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The simulation of the effect of the geometry of the Rectangular Double Barrier structure about the transmission and reflection coefficient

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Abstract - This paper is focused on the simulation of the effect of the geometry of the quantum Rectangular Double Barrier (RDB) structures about the transmission and reflection coefficient of them, in view of obtained electronics devices with good transmission performances. The theoretical base of this study is finding out in the Generalized Impedance Method (GIM) and the practical simulation is realized using PHP and JAVA scripts.

This simulation shows that, the transmission performances of these devices can by easy modified by the changing of the height and thickness sizes of the potential barriers and quantum well.

Keywords: simulation, Rectangular Double Barrier structures, transmission coefficient, reflection coefficient, electronics devices

I. INTRODUCTION

Since the demonstration of the resonant tunneling in semiconductor heterostructure, the Double Barrier Resonant Tunneling (DBRT) structure has become a generic device, stimulating a large number of theoretical and experimental works [1-6]. The study of the resonant states and the power transmission coefficient across such potential barriers is important both from a fundamental and a practical point of view. Several methods have been reported in literature. The Generalized Impedance Method (GIM) [1] and the Complex Valued Equivalent Circuit Method (CVECM) [3] treat the quantum effect devices by using the analogy between the Schrödinger equation and the equation voltage-current in the transmission lines theory.

In this paper, the theoretical base is finding out in the Generalized Impedance Method, witch is used to study the transmission and reflection coefficient of the GaAs-$Al_xGa_{1-x}As$ RDB structures with different geometry sizes. This theoretical study is completed with a practical simulation realized using PHP and JAVA scripts, in which are calculated and graphic represented the transmission coefficient, T, and the reflection coefficient, Γ, of the devices. The parameters of the RDB structures (the thickness and the height barrier) are introduced using a HTML fail. In this way, you can obtain the quantum structure with the wished transmission performances. This spectral simulation is an interactive Java applet, in witch you can set parameters, obtained from PHP calculation script.

Making experiments with this simulator you can predict the geometry of the RDB witch leads of the structures with grate power transmission coefficient and small reflections. The simulation shows that the better choose is to use a structure with the thickness of the potential barriers equal with them, the thickness of the quantum well much grater of them and the small height of structure. In this case, the T coefficient $\rightarrow 1$, and the Γ coefficient is approximated null.

Our results show that, the transmission performances of these devices can by easy modified by the changing of the height and thickness of the potential barriers and quantum well.

II. THEORY

A. *The Generalized Impedance Method applied in Rectangular Double Barrier structures*

To study the properties of the transmission in the GaAs-$Al_xGa_{1-x}As$ quantum structures, we used the GIM method to calculate the reflection and transmission coefficients.

Let us assume that an electron with the energy E is incident on the potential barrier (Fig. 1).

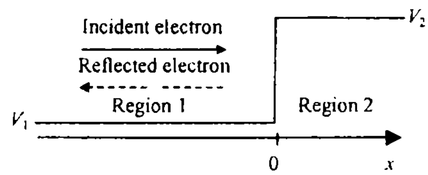

Fig. 1. A potential barrier with an incident electron

The complex conjugate of the wave functions can be written as

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$$\Psi_1^*(x) = A_1^+(e^{-\gamma_1 x} + \rho e^{\gamma_1 x}), \quad x < 0, \quad (1)$$

$$\Psi_2^*(x) = A_2^+ e^{-\gamma_2 x}, \quad x > 0, \quad (2)$$

where

$$\gamma_i = \mathrm{j}\sqrt{(2m_i/\hbar^2)(E - V_i)}, \quad (3)$$

m_i and V_i (i=1,2) are the propagation constant, the effective mass and the potential, respectively, for the i^{th} region; ρ is the wave amplitude reflection coefficient.

Obs.: For to obtained a better accurate of the calculation, the effective mass m_i is assumed to be the different in both materials, depending of the Al concentration, X, from the structure.

Based on this observation, m_i is calculated thru:

$$m_b = (0.0667 + 0.083 \cdot X) \cdot m_0 \quad (4)$$

$$m_w = 0.0667 \cdot m_0 \quad (5)$$

where

m_0 is the effective mass of the free electron;

m_w - the effective mass of the electron in the quantum well;

m_b - the effective mass of the electron in the potential barrier.

V_i function of Al concentration, X, is:

$$V_b = 0.57 \cdot (1.155 \cdot X + 0.37 \cdot X^2). \quad (6)$$

Using equation (1) we obtain relation (7):

$$\Phi_i(x) = j(\hbar/m_i)(\mathrm{d}\Psi_i^*/\mathrm{d}x) = A_i^+\left(e^{-\gamma_i x} - \rho e^{\gamma_i x}\right)$$

with

$$Z_{0i} = \mathrm{j} m_i / \gamma_i \hbar \ . \quad (8)$$

Let us now write the equation for voltage (U) and current (I) used in the transmission lines with generalized distributed impedance. These are:

$$U(x) = I^+ Z_0 (e^{-\gamma x} + \Gamma e^{+\gamma x}), \quad (9)$$

$$I(x) = I^+ (e^{-\gamma x} - \Gamma e^{+\gamma x}), \quad (10)$$

where

$$\Gamma = \frac{Z_l - Z_0}{Z_l + Z_0} \quad (11)$$

is the voltage reflection coefficient, Z_l and Z_0 are the load and the characteristic impedances of the transmission line, respectively. If we compare the equations for Ψ_i^* and Φ_i and the corresponding expressions for U and I for a transmission line we see that these are analogous equations. Thus, we can regard Z_0 as the characteristic impedance of a region. Also, the ratio of Ψ_i^* and Φ_i (analogous to the ratio of the voltage and current), will define, at any plane x, the quantum mechanical wave impedance

$$Z_i(x) = \Psi^*{}_i(x) / \Phi_i(x) \quad (12)$$

Thus, the input value of impedance, $Z_i = Z(-l)$, may be expressed in terms of the load impedance $Z_l = Z(0)$ [1] as:

$$Z_i = Z_0 \frac{Z_l \cosh(\gamma l) + Z_0 \sinh(\gamma l)}{Z_0 \cosh(\gamma l) + Z_l \sinh(\gamma l)} \quad (13)$$

The method can be used for the arbitrary potential barrier structures, so that we consider a symmetrical double barrier structure with a rectangular quantum well (RDB), as shown in figure 2:

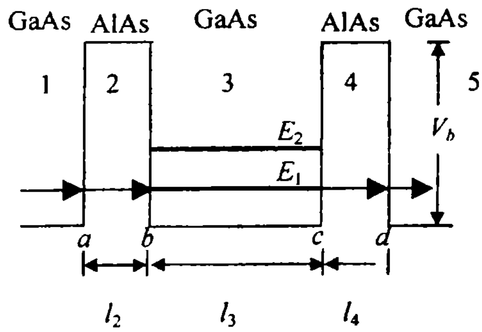

Fig. 2. Schematics of the resonant tunneling effect and resonant transmission obtained for $E = E_n$, when electrons tunnel resonantly into the n^{th} bound state of the well

The characteristic impedance for the rightmost section serves as the load and, because the region 5 is theoretically infinite, $Z_l = Z_{0,5}$. Having the load impedance at point d, the input impedance Z_c at the point c is calculated using relation (13), with $Z_0 = Z_{0,4}$ and $l = l_4$. With Z_c as the load at point c, the input impedance at point b is computed and this process is repeated until the point a is reached. The reflection coefficient is calculated using the equation (11) with Z_a as the load impedance and $Z_{0,1}$ as the characteristic impedance. The transmission coefficient $T(E)$ is given by:

$$T(E) = 1 - |\Gamma(E)|^2. \quad (14)$$

We have used this method in the PHP script from the simulator of paper, for to obtained the better RDB quantum structures which lead at electronic devices with good transmission performances. Also, for to realize a complete study, we have utilized the Smith chart by using an interactive Java applet, in witch you can set parameters, obtained from PHP calculation script. The theory and the mode of work of this interactive Java applet will be presented in the next subsection.

B. *The description of the interactive Java applet*

In any transmission system, a source sends energy to a load, such as an antenna. Ideally, we design the transmission network such that the characteristic impedances of the source, the transmission line and the load are all identical. Unfortunately, many real-world situations prevent the match from being perfect. For example, we might want an antenna (the load) to be useful over a broad range of frequencies. But the characteristic impedance of an antenna is unlikely to stay constant with frequency, especially if the frequency span is great.

When the transmission line impedance does not match that of the load, part of the transmitted waveform is reflected back towards the source. The reflected wave, which varies in phase and magnitude, adds to the incident (transmitted) wave and the sum is called a *Standing Wave*. The reflected wave causes the amplitude to vary as a function of position along the transmission line. The Standing Wave Ratio (SWR), which is the ratio between the maximum and minimum amplitudes of the total waveform, will in this case be greater than one. If there is no reflected wave, i.e., if the impedance match is perfect, the amplitude of the total waveform (incident plus reflected wave) will be the constant, regardless of where we measure it along the transmission line. The result is a SWR of 1. SWR = 1 indicates maximum power transfer to the load. SWR can be inferred by measuring the reflection coefficient of the circuit. The network analyzer is a tool that enables us to do just that. If we know the reflection coefficient, we can determine the characteristic impedance of the load by using a Smith Chart. The Smith Chart has circles of constant resistance and arcs of constant reactance. The relationship between reflection coefficient and [illegible] (fig. 3).

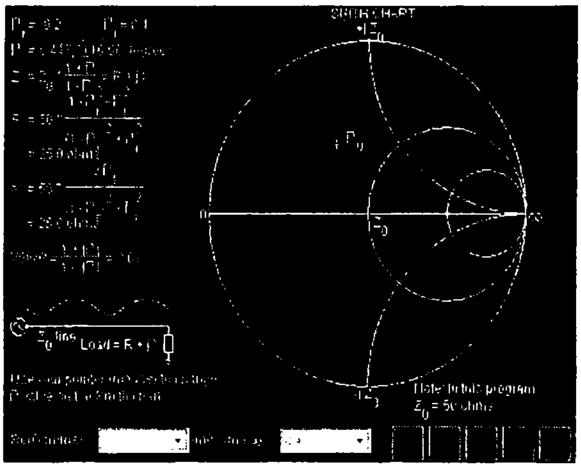

Fig 3 Position Γ using the pointer device (mouse)

The Smith Chart can help us translate the reflection coefficient into impedance. First, we calculated the reflection coefficient using the PHP script. Place the reflection coefficient, by using either the mouse or the drop-down input boxes, at the desired value (real + imaginary) on the Smith Chart. Hit the Play button (triangle), and the program will display (fig. 4) a circle with a radius equal to the reflection coefficient magnitude (constant VSWR circle). Notice that if you move the reflection coefficient anywhere on this circle, you can see from the waveform at the left that the SWR is the same, only its phase changes. (Phase values are not shown around the chart in this program; however, the phase is calculated and shown at the left side of the screen.)

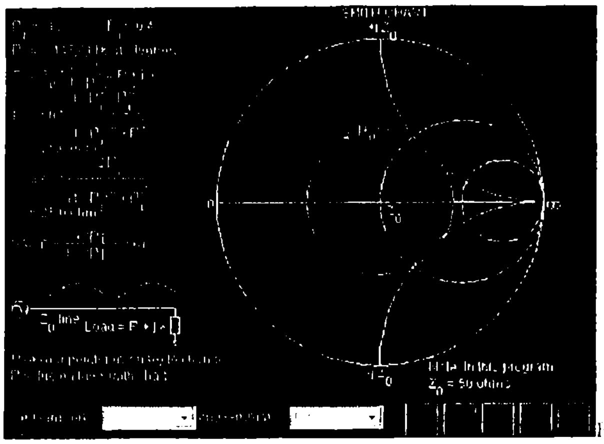

Fig 4 Drawing the VSWR circle

In general, only the horizontal line (diameter) is labeled with (normalized) resistance values and only the unit (outer) circle is labeled with (normalized) reactance values. To read the desired values, it is necessary to follow the appropriate circle of constant resistance to the diameter line, and to follow the appropriate arc of constant reactance to the unit circle. Hit Play again, and the program will display the constant-resistance circle and the constant-reactance arc for you (fig. 5). The actual values are calculated and shown at the left side of the screen.

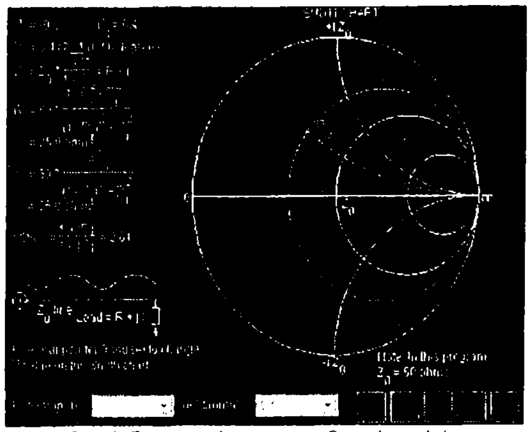

Fig 5 Drawing the constant R circle and the constant X arc

Experiment with the simulator and you will see that you can predict the geometry size of the symmetric RDB structure witch leads of the electronic devices with grate power transmission coefficient and small reflection.

III. THE SIMULATION DESCRIPTION AND RESULTS

Since the our final goal is to obtain electronics devices, with good transmission performances, from RDB structures, this present simulator helps us to calculate and graphic represent the transmission coefficient and the reflection coefficient on the Smith Chart. The mode of work of the simulator is present step by step in following.

First, using a HTML file, we can introduce the geometry size of RDB. Having these input dates, the next step is to determine the transmission coefficient and the reflection coefficient of the chosen structure.

These coefficients are obtained from PHP script. The last step is the graphic representation of the transmission coefficient function of the incident electron energy (using another PHP script) and the representation of the reflection coefficient on the Smith Chart by utilizing the interactive JAVA applet witch receives the dates from the first PHP script.
By realize more experiments with this simulator we can anticipate the RDB geometry witch leads to electronic devices with wishing transmission performances.
Thus, we can observe that, if we chose an asymmetric RDB structure (l_2 = 20Å, l_3 = 100Å, l_4 = 35Å and V = 0.45 => E_{rez} = 338.96 meV) it will obtained a devices with small transmission coefficient (T < 0.7 - fig. 6) and with grater reflection ($\Gamma \in$ Ox axis of the Smith Chart – fig.7).

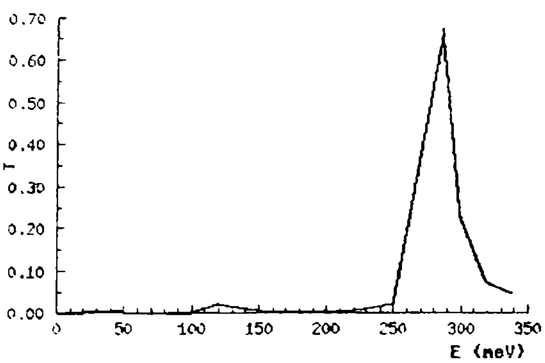

Fig 6. Transmission coefficient function of the incident electron energy, $T(E)$, for the asymetric RDB structure: E_{rez} = 287 meV

The better choose is to use a symmetric RDB, for example, a structure with the thickness of the potential barriers equal with them (l_2 = l_4 = 20Å) and the thickness of the quantum well much grater of them (l_3 = 100Å). In this case, the T coefficient → 1 (fig. 8), and the center of the VSWR circle is near the center of Smith Chart (fig. 9).
From figure 8, we can see that using thus symmetrical structures it obtained filters with good transmission performances, witch permit to pass only the electrons with energy, $E = E_{rez}$. The asymmetric RDB structures have this function (fig. 6), being disadvantage from this point of view. At this conclusion arrived thru the studies from another papers [7-9], too. Thus, this simulator proves that we can obtain electronics devices, with wished transmission performances, from RDB structures by simple changing of the geometry size of them.
Using the analogue PHP script, we can create a Data Base in MySQL, in witch it stockade the values of the transmission coefficients and resonant frequencies of the submilimetric filters obtained with symmetric RDB structures, for different height and thickness of the potential barriers, keeping constant the thickness of the quantum well (l_3 = 100Å).

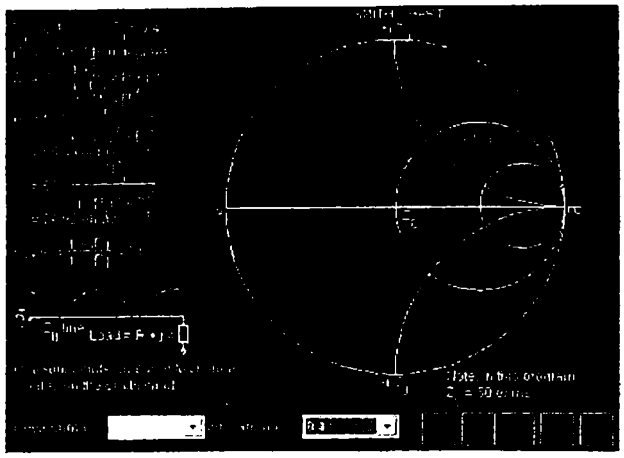

Fig 7. Reflection coefficient for the asymetric RDB structure

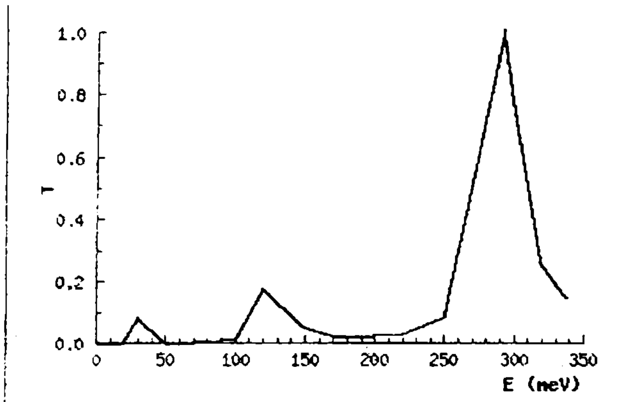

Fig 8. Transmission coefficient function of the incident electron energy, $T(E)$, for the symmetric RDB structure: E_{rez} = 292 meV, T = 0.99942

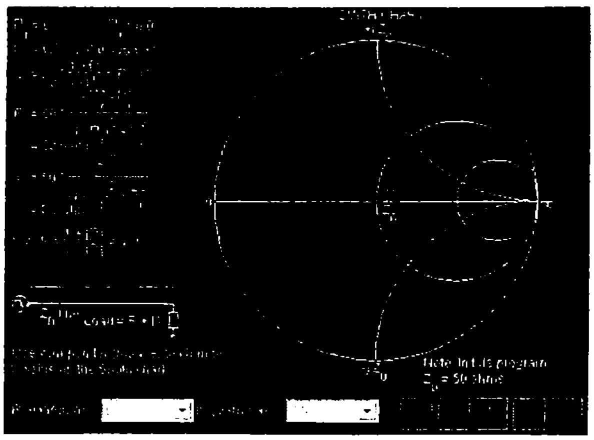

Fig 9. Reflection coefficient for the symmetric RDB structure

In this moment, the Data Base contains 40 records (table 1), but it can be up gradated and interrogated using another PHP scripts. The task of the interrogation PHP script is to permit an easy identification of the symmetric RDB structures witch lead at the electronic devices (filters in THz range) with wished transmission performances.
Using table 1, in figure 10 it represent the dependences: $T(V_b)$, $F_{rez}(V_b)$, $T(G_b)$, $F_{rez}(G_b)$, for to help us to identification the better geometry structure for our applications.

Table 1

Thickness of the potential barriers [Å]	Height of potential barriers [meV]	Resonant frequency [THz]	Transmission coefficient
10	193.12	5.803	0.99999
10	297.08	30.225	0.99971
[illegible]	313.7	[illegible]	[illegible]
10	305.37	30.467	0.99999
10	322.08	74.718	0.99999
10	330.5	74.959	0.99995
10	338.96	74.959	0.99999
10	103.49	4.594	0.99937
10	147.55	28.049	0.99996
10	232.26	29.258	[illegible]
11	305.37	73.75	0.99999
12	338.96	[illegible]	0.99999
13	297.08	30.225	0.99983
13	313.7	72.783	0.99986
13	103.49	4.836	0.99892
14	170.15	27.807	0.99987
15	272.46	29.742	0.99977
15	313.7	71.574	0.99994
15	322.08	71.816	0.99999
15	103.49	5.078	0.99963
16	297.08	30.225	0.99998
17	338.96	30.951	0.99981
17	216.48	28.533	0.99997
17	82.038	4.8361	0.99731
18	103.49	24.906	0.99823
20	272.46	29.742	0.99884
20	103.49	24.906	0.99999
23	272.46	29.742	0.99273
24	103.49	24.18	0.9998
25	193.12	27.565	0.99635
26	103.49	23.938	0.99993
27	118.01	5.8033	0.99998
28	216.48	28.049	0.99892
29	103.49	23.697	0.9995
32	67.944	4.836	0.99611
32	67.944	4.836	0.99611
34	103.49	22.971	0.99866
35	67.944	4.836	0.99982
38	67.944	4.836	0.99761
41	103.49	22.487	0.9995

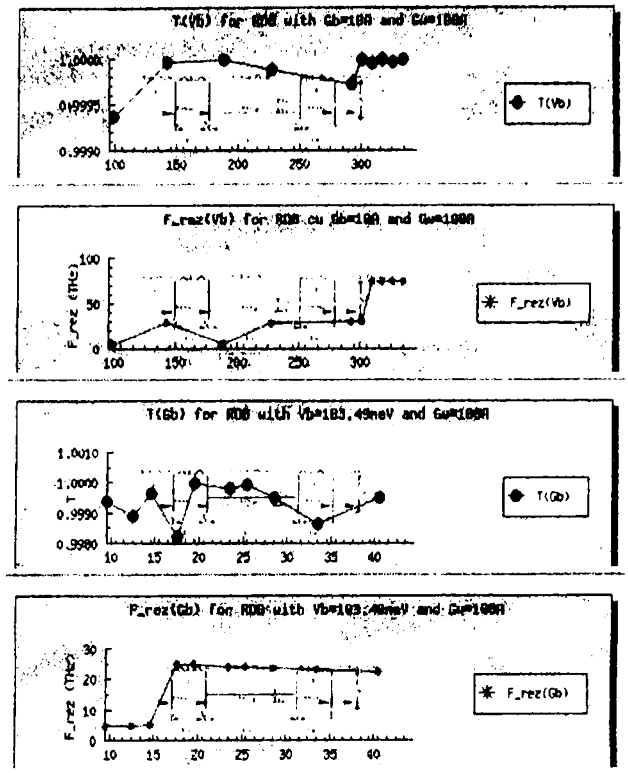

Fig 10. The dependences $T(V_b)$, $F_{rez}(V_b)$, $T(G_b)$, $F_{rez}(G_b)$, for symmetric RDB structure with G_w = 100 Å

IV. CONCLUSIONS

In conclusion, making more experiments with this simulator you can predict the geometry of the RDB witch leads of the electronic devices with wishing transmission performances. In this way, our present study clear proved that, for to obtained the circuits with good transmission power coefficient, it is necessary to use a symmetric RDB structure with the thickness of the potential barriers equal with them and the thickness of the quantum well much grater of them. Thus, the transmission performances of the electronic devices can by easy modified by the changing the geometry size of the RDB structures. Much more, for a easy identification of the geometry structure with leads at the wishing performances, using MySQL, in this paper we created a Data Base, in witch it stockade the values of the transmission coefficients and resonant frequencies of the submilimetric filters obtained with symmetric RDB structures, for different height and thickness of the potential barriers. This Data Base can be anytime up gradated and interrogated using PHP scripts.

So, our paper present an original and modern simulator, realized with PHP scripts and interactive JAVA applet (two language programs very much used in Internet, in the last time) witch permit us to determinate the transmission performances of the electronic devices obtained from RDB quantum structures.

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