Energy spectrum of a hierarchical superlattice with impurities in potential barriers

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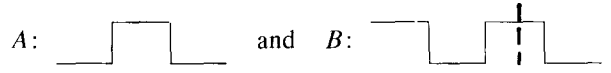
A 1D superlattice in which a hierarchical modulation of the potential is caused by impurity centers in potential barriers is discussed. A transfer-matrix method is used to calculate and analyze the tunneling spectra of this hierarchical superlattice.

Hierarchical structures are attracting interest for several reasons. First, reaching an understanding of the properties of such structures is a necessary step in describing several physical effects, such as classical diffusion,[1] molecular diffusion in complex macromolecules,[2] anomalous relaxation in spin glasses,[3] and processes which occur in computer systems.[4] Second, hierarchical structures are distinguished by some unusual physical properties, in particular, Cantor energy spectra, self-similarity, and crystal wave functions (see, for example, Refs. 5–8). Hierarchical structures are thus important topics for research, from both the theoretical and practical standpoints. We might add that the popular quasiperiodic Fibonacci series can also be thought of as hierarchical models.[7]

In the present letter we discuss one type of semiconductor hierarchical heterosystem. The reason for the large interest in semiconductor structures, in particular, is that technological progress has made it possible to realize some complex structures experimentally. We suggest creating a hierarchical modulation by means of deep impurity centers implanted in potential barriers of a semiconductor superlattice. Since technological procedures for doping semiconductor heterostructures with deep impurities are well known,[9] we believe that the model of hierarchical systems discussed in this letter is relatively simple and convenient for both experimental and theoretical research. We might add that it was shown in Ref. 10 that deep levels have a very strong effect on the energy spectrum of a periodic superlattice. The first experimental confirmation that deep centers play an important role in barriers and electronic processes in superlattices was found in Ref. 11. Below we calculate the transmission coefficient T of a superlattice constructed in accordance with a hierarchical principle. The intervals of the energy E in which the condition $T(E)\approx 1$ holds make up the energy structure of these superlattices. The analysis is carried out by an effective-mass method with the help of the technique of transfer matrices.

We consider a semiconductor superlattice made up of 1D rectangular barriers of height V and width b. The superlattice is constructed from elements of two types,



which differ in that a B element contains a deep-center impurity plane[10] (the dashed line). There are no such planes in the A elements. The order number of a barrier with impurities (of the corresponding B element) in the chain of the superlattice is 2^s for each level of the

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hierarchy, $s=2, 3, 4, \ldots$. A flux of electrons of energy E is incident on the superlattice from the left. This flux moves along the axis of the superlattice, which coincides with the x axis, which runs from left to right. The potential of the deep centers is modeled by a δ-function: $U(x)=\Omega\cdot\delta(x-x_j)$, where Ω is the strength of the potential, and x_j is the coordinate of the impurity center. In the effective-mass method, the motion of the electrons in the potential barriers is described by the equation

$$(d^2/dx^2-\kappa^2)\psi(x)=\beta\delta(x-x_j)\psi(x), \tag{1}$$

where $\beta=2m_b\Omega$, $\kappa^2=2m_b(V-E)$, $\hbar=e=m_0=1$, and m_b is the effective mass of the electrons in the barriers. A solution of Eq. (1) and of the equation describing the state of the electrons in the quantum wells is written in the form

$$\psi_p=C_pe^{ikx}+D_pe^{-ikx}, \tag{2}$$

where we have $k=-i\kappa$ in the barriers. We also assume that the wave numbers with the same energy in different quantum wells are identical ($k^2=2m_wE$, where m_w is the effective mass of the electrons in the wells). The same comment applies to the barriers, without regard to the wells. We set $C_1=1$. We set the coefficient D with the highest index equal to zero. This condition corresponds to the absence of a reflected wave beyond the last barrier. We seek a solution of the system of equations for the coefficients C and D by the method of transfer matrices. The matrix which transfers the solution across the barrier–well interface is

$$R_n=\frac{1}{2k_n}\begin{pmatrix}(k_n+k_{n+1})\exp\{i(-k_n+k_{n+1})x_n\} & (k_n-k_{n+1})\exp\{-i(k_n-k_{n+1})x_n\}\\ (k_n-k_{n+1})\exp\{i(k_n+k_{n+1})x_n\} & (k_n+k_{n+1})\exp\{i(k_n-k_{n+1})x_n\}\end{pmatrix}, \tag{3}$$

where n is the index of the heterojunction. The matrix which transfers the solution through impurity centers is[12]

$$M_j=\frac{1}{2\kappa}\begin{pmatrix}2\kappa-\beta & -\beta e^{2\kappa x_j}\\ \beta e^{2\kappa x_j} & 2\kappa+\beta\end{pmatrix}. \tag{4}$$

The coefficient of the transmission of an electron through the superlattice is

$$T(E)=\left|\left(\prod_{n=1}^{\tau}R_n'\right)_{11}\right|^{-2}, \tag{5}$$

where r is the number of heterojunctions. For odd values of n we have $R_n'=R_{2l-1}M_l$; for even values we have $R_n'=R_{2l}$, where $l=1, 2, 3, \ldots$.

Calculations were carried out from Eq. (5) for a broad range of values of the parameters of the problem. Figure 1 shows energy spectra for levels $s=2,3,4$ of the hierarchy with specific parameter values corresponding to GaAs/GaAlAs superlattices: $V=0.01$ a.u., $m_w=0.07m_0$, $m_b=0.09m_0$, $w=75$ a.u., $b=50$ a.u., and either $\beta_1=-0.04$ a.u. (for Fig. 1a) or $\beta_2=-0.06$ a.u. (Fig. 1b). The impurity planes are at the centers of the barriers. We can generalize certain features of these spectra.

1. Analysis shows that the energy spectra of this hierarchical superlattice are largely determined by the spectra of the one- and two-barrier tunneling-resonance structures

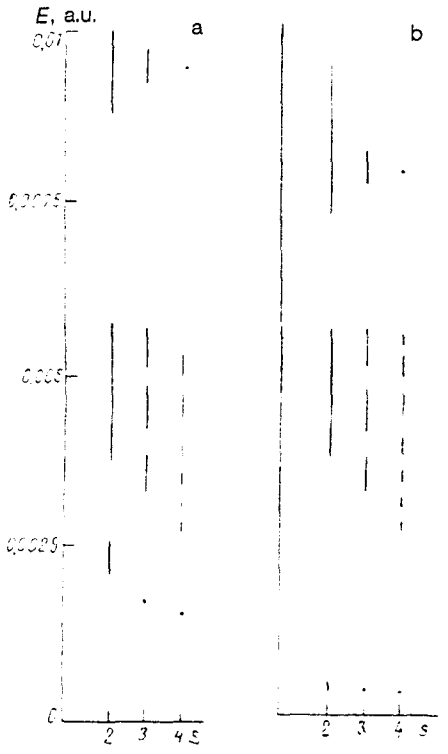

FIG. 1. Energy spectra for levels $s=2,3,4$ of the hierarchy for two values of the δ-function potential. a—$\beta_1=-0.04$ a.u.; b—$\beta_2=-0.06$ a.u. The values of the other parameters are given in the text proper.

from which the superlattice is constructed. For example, it follows from the calculations that a hierarchical modulation can arise only if there is a resonance in the interval $[0,V]$ in a one-barrier structure. Otherwise, the impurities do not have a sufficient effect on the spectrum of the superlattice.

2. These spectra are clearly of a triad nature, by which we mean that they consist of three groups of bands, with the distance between groups being much larger than the distance between the bands within a group.

3. The number of bands in the energy spectra depends on the values of the parameters. For the values corresponding to Fig. 1a (at these values, the quantum well of the two-barrier tunneling-resonance structure without impurities has a single resonance), the outermost groups have one band each. The total number of bands at each level of the hierarchy, $N=2^s+1$, is equal to the number of elements in a cell of the superlattice, i.e., 2^s, plus one additional band which is due to impurity states in the barriers. The number of bands in the central group is equal to the number of elements A (which do not have impurities) in a cell of the superlattice, i.e., 2^s-1.

4. As we move to a higher level in the hierarchy, we find a decrease in the total width of the allowed energy bands within each group of bands.

5. The positions of the two outermost groups of bands depend strongly on the strength of the δ-function potential, β. As β is raised, the bands shift down the energy scale (so that some of the bands may descend partly or completely into the below-barrier

region). The situation is different for the central group of bands. This group is determined fairly rigidly by the resonance lines of the quantum well of the two-barrier structure in their vicinity. Its position depends weakly on β. At the parameter values corresponding to Fig. 1, the resonant energy in the two-barrier structure is $E_p \approx 0.004$ a.u.

6. The widths of the bands depend on the strength of the δ-function potential. For the $s=2$ level, this dependence is extremely strong. The widths of the allowed bands reach their maximum values at a certain value of β_k, and they decrease as β deviates from β_k. For the higher levels in the hierarchy, the β dependence of the band widths weakens considerably. The width of the central band, which (as mentioned above) is rigidly tied to the resonances of the quantum well of the two-barrier structure, is much greater than the widths of the outermost bands.

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