LOW-DIMENSIONAL SYSTEMS

On transport parameters of a mesoscopic crystal with impurities at potential barriers

A. N. Korol'

Ukrainian State University of Food Technology, 252601 Kiev, Ukraine

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A one-dimensional ballistic superlattice (mesoscopic crystal) containing impurity centers at potential barriers is considered. The dependence of the transmission coefficient T on the energy B is evaluated for this structure in the effective mass approximation. It is shown that scatterers are responsible for an increase in T by several orders of magnitude, a significant shift of resonant peaks, and the reappearance (at certain energies) of the plateau on the $T(e)$ dependence, which is typical of the case $V=0$ (V is the barrier height). The possibility of varying the energy spectra of the mesoscopic crystal over a wide range is thus demonstrated. © *1996 American Institute of Physics.* [S1063-777X(96)01204-3]

A new class of semiconducting nanostructures, viz., the so-called mesoscopic crystals (or mesocrystals), has been discovered quite recently.[1,2] These materials form a one-dimensional superlattice (SL) in which electrons move under ballistic conditions. Technological progress makes it possible to obtain such structures, which are characterized by a unique combination of the properties of superlattices with a high level of quantum coherence and low dimensionality, and hence become important and promising objects of investigation. It should also be noted that mesocrystals actually combine the properties of tunnel-resonant structures and quantum waveguides which were previously studied independently. At the same time, the important role of impurity centers in phenomena occurring in various nanostructures, tunnel-resonant structures, etc. is well known. For example, a very strong influence of impurities on the energy spectrum of an infinite periodic superlattice was demonstrated by Bel- tram and Capasso,[3] while the role of impurities in disordered, hierarchial, and quasi-periodic (Fibonacci) superlattices was analyzed in our previous publications.[4-6] We can rightfully expect that the energy spectrum, and hence transport properties of mesocrystals can also be varied over a wide range with the help of impurity level. This research is devoted to the verification of this statement.

A mesocrystal can be formed, for example, on the basis of the heterostructure GaAs-Al^Gaj .....,As containing a two-dimensional electron gas. A negative voltage applied to metal electrodes creates a narrow ballistic channel, whose overlapping with potential barriers results in a one- dimensional superlattice, or mesocrystal.[1,2] In the case of high potentials, we obtain a sequence of quantum points. As usual, a quantum wire is regarded as a two-dimensional waveguide. In the effective-mass method, the wave function satisfies the following two-dimensional equation (in atomic units):

$$\left[-\frac{1}{2}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)+U(x)\right]\psi=E\psi \qquad (1)$$

As the modulating potential depends only on the longitudinal coordinate x, it can be separated from the transverse coordinate y, and the function ψ can be written in the form

$$\psi_n(x,y)=\varphi(x)\sin\frac{n\pi y}{d}, \qquad (2)$$

where d is the channel width. We assume that each potential barrier has only one "plane of impurity levels" (PIL).[3,7] The wave functions corresponding to impurity levels are assumed to be strongly localized only in the direction normal to heteroboundaries. Following Refs. 3 and 7 we model the potential of impurity centers by the δ-function $U(x)=\alpha\delta(x-x_c)$, $\alpha<0$, where x_c is the coordinate of an impurity. Assuming that the potential barriers in the x direction are rectangular (see Ref. 1), we can write the equation for the function φ in the barrier regions:

$$\varphi''+[V(x)+\alpha\delta(x-x_c)]\varphi=\beta\varphi, \qquad (3)$$

where

$$\beta=\left(\frac{n\pi}{d}\right)^2, \qquad V(x)=2m^*v(x), \quad E<v,$$

and $v(x)$ is the height of potential barriers. In the regions between the barriers, the right-hand side of Eq. (3) is equal to zero. According to Wu *et al.*,[2] the conductivity $G(E)$ of a mesocrystal in the two-dimensional case can be expressed in terms of the one-dimensional conductivity g(e): $G(E)=\sum_n g(e_n)$, where the sum is taken over all open channels. In this case, the $G(E)$ curve is the superposition of displaced curves $g(\varepsilon_n)$: the first term is shifted by e_0, the second by 2^2e_0, the third by 3^2e_0, and so on, where e_0 is the threshold transverse energy $(\pi/d)^2$. Here we calculate the transmission coefficient T which is connected with $g(e)$ through the well-known relation $g(e)=2e^2T/h$.

We represent the wave functions at barriers and quantum wells in the form

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e^{ikx} (4)

$(P_j(x) = A_j e^{ikx} + B_i e$

where $k = \sim i K = -I\backslash je$ — $-fit$ $2KX_i$ V for the barrier $2KX_i$ $2K + P$ (5) regions and $k = \backslash /e$ for the quantum wells. The coefficients Aj and Bj can be determined with the help of the method of transfer matrices, where we assume that the coefficient for an incident wave is equal to unity, and the coefficient Bj with the highest index is equal to zero (the absence of the reflected wave behind the last barrier). The form of the matrices transferring the solution through heteroboundaries R and PIL is well known (see Refs. 8 and 9 respectively). For example, the matrix transferring the solution through the PIL has the form[9]

$T(s) \sim -$ (6)

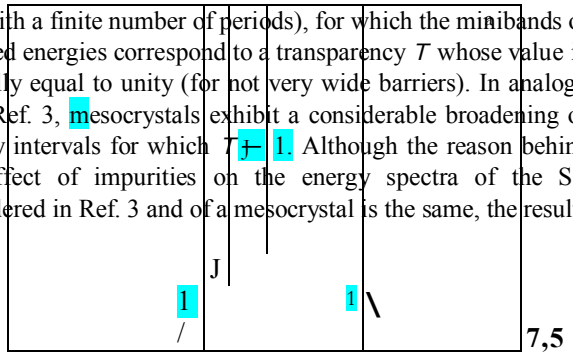
$$M_R \quad \begin{matrix} 1 & 2K-P \\ 2K & F3E \end{matrix}$$

The transmission coefficient $T(E)$ under these conditions has the form

$$UK \qquad n = I \qquad 11$$

where r is the number of boundaries between barriers and wells; $R'_N = R_{LS}$ for even N and $R'_N = R_{2S} \sim IM_S$ for odd N (S = 1,2,3,...).

We now calculate the coefficient $T(E)$ by formula (6) for a structure with the following parameters: V= e_0, $M^* = 0.07M_0$, and PIL are located at the centers of the barriers. Let us analyze the initial region of the spectrum. Figure 1 shows the $T(E)$ dependences for $/3 = 0$ (the barriers contain no scatterers), 0.01, and 0.0074 at. units; the barrier thickness is $b = 0.5d$, and the number of barriers is six as in Refs. 1 and 2. Figure la demonstrates that the presence of super- lattice modulation of the potential leads to sharp oscillations of the quantity $T(E)$ in the region of the plateau observed for V=0. (As the number of periods in the superlattice increases, the group of resonances is transformed into a mini- band of resonant (allowed) energies.) Figures lb and c show that impurity centers strongly affect the spectrum of the me- socrystal. The observed effect has the same physical nature as that manifested in the effect of impurities on the energy spectrum of a periodic SL described by Beltram and Capasso.[3] The authors of Ref. 3 demonstrated that the introduction of impurities into the potential barriers of one-dimensional infinitely long periodic SL leads to an increase in the widths of allowed minibands of the SL under consideration by several orders of magnitude. The maximum effect is observed when impurity levels are located most closely to the energy levels in the quantum well of the SL. According to Ref. 3, this is explained by the interaction (mixing) of impurity states with the states in the wells. A mesocrystal can be regarded as a periodic SL (with a finite number of periods), for which the minibands of allowed energies correspond to a transparency T whose value is virtually equal to unity (for not very wide barriers). In analogy with Ref. 3, mesocrystals exhibit a considerable broadening of energy intervals for which $T \to 1$. Although the reason behind the effect of impurities on the energy spectra of the SL considered in Ref. 3 and of a mesocrystal is the same, the results of this



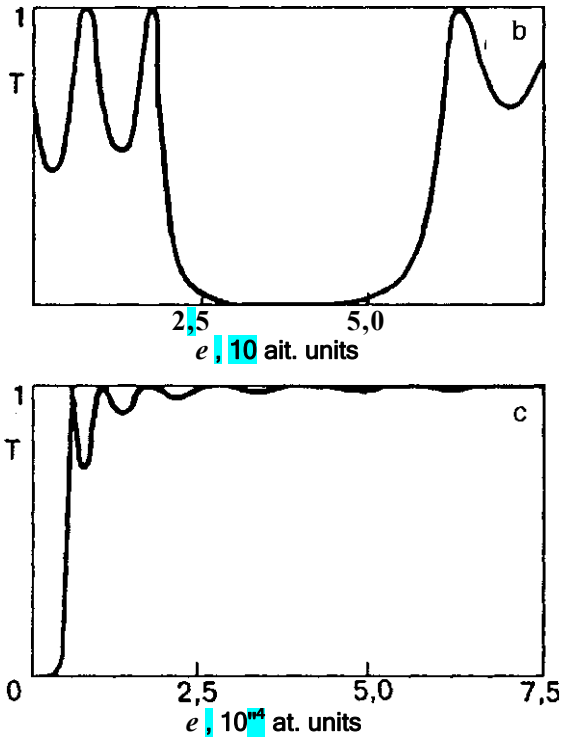


FIG. 1. Dependence of the transmission coefficient T on energy e for three values of fi, at. units: 0 (a), 0.01 (b), and 0.0074 (c). The values of other parameters are given in the text.

2,5 _4 5,0 £,10 at. units

effect in the mesocrystal have some peculiarities. It can be seen in Fig. lb that under the effect of scatterers, the resonances are shifted significantly towards lower energy, some of them being lowered to the under-the-barrier region. The resonances become less sharp, and the separation between them increases. It should be noted that for a large barrier width the maximum value T_M becomes noticeably smaller than unity, but the presence of impurities leads to an increase in T_M. For example, the value of T_M increases due to the presence of scatterers by approximately two orders of magnitude and becomes virtually equal to unity (T~ 0.999) for $b = d =$ 2000 at. units.

A very strong change in the spectrum is observed in Fig. lc: instead of individual resonances, we have an energy interval in which $T \to 1$ almost everywhere. In other words, the presence of scatterers restores the plateau in the $T(E)$ dependence, which was destroyed by superlattice modulation of the potential. It should be noted that this is observed for the values of (3 for which resonant tunneling through an

isolated (individual) barrier is possible. In the case of "barrier

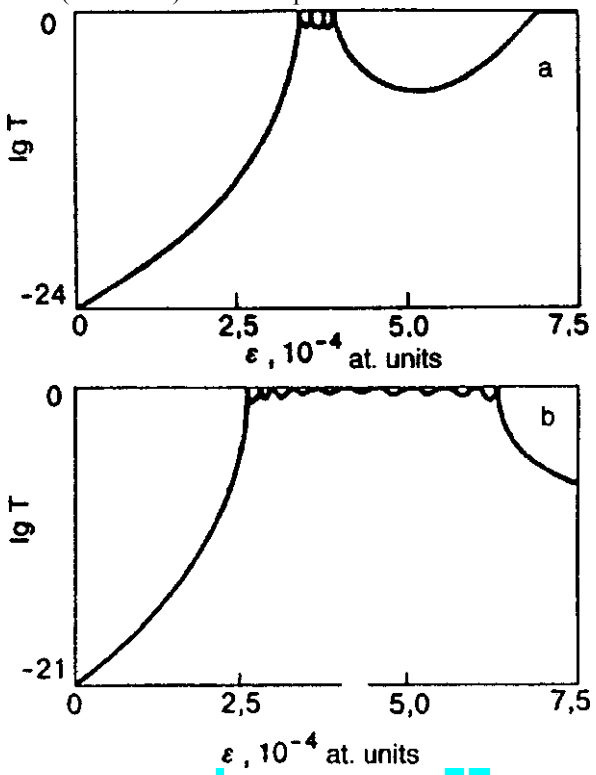


FIG. 2. Dependence of log7"(e) for broad barriers with *b*— 1500 at. units for /?=0.008(a) and 0.012 at. unit(b). The number of barriers is six.

resonances," the interaction of impurity states with one another and with the states in quantum wells is very strong, and new resonant states emerging as a result of this interaction cannot be identified by indicating their origin (in contrast to the case illustrated in Fig. 2a when this can be done easily).

Thus, the position of resonant peaks e, depends considerably on the intensity of the ^-potential and on the barrier width. The dependence of e, on /? is approximately the same for all resonances and is close to linear. For example, the resonance depicted in Fig. la are displaced by Ae,= 10"[4] at. unit when p changes by 0.001 at. unit.

Figure 2 shows the dependences logHe) for rather broad barriers with *b* = 1500 at. unit for 0.008 and 0.012 at. unit. For the two groups of resonance clearly seen in Fig. 2a, the right group is due to impurity states. With increasing

the energies corresponding to the two groups of resonances become closer, and the interaction between various states becomes stronger, leading to broadening of both energy intervals with high values of T. Figure 2b illustrates the case when the energy intervals corresponding to high values of T overlap.

It should be noted that the values of fi for which the case of "barrier resonances" is realized also depend on the barrier width. As the value of *b* increases, the range of corresponding to this case is broadened and displaced towards higher energies. For example, the case of "barrier resonances" is realized for the barrier width *b*- 700 at. units for the values of j3 belong to the interval [0.005; 0.008], while for *b*= 1500 at. unit this interval is [0.007; 0.014],

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