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Effect of the Aluminium Fraction "x" in Subminiband Structures of Fibonacci $\text{Al}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$ Superlattices

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Abstract: We study numerically the effects of a quasiperiodicity on the transport properties of $\text{GaAs}/\text{Al}_x\text{Ga}_{1-x}\text{As}$ superlattices. We consider layers having identical thickness where the Al concentration x takes at two different values. We study the transmission coefficient of a plane wave through a 1D finite Fibonacci in height of barrier superlattices by computed by means of the transfer-matrix formalism.

Key words: Fibonacci in height of barrier superlattices, pseudo-bandgaps, singular localised states

INTRODUCTION

Heterostructures and superlattices consisting of semiconductors have been investigated as a source of new physical properties as well as for their applications in devices (Dominguez-Adame *et al.*, 1995). Some years ago, the advances achieved in nanotechnology mainly those technique based on molecular beam epitaxy-made it possible to fabricate a quasi periodic semiconductors superlattices (Merlin *et al.*, 1985).

Following the first fabrication of quasiperiodic semiconductor superlattices, there has been an increasing interest in the study of one-dimensional systems describing quasiperiodic structures because they are structures being intermediate between periodic and fully disorder (random) ones (Dominguez-Adame *et al.*, 1994; Dominguez-Adame and Sanchez, 1991; Bentata *et al.*, 2001; Bentata, 2005).

In particular, the Fibonacci quasiperiodic superlattices have been extensively studied and a lot of experimental work has been concerned with the propagation of electrons or other classical waves in one-dimensional quasiperiodic superlattices or dielectric multilayer. Merlin *et al.* (1985) have grown a Fibonacci lattice made of GaAs and AlAs for the first time and have studied its x-ray diffraction and Raman scattering properties. Diez *et al.* (1996) have demonstrated that periodic coherent-field-induced oscillations, which we are able to observe in our simulations of periodic SLs, are replaced in Fibonacci SLs by more complex oscillations displaying quasiperiodic signatures.

Xiangbo *et al.* (1999) have investigated the transmission properties of light through the Fibonacci-class quasiperiodic multilayer and found some interesting results. The trace map of propagation matrices is deduced

and the invariant of motion is found. They obtained the expression of the coefficient T analytically for general incidences and normal one.

Arunava *et al.* (1992) have reexamined the conventional idea of determining the nature of the electronic eigenfunction of a Fibonacci lattice from a study of the associated with the trace map. They have demonstrated that this is insufficient and a more detailed study of the renormalisation group transformation itself is required to ascertain the nature of the eigenfunctions.

Very recently, Dong *et al.* (2003) reported a broad omnidirectional bandgap. They designed a structure composed of both Fibonacci multilayer and periodic structures.

The main aim of this research treat the transfer-matrix formalism with the calculation of the miniband structures, the transmission coefficient of Fibonacci in height barrier superlattices (FHBSL).

MODEL

Here, we calculate the transmission coefficient of FHBSL in the stationary case. we consider quantum well-based SL constituted by two semiconductor materials with the same well width d_w and barrier thickness d_b in the whole sample which in turns preserves the periodicity of the lattice along the growing axis; the unit supercell having the period $d = d_w + d_b$. The physical picture may be handled through the investigation of states close to the bottom of the conduction miniband with $k_{\perp} = 0$. As usual, nonparabolicity effects can be neglected without loss of generality. Under these circumstances, the one-electron one-band effective-mass Hamiltonian provides a satisfactory description:

$$\left[-\frac{\hbar^2}{2} \frac{d}{dz} \frac{1}{m^*(z)} \frac{d}{dz} + V_{SL}(z) \right] \Psi(z) = E\Psi(z) \quad (1)$$

Here the SL potential V_{SL} derives directly from the different energies of the conduction band-edge of the two semiconductor materials (GaAs and $Al_xGa_{1-x}As$) at the interfaces.

The structure of FHBSL is starting from two basic building blocks A and B. Here A and B consists the two height of barrier of the potential. A usual method to construct the Fibonacci sequence is to use an inflation process according to the rule $B \rightarrow A$ and $A \rightarrow AB$. This sequence comprises S_{n-1} elements A and S_{n-2} elements B. The initial sequences is $S_0 = A = V_1$ and $S_1 = B = V_f$.

In this model of SL, we consider that the height of the barriers takes only two values, namely V_1 for a basic block A and V_f for B. These two energies are proportional to the two values of the Al fraction in the $Al_xGa_{1-x}As$ barriers. The fifth sequence for example of energies is correlated the: $V_1 V_f V_1 V_1 V_f V_1 V_f V_1$.

In the following treatment, we include the electron effective masses according to the different regions of the potential: m_{b1} and m_{bf} corresponding to barrier heights V_1 and V_b respectively and m_a to the well. The transmission coefficient and all the related physical quantities of interest at zero temperature can be conveniently computed within the framework of the transfer matrix formalism.

Using the Bastard conditions of continuity (Bastard, 1981), for an incident electron coming from the left one has the relation between the reflected and transmitted amplitude, r and t, respectively:

$$\begin{pmatrix} 1 \\ r \end{pmatrix} = M(0,L) \begin{pmatrix} t \\ 0 \end{pmatrix} \quad (2)$$

A simple algebra yields the transfer matrix $M(0, L)$ as:

$$M(0,L) = -\frac{m_w^*}{2ik} \begin{pmatrix} -\frac{ik}{m_w^*} & -1 \\ -\frac{ik}{m_w^*} & -1 \end{pmatrix} S(0,L) \begin{pmatrix} 1 & 1 \\ \frac{ik}{m_w^*} & -\frac{ik}{m_w^*} \end{pmatrix} \quad (3)$$

Here the diffusion matrix $S(0, L)$ can be formulated in terms of the elementary diffusion matrices G_j (1) associated to each region j of the potential having a width l as the product:

$$S(0,L) = \prod_{j=0}^N G_j(1) = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} \quad (4)$$

The transmission coefficient is then given by:

$$\tau = \frac{4}{(S_{11} + S_{22})^2 + \left(\frac{k}{m_w^*} S_{12} - \frac{m_w^*}{k} S_{21} \right)^2} \quad (5)$$

This expression measures the electron interaction with the structure through the elements of the diffusion matrix $S(0, L)$ and the wave vector defined by:

$$k^2 = \frac{2 m_w^* E}{\hbar^2}$$

RESULTS AND DISCUSSION

Within the following description, several parameters can be varied, namely: the height of the potential barriers V_1 and V_b , the width of the Quantum Wells (QW) a, the thickness of the potential barriers b and the length of the system L through the number N of supercells. Each of these parameters has a specific physical bearing: the width a determines the number of minibands while the thickness b acts on the spread of these minibands by controlling the strength of the interaction between neighbour states belonging to neighbour wells.

For a proper understanding, we have treated the overquoted GaAs/ $Al_xGa_{1-x}As$ as the semiconductor SL. This material has a long and rich history and presents a great challenge for technological purposes. Moreover all the desired experimental parameters involved in our calculations are available in the literature and, besides, it serves as test for our computed magnitudes. In particular, the SL potential V_{SL} may be expressed in terms of the aluminium concentration x in $Al_xGa_{1-x}As$, using the rule 60% for the conduction-band offset (Adachi, 1985):

$$V_{SL} = 0.6 (1.247 x) \text{ for } 0 \leq x \leq 0.45 \quad (6)$$

This interval of x delimits the region where $Al_xGa_{1-x}As$ presents a direct gap in the direction Γ . As well as the effective mass in this region:

$$m(x) = (0.067 + 0.083 x) m_0 \quad (7)$$

m_0 being the free electron mass.

We have chosen the physical parameter values, such as $d_w = 20 \text{ \AA}$, $d_b = 20 \text{ \AA}$, $V_1 = 260 \text{ meV}$ and $V_f = 200 \text{ meV}$, to obtain allowed minibands lying below the barriers. The corresponding effective masses are taken to be

$m_a = 0.067 m_0$, $m_{b1} = 0.096 m_0$ and $m_{br} = 0.089 m_0$ for, respectively the quantum well and the two barrier height V_l and V_r (Adachi, 1985), where m_0 is the free electron mass.

For the above parameters, transmission coefficient versus electron incident energy $\tau(E)$ is plotted.

Figure 1 shows the position of the lower and upper band edges of the minibands corresponding to the two ordered superlattices with the two barrier heights V_l and V_r . One can observe the existence of one miniband under the well, ranging from 118 up to 309 meV for V_l and from 93 up to 314 for V_r .

In Fig. 2 we present the curves of transmission coefficient versus electron incident energy $\tau(E)$ of FHBSL

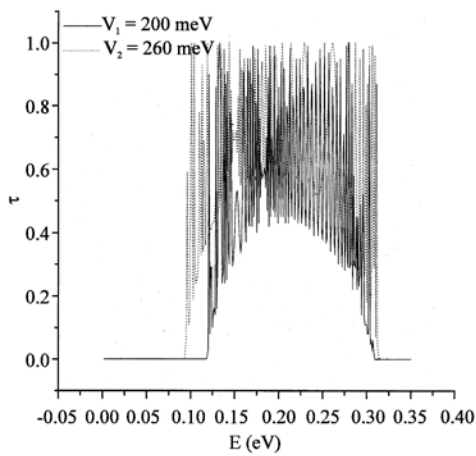


Fig. 1: Transmission coefficient of incident electron energy E for the two ordered superlattices with $N = 377$ barriers. (a) for $V_1 = 200$ meV and (b) for $V_2 = 260$ meV

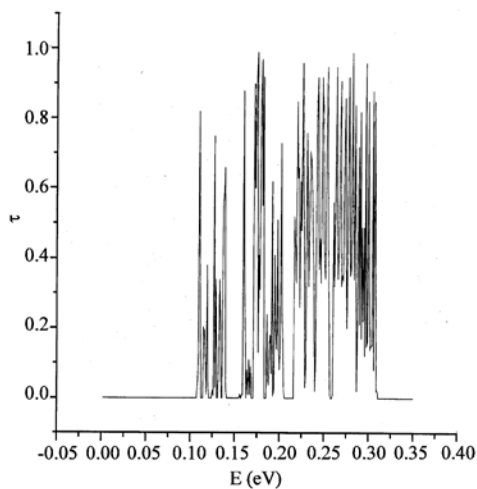


Fig. 2: Transmission coefficient of incident electron energy E for the structure of FHBSL with $N = 377$ barriers, $V_1 = 260$ meV, $V_r = 200$ meV, $d_w = 20 \text{ \AA}$, $d_b = 20 \text{ \AA}$

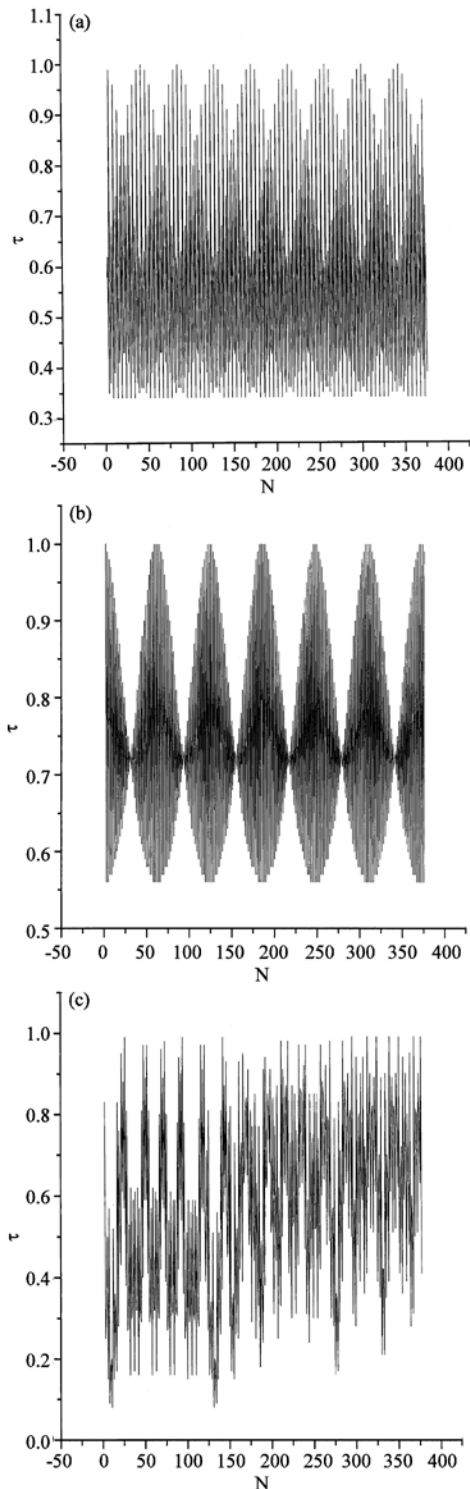


Fig. 3: The transmission coefficients according to the barrier number of the structure with $N = 377$ barriers of the: (a) ordered superlattices with $V_1 = 260$ meV, (b) ordered superlattices with $V_r = 200$ meV, (c) FHBSL with $V_1 = 260$ meV and $V_r = 200$ meV

or $N = 377$. The overall structure of the energy spectrum is characterized by the presence of four main subminibands and three minigaps. The first minigap is clustered around energies 140 and 159 meV, the second between 205 and 216 meV and the last minigap is ranging from 252 and 257 meV.

By introducing the potential of Fibonacci V_f , the system tends toward a loss periodicity to long range induced for the destructive interferences of the functions wave in these areas from where the creation a singularly localised states. For the short range the system tends toward a quasiperiodicity induced for constructive interferences of the functions wave. The potential of Fibonacci play the role of the specific defect.

Figure 3 represents the transmission coefficient versus number of barrier energy $\tau(N)$ of the two ordered superlattices with the two barrier heights V and V_f of FHBSL for energies 162 meV.

One observes that the coefficient of transmission varies between 1 and 0.34 and the width of the envelope is equal to 860 Å corresponding to the first ordered

superlattices (Fig. 3a). For the second ordered superlattices, the coefficient of transmission varies between 1 and 0.56 and the width of the envelope equal to 1260 Å (Fig. 3b).

This result is due to the difference in height of potential of the two structures and the position of energies states in basic cell where the effective masse is different. We have observed in (Fig. 3c), the appearance of the fragmentation of the structure, the disappearance of the periodic envelopes and the rupture of the periodicity in height and effective mass due to the overlap of the two structures (V_1 and V_f).

Then we studied the influence of the variation the barrier height as the form of the quasiperiodic structure by representing the coefficient of transmission according to the energy of the electron for (a) $V_f = 247$ meV; (b) $V_f = 210$ meV; (c) $V_f = 200$ meV and (d) $V_f = 150$ meV as plotted in Fig. 4. It is noted that the width of minigap increases while reducing the potential height of Fibonacci. The electron feels the quasiperiodicity of the system when the height of potential is quite different.

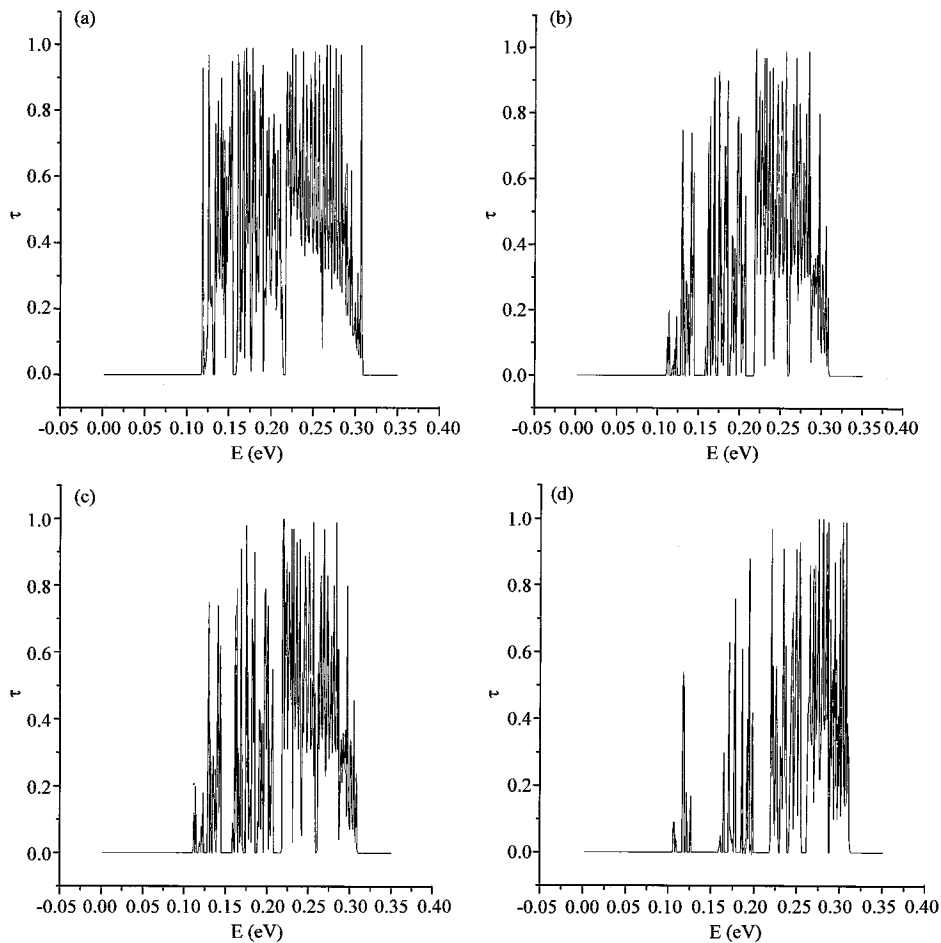


Fig. 4: The transmission coefficients incident electron energy E for the structure of FHBSL with $N = 377$ barriers for different values of the Fibonacci potential V_f : (a) $V_f = 247$ meV, (b) $V_f = 210$ meV, (c) $V_f = 200$ meV, (d) $V_f = 150$ meV

CONCLUSIONS

In this research, we have calculated the transmission coefficient of FHBSL by making use of the transfer-matrix method. We have noted that the difference in height of the potential of the two structures V_1 and V_2 influences on the structure of miniband (number of sub-minibands and minigaps). The width of minigap increases while reducing height of potential of Fibonacci it plays the role of specific defect.

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