs between two leagues of GaAs.



**Figure 4.** a) Quantum well; b) Potential profile of quantum well;  $z$  is the direction of growth in quantum well;  $L_w$  represents the width of quantum;  $e1$  is the first level of electrons;  $hh1$  indicates the first level of heavy holes and  $lh1$  is the first level of light holes.

The origin of the potential in Figure 2 is explained by the difference of energy  $\Delta E_g$  as follows:

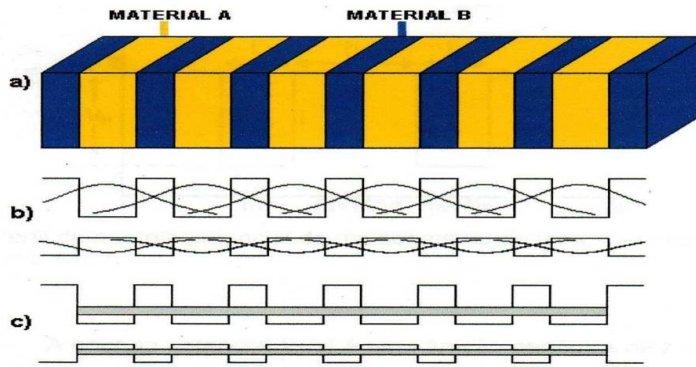
$$\Delta E_g = E_g^{AlGaAs} - E_g^{GaAs} \quad (4)$$

In the above equation,  $E_g^{AlGaAs}$  is the gap of AlGaAs material and  $E_g^{GaAs}$ , i.e., the gap of GaAs material. The difference of energy  $\Delta E_g$  is distributed between the bands of valence and of conduction in several ways. In bulk GaAs at the point of symmetry of holes states have the same energy, i.e., are degenerate. For this reason, the transitions between electrons and holes occur between levels of electrons and heavy hole levels, because it distinguishes light heavy hole because of this degeneracy. Alloys AlGaAs /GaAs/AlGaAs, electrons are trapped in layers of GaAs by potential barriers of AlGaAs due to discontinuities of the conduction bands of both. Likewise, holes are trapped by the discontinuity in the valence bands.

For a stoichiometric composition of the alloy  $Al_xGa_{1-x}As$  has the same structure of GaAs, except that a fraction  $x$  of Ga atoms has been replaced by Al atoms quantities such as the lattice parameter, the dielectric constant, the effective mass of the charge carriers in the energy gap, among others, depend on aluminum concentration ( $x$ ) (Oliveira; Meneses; Da Silva,1999).

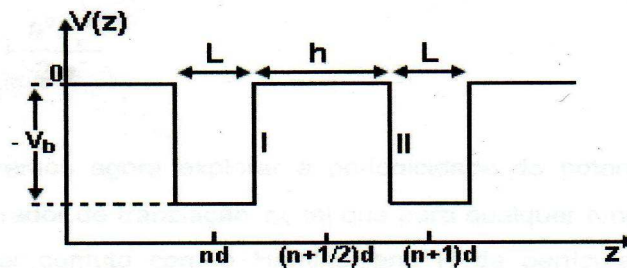
### 3 DEVELOPMENT OF A THEORETICAL MODEL FOR SUPERLATTICE

In order to obtain a superlattice it is necessary to repeat the same process for building a quantum well. Figure 5 below shows the construction of superlattices.



**Figure 5.** a) Superlattice builds by the over position of layers of A and B semiconductor materials; b) Penetration of wave functions at the barrier and wells and; c) Formation of energy minibands (for electrons and holes) along the superlattice.

With the help of Quantum Mechanics it is possible to study the interaction between wave functions which describe the electrons in the potential wells. Consequently, the existence of an energy band (miniband) affects the transportation phenomenon of loads through the structure. Figure 6 shows an infinite sequence of quantum wells of width  $L$  separated by barriers of thickness  $h$ .



**Figure 6.** Profile of potential energy of a segment of a superlattices with period  $d = L + h$ .

Calculations for determining energies and wave functions in a potential well made by two semiconductor materials are shown below. The potential energy  $V_b(z)$  is a periodic function with period  $d = L + h$  is given by (Akiyama et al., 2003).

$$V_b = \sum_{n=-\infty}^{+\infty} V_b(z - nd) \quad (5)$$

Where:

$$V_b(z - nd) = \begin{cases} -V_b, & \text{for } (z - nd) \leq \frac{L}{2} \\ 0, & \text{for } (z - nd) \geq \frac{L}{2} \end{cases} \quad (6)$$

For a superlattice with energy greater than the height of barrier, the following equations are defined:

$$\psi_w(Z) = \alpha e^{ik_w(z-nd)} + \beta e^{-ik_w(z-nd)} \quad (7)$$

$$\text{For } |z - nd| \leq \frac{L}{2} \quad (8)$$



$$\psi_w(Z) = \gamma e^{ik_b(z-nd-\frac{d}{2})} + \delta e^{-ik_b(z-nd-\frac{d}{2})} \quad (9)$$

$$\text{For } \left| z - nd - \frac{d}{2} \right| \leq \frac{\hbar}{2} \quad (10)$$

However, when an electron with energy higher than the barrier height ( $E > 0$ ) is affected by superlattice potential, its energy is given by:

$$\varepsilon = \frac{\hbar^2 k_b^2}{2m^*} = -V_b + \frac{\hbar^2 k_x^2}{2m^*} \quad (11)$$

The periodicity of a potential can be determined by the operator of the superlattice. The autofunctions and autovalues can be demonstrated via Schrödinger equation, as follows (Schrödinger equation in one-dimensional case in the  $z$  direction) (Ter Haar D, 2004).

$$i\hbar \frac{\partial \psi(z,t)}{\partial t} = -\frac{\hbar^2}{2m^*} \frac{\partial^2 \psi(z,t)}{\partial z^2} + V(z,t)\psi(z,t) \quad (12)$$

The crystal size is  $nd$ , where  $n$  is an integer, and impose periodic boundary conditions so that we,  $\psi_q(z+nd) = \psi_q(z)$ ,  $L$  is the length of the shaft. Thus, using the Bloch theorem, we find that  $qnd = 2\pi p$  with  $p$  integer. I.e.,  $q$  is real and discrete, being  $\frac{2\pi}{nd}$  the spacing between two consecutive values. Is well defined space of vectors  $q$ , which is called reciprocal space. The segment  $\left[-\frac{\pi}{d}, \frac{\pi}{d}\right]$  in reciprocal space is known as the first Brillouin zone (Laureto, 2002). The functions  $\psi_q$  must be continuous, as its first derivative. Thus, the interface between a well and a barrier, we have:

$$\alpha e^{(ik_w L/2)} + \beta e^{(-ik_w L/2)} = \beta e^{(-ik_b L/2)} + \delta e^{(ik_b L/2)} \quad (13)$$

$$ik_w \left\{ \alpha e^{(ik_w L/2)} - \beta e^{(-ik_w L/2)} \right\} = ik_b \left\{ \gamma e^{(-ik_w L/2)} - \delta e^{(-ik_w L/2)} \right\} \quad (14)$$

In the interface between a barrier and a well are:

$$\psi_q(z = (n+1)d - L/2) = \gamma e^{(ik_w L/2)} + \delta e^{(-ik_b L/2)} \quad (15)$$

Again using the Bloch theorem we can rewrite,

$$\psi_q(z = (n+1)d - L/2) \quad (16)$$

as,

$$\psi_q(z = (n+1)d - L/2) = e^{(iqd)} \psi_q(z = nd - L/2) \quad (17)$$

Proceeding with the calculations for the derivatives, we arrive at a system of four equations and four unknowns  $(\alpha, \beta, \gamma, \delta)$ , admits nontrivial solution if the following equation is satisfied:

$$\cos(qd) = \cos(k_w L) \cos(k_b h) - \frac{1}{2} \left( \xi + \frac{1}{\xi} \right) \text{sen}(k_w L) \text{sen}(k_b L) \quad (18)$$

$$\xi = \frac{k_b}{k_w} \quad (19)$$

Above only consider the situation where we have propagating states with energies above the top of the barrier ( $\varepsilon \geq 0$ ). Thus, equation (16) gives us the levels of virtual states such heterostructures. However, states that interest us most are the quasi-particle states in which bound  $-V_b \leq \varepsilon \leq 0$ . In this case, the wave functions are evanescent in the barrier and simply make the substitutions:

$$kb \rightarrow i\kappa_b \text{ with } \kappa_b = \sqrt{\frac{-2m^* \varepsilon}{\hbar^2}}, \xi \rightarrow i\xi, \text{ being } \xi = \frac{\kappa_b}{k_b} \quad (20)$$

in equation (16) and she is:

$$\cos(qd) = \cos(k_w L) \cosh(\kappa_b h) - \frac{1}{2} \left( \xi + \frac{1}{\xi} \right) \text{sen}(k_w L) \text{senh}(\kappa_b h) \quad (21)$$

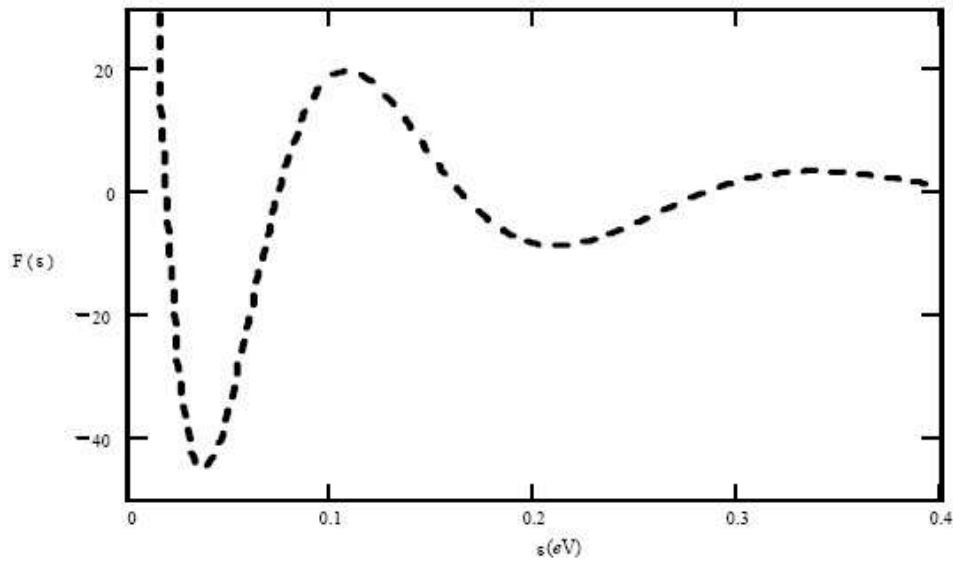
We note that equation (21) diverges exponentially with increasing  $h(e^{\kappa_b h})$ . To maintain the convergence of the solution; we must have the coefficients which multiply these terms may be null, which occurs when:

$$\cos(k_w L) - \frac{1}{2} \left[ -\xi + \frac{1}{\xi} \right] \text{sen}(k_w L) = 0 \quad (22)$$

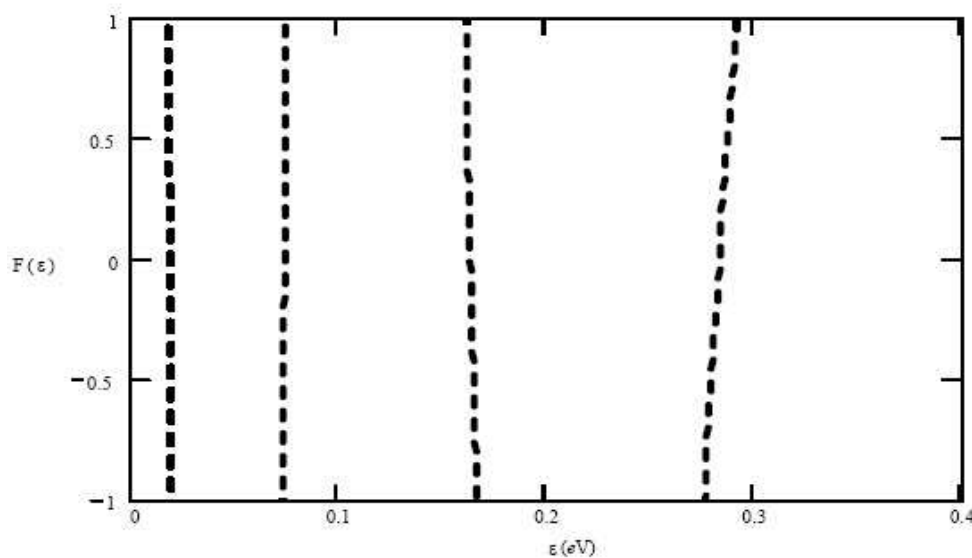
Equation (20) is the same which gives the values of the energy levels of simple square shaft. Thus, we conclude that the energy levels of the structure of the superlattices semiconductor multi-quantum wells are a hybridization of the energy levels of the well isolated. These levels hybridized form miniband energy when the overlap of the wave functions of each well through the finite barrier is very large (Vurgaftman; Meyer.; Ram-Mohan, 2001). Equation (20) provides an implicit relationship between the energy levels of states allowed in the pit and the parameters of the sample. The interval  $[-1, 1]$ , the right side of this equation,

$$F(\varepsilon) = \cos(k_w L) \cosh(\kappa_b h) - \frac{1}{2} \left( \xi - \frac{1}{\xi} \right) \text{sen}(k_w L) \text{senh}(\kappa_b h) \quad (23),$$

shows the states allowed to structure multi-quantum wells as it is equal to  $\cos(qd)$ . The following Figures 5 and 6 show the function  $F(\varepsilon)$  to a structure with the following parameters: width of the barrier,  $h = 5$  nm, pit width,  $L = 15$  nm; effective mass of the barriers and wells equal a  $m^* = 0.067$  m, and barrier height,  $V = 400$  meV. Figure 5 shows the graph of the function  $F(\varepsilon)$  as a function of electron energy,  $\varepsilon$ , as a whole, and the Figure 7 shows the detail of the same function in the range  $-1 < F(\varepsilon) < 1$ .



**Figure 7.** Graph of the right side of equation (19) for barrier height  $V = 0.4$  eV,  $m^* = 0.067$  m,  $G = 15$  nm and  $h = 5$  nm.



**Figure 8.** Figure 5 illustrates detail of the allowed states for the same superlattices.

For the situation shown above, Figures 5 and 6 wells of the structure of multi-quantum wells have four energy levels are allowed. We observed that the slope of the curves indicate the widths of these energy levels for delimit an energy band permitted for the electron in the crystal structure.

#### 4 CONCLUSIONS

Structural imperfections in semiconductor superlattices have a strong influence on the optical properties of semiconductor heterostructures that form the basis of many current photonic and optoelectronic devices. A clear understanding of the origin of these defects is essential for their control and minimizes its effects. In this work, we discuss the general features related to structural imperfections of interfaces and the formation of compound semiconductors involving mixing of three or more chemical elements. Through the analysis of different systems forming semiconductor quantum wells, we found a high degree of sensitivity of the energy spectra of the effects of these imperfections the superlattices.

Many advantages are observed in the utilization of these materials, principally when concerns its optic and electric properties. Valuable informations are obtained from temperature studies such as the electron confinement in quantum wells, quantum threads and quantum points.

This theoretical Model evidenced some properties of heterostructures where disorders are diversified leading to interesting and surprisingly results.

Calculations made at level of band energy can be solved through equation of Schrödinger. This Model also showed that the introduction of dopants in a semiconductor crystal determine the bearers (electron or hole) responsible for its conductivity as predicted by the laws of quantum mechanics.

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