SYNCHROINFO JOURNAL

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RESTRUCTURING RESONANCE TUNNEL LEVELS DURING THE SUPERLATTICE FORMATION

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ABSTRACT

Reducing the active dimensions of semiconductor structures leads to the manifestation of new edge-mechanical phenomena. The characteristic sizes of structures at which these effects appear are 1...100 nm. In this range, quantum effects begin to fully manifest themselves, and the physics of conductivity is determined by the quantum mechanical interference of electron waves. It has been established that during the formation of a superlattice consisting of a sequence of potential wells and barriers, resonant levels arise, the energy of which is determined by the number of de Broglie waves that fit across the width of the well. For particles with energy equal to the energy of the levels, the transparency of the structure is equal to unity. As the number of units increases, these levels split into similar sublevels. The scheme and mechanism for rearranging levels in the chain are considered. This mechanism is based on ideas about the points of change in the phases of oscillator oscillations during the formation of a chain. It has been established that the parameters of these sublevels (energy, half-width and wave function) depend on the parameters of the barriers and the number of cells in the chain. A model is proposed that makes it possible to determine the characteristics of these sublevels, in particular their energy and wave functions.

KEYWORDS: *Quantum Mechanics, Quantum Barrier, Wave Function, Transparency, Superlattice, Tunneling.*

DOI: 10.36724/2664-066X-2023-9-3-22-28

Received: 15.04.2023
Accepted: 27.05.2023

Citation: Vladimir F. Degtyarev, Alexey P. Zhilinsky, "Restructuring resonance tunnel levels during the superlattice formation," *Synchroinfo Journal* **2023**, vol. 9, no. 3, pp. 22-28.

1 Introduction

It is known that a decrease in the active dimensions of semiconductor structures leads to the manifestation of new edge-mechanical phenomena. The characteristic sizes of structures at which these effects appear are 1...100 nm [1]. In this range, quantum effects begin to fully manifest themselves, and the physics of conductivity is determined by the quantum mechanical interference of electron waves. Due to the strong spatial limitation of charge carriers in these structures (*a* ~ 1 nm), the size quantization energy is of the order of $\Delta E \sim \frac{\hbar^2}{2m^* a^2} = 340 meV$.

This value is comparable to the band gap of typical semiconductors and is an order of magnitude greater than the thermal energy of charge carriers at room temperature. Thus, in semiconductor nanostructures, size quantization effects will play a significant role, determining their basic electrical properties. In this case, the possibility arises of using quantum effects for qualitatively new technologies. The physical and mathematical description of such structures and their properties are quite widely presented in the literature, both in periodicals and in various monographs [2-4]. Of particular interest is the resonant passage of charged particles through a periodic structure. A number of publications are devoted to the study of this problem, for example [2,3,5]. These works address important issues related to the behavior of electrons in ideal infinite structures. The main attention was paid to band theory, the energy spectrum of electrons in ideal and non-ideal systems. Currently, the effect of resonant tunneling in thin-film heterostructures is the basis for the creation of a number of new devices.

Problems related to the propagation of waves (electromagnetic, electronic) in layered media also arise in many other areas of science and technology. In particular, media such as plasma, ionosphere, atmosphere, and ocean contain layered structures. Solving problems on the passage of waves in these media, calculating the reflection and transmission coefficients during the propagation of electromagnetic waves are of great importance both for calculating radio paths with reflection from the ionosphere, and for many problems of remote diagnostics of ionospheric plasma [6]. Therefore, the issues discussed in this work may be of interest to specialists in these areas.

2 Simulation methodology

Solving nanoelectronics problems is impossible without the use of modern mathematical methods. In this work, the wave functions and transparency coefficients of the barrier system were found by directly solving the Schrödinger equation for a given potential with the corresponding boundary conditions in the MAPLE computer algebra system. This system has extensive capabilities for numerical and analytical solutions of many problems, as well as for graphical presentation of the results obtained. In this work, as an example, we consider a superlattice consisting of wells and barriers with the following parameters: barrier width (*a*) – 1 nm, its height (*U*) – 2 eV, well width (*b*) – 1 nm, period d = 2 nm. The amplitude of the incident wave was taken equal to unity ($\Psi_{in}(x) = e^{ikx}$). The dependence of the transparency of the structure on the particle energy was studied. From the dependence *T*(*E*) (*T* is the transparency coefficient of the chain), the position of the peak maximum (E_0), its energy width ΔE_{05} at half its height, and the quality factor were determined. The results obtained in this work, as well as the developed methodology, also apply to chains with other parameters.

3 Resonance tunnel levels in an elementary chain link

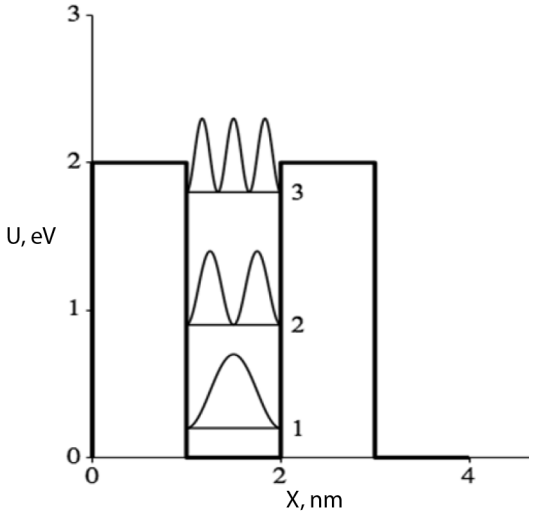

Fig. 1: Chain elementary link diagram and wave functions in the case when:
1 – one half-wave; 2 – two half-waves; 3 – three half-waves fit across the width of the well

In the structure under consideration, the elementary link is a double-barrier quantum structure (DBQS), shown in Figure 1. The case is considered when the particle energy is less than the barrier height. Resonance levels and wave functions for this case are shown in the figure. The main results of the computer simulation are listed below.

1. In an elementary link, as well as in a potential well of finite depth (the thickness of the barrier is considered infinitely large) at E < U, a system of resonant tunnel levels is formed [7], the position of which is determined by the condition $b = n\frac{\lambda}{2}$, where b – well width, λ – wavelength for a particle with energy E, n= 1, 2,… – number of half-waves that fit within the well width (Fig. 1 curves 1, 2, 3). The transparency of the structure for particles with such energy is equal to unity.

2. In the elementary link of the structure under consideration, the number of such levels is 3 (Fig. 1). As calculations show, their energy position is as follows: E_{01} = 0.228949 eV, E_{02} = 0.887202 eV and E_{03} = 1.818140 eV. The energy of these peaks corresponds to the position of energy levels in a well of the same width and depth, which is not surprising given the low transparency of the barriers separating the cells. This is easy to understand if we consider that both types of peaks meet the condition that the same number of half-waves fits across the width of the well.

4 Splitting of resonant levels into sublevels with increasing number of links

Let us consider the electron motion in a superlattice. The motion of a chain particle is described by the Schrödinger equation [7,8]

$$\frac{d^2\Psi(x)}{dx^2} + \frac{2m}{\hbar^2}(E - U(x))\Psi(x) = 0\ ) \qquad (1)$$

U – potential energy of interaction of an electron with a barrier. Since the chain consists of N identical links, then U and Ψ are periodic functions.

According to the principle of superposition [7,8] $\Psi = \sum_n C_n \Psi_n$ Here C_n – amplitude of the finding probability an electron at the *n*th atom.

Since the chain dimensions are limited, it is necessary to take into account the boundary conditions

$$\Psi(0) = 0 \text{ and } \Psi(x_{N+1}) = 0 \tag{2}$$

We will take into account the electron interaction only with its nearest neighbors. Then the equation describing the electron behavior in the nth cell takes the form [7-9]:

$$(E_m - E_{0m})C_n = -A_m C_{n-1} - A_m C_{n+1} \tag{3}$$

Here for the level with number m (m=1, 2, 3 in Fig. 1) $-A_m = -H_{n,m} = \int \Psi_n^* H \Psi_m dx$ initial level energy is E0m. Since the dimensions of the chain are limited, waves are reflected from the front and rear boundaries and a standing wave is formed. Therefore, one should look for a solution to equation (3) in the form

$$C_n = (\alpha \exp(ikx) + \beta \exp(-ikx)) \tag{4}$$

The first term in (4) represents a direct wave, and the second – a reflected one. The values of the coefficients α and β are determined from the boundary conditions. Substituting expression (4) into (3), after simple transformations we obtain

$$E_m = E_{0m} - 2A_m \cos(kd) \tag{5}$$

This relationship gives the connection between the energy of the electron and its wave number (dispersion equation).

Using boundary conditions (2), we obtain

$$\alpha + \beta = 0$$
$$\alpha \exp(ik(N+1)d) + \beta \exp(-ik(N+1)d) = 0$$

From here

$$\exp(ik(N+1)d) - \exp(-ik(N+1)d) = 0 \text{ or } \sin(k(N+1)d) = 0 \tag{6}$$

In a lattice consisting of *N* links, there are *N* possible solutions corresponding to certain vibration modes. These modes (j – number of the vibration mode) correspond to the wave number values

$$k_j = \frac{\pi j}{(N+1)d}, \text{ where } j = 1, 2, \ldots N. \tag{7}$$

Substituting (7) into (5), we obtain the following relation for the sublevels energy

$$E_{mj} = E_{0m} - 2A_m \cos\left(\frac{\pi j}{N+1}\right), \text{ where } j = 1, 2, \ldots, N \tag{8}$$

The above consideration leads to the energy distribution states band nature and allows us to find the energy spectrum of particles depending on links number in the chain [8,9].

This model, however, does not reveal the process physical essence. This can be done by considering the wave function configuration (Fig. 2) [4,9-15]. Here we are talking specifically about the wave function itself (Fig. 2b), and not about the square of its modulus, as shown in Figure 2a.

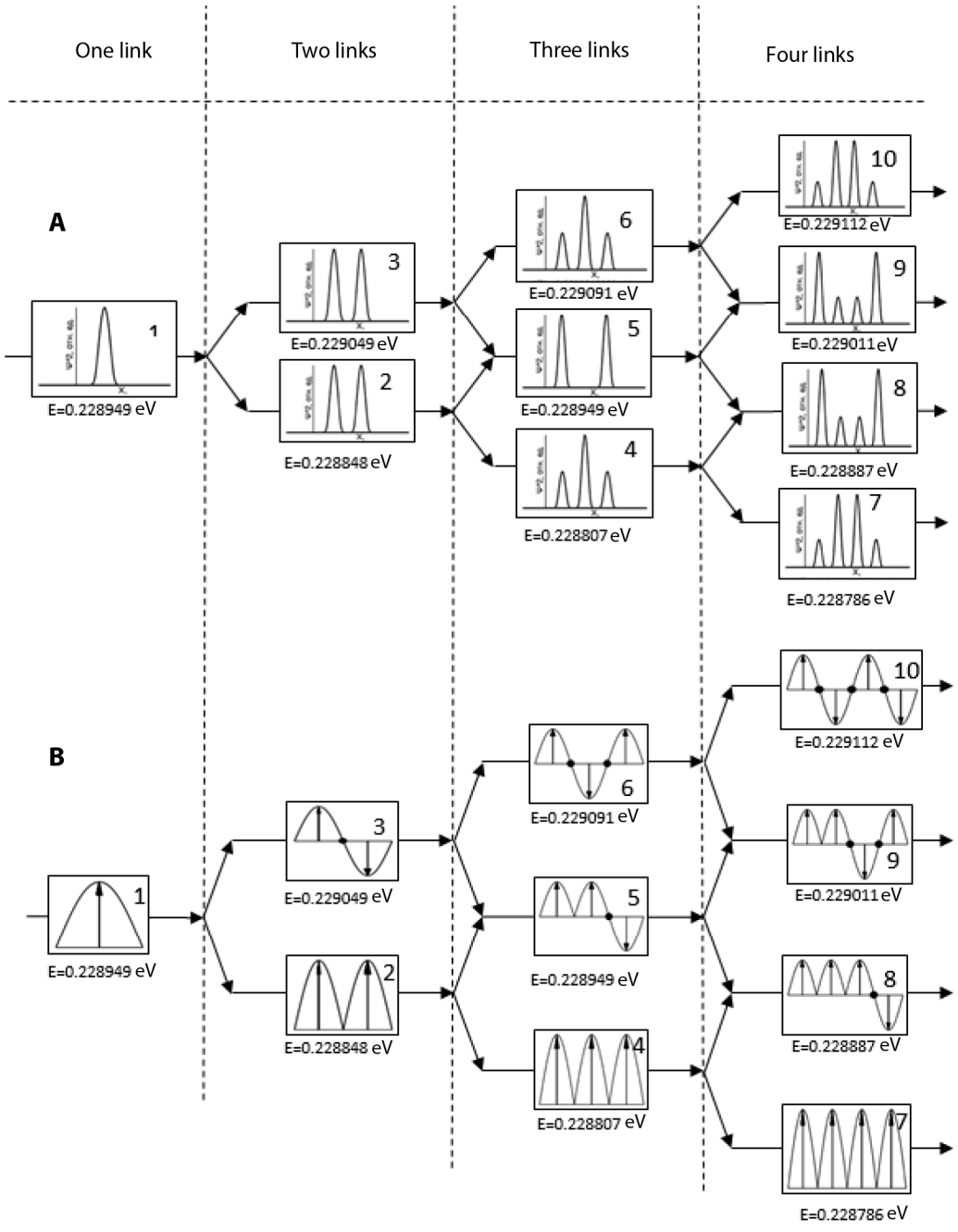

Fig. 2: A. Scheme of level splitting with an energy of 0.228949 eV in a simple chain (the squares show the corresponding wave functions modulus squares).
B. Diagrams illustrating possible configurations of wave functions. When the oscillation phase changes to the opposite, the oscillation energy increases and the energy of the sublevels increases accordingly. The places where the oscillation phases change are marked with a dot. In the figure, the configuration of the wave function in an elementary unit is conventionally represented by the icon

5 Wave functions reorganization during the chain formation

When a layered quantum-size structure is formed, not only energy levels, but also wave functions undergo significant changes. Let us consider, for example, the wave functions corresponding to the first level in a unit cell in a four-link chain. The squared modulus of these functions are shown in Figure 3. Figure 3a corresponds to the first oscillation mode, and Figure 3b to the second mode. The length of the arrows in the figure is proportional to the probability of detecting a particle in a given link.

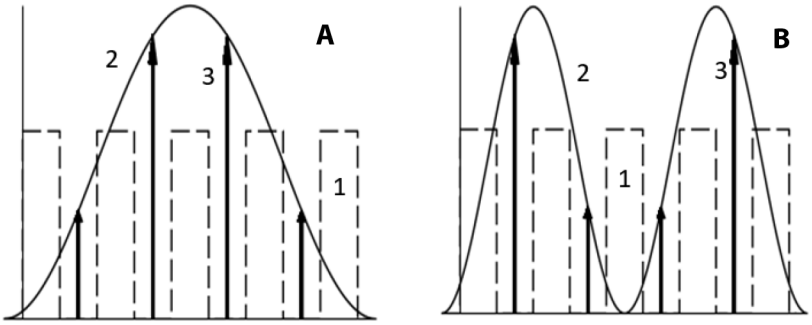

Fig. 3: Fig. 3: Scheme of the a wave function formation in a four links chain: A – first mode (*E* = 0.228786 eV; *B* – second mode (E = 0.228887 eV). 1 – diagram of barriers; 2 – envelope $\Psi^2(x)$ for the first (A) and second (B) modes; 3 – arrows, the length of which is proportional $\Psi^2(x)$

In an elementary unit, the square of the wave function modulus has a characteristic bell-shaped appearance (Fig. 2a, curve 1). When a chain is formed, the wave function takes on a complex form. The configuration of the wave function is largely determined by the structure of the layers of the chain. An important role in this is played by the ideas developed in the previous section about the points of change of phases of oscillations. The number of vibration modes is determined by the number of cells. The vibrations corresponding to the first mode have the lowest energy, when one half-wave fits along the length of the chain. Oscillator oscillations here in all links occur in the same phase (there are no phase change points (Fig. 2)). For the second oscillation mode, two half-waves are placed along the length of the chain. This configuration corresponds to one point of oscillation phase change and the level energy E = 0.228887 eV. The squared modulus of the wave function in this case is shown in Figure 2b.

The considered situation remains the same for subsequent oscillation modes. Here, too, an increase in the mode number corresponds to an increase in the number of phase change points and an increase in the energy of sublevels. Noteworthy is the symmetrical appearance of the wave functions relative to the middle of the chain. It is this type of wave function that ensures, in our opinion, the equality of particle fluxes from left to right and from right to left, which leads to high transparency of the chain. It should also be noted that the wave functions of the m-th and (N+1-m)-th modes have exactly the same form.

Indeed, from (4) and (6) it follows that the probability of detecting a particle in cell number n can be represented as

$$\Psi^2 = a \cdot \sin^2(kx_n) = a \sin^2\left(\frac{\pi jn}{N+1}\right) \tag{9}$$

$x_n = nd$, n – cell number (n=1…N), d – period structure, j – mode number (j = 1..N). From this relationship it is clear that when $j_1 + j_2 = N+1$ $\Psi_1^2 = \Psi_2^2$, and $n_1 + n_2 = N+1$ $\Psi_1^2 = \Psi_2^2$

Thus, the considered model makes it possible to explain the main features of wave functions restructuring of during the layered structure formation.

6 Conclusion

In this work, the rearrangement process of resonant tunnel levels (RTLs) during the layered quantum-size structure formation is studied. It has been established that the wave function also undergoes significant changes.

1. It has been established that when a chain is formed, RTUs are split into a system of sublevels, the number of which is equal to the number of links in the chain.

2. The energy values of these sublevels and the corresponding wave functions are determined depending on the number of links. The transparency of the chain for these energy values is equal to one. A technique is proposed that allows one to calculate these energies and construct the corresponding wave functions.

3. To explain the mechanism of level restructuring, ideas about the points of change of phases of oscillations have been developed. These are the points at which the phases of oscillations in neighboring links change to the opposite. The number of such points varies from zero to N-1. Accordingly, the number of sublevels into which the initial state is split is equal to the number of links in the chain. The more such points, the higher the oscillation energy.

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