INFLUENCE OF QUANTUM WIRE CROSS SECTION FLUCTUATIONS ON TRANSPORT PHENOMENA

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For all currently available methods of quantum wire (QWI) fabrication the cross section of the QWI varies along the length, producing fluctuations in the energy position of the subband energy along the QWI. This fluctuation leads to a smearing of the peak-like structure of the dependence of the average density of states on carrier energy. This, in turn, results in a smearing of the peak-like structure of the dependence of the resistivity of a QWI on the Fermi energy and/or total electron concentration, and in an increase of resistivity. In previous attempts to obtain agreement between theory and experiment the subband energy fluctuation was not taken into account, that is why the importance of other factors, such as impurity scattering, have been overestimated.

Introduction

Interest in quantum wires (QWI) (systems containing a 1-D electron gas) is now increasing very rapidly [1-7] because they could serve in a variety of high-speed electronic devices. A 1-D electron gas implies that electrons are free to move only in one direction. Let us define this as the x-direction. The energy in the y- and z-directions is fixed because electrons are confined to a QWI of small cross sectional area $A = d_y d_z$, where the linear dimensions d_y and d_z along y and z are of the order of the de Broglie wavelength, λ_0, of the electrons. (We can also have $d_y, d_z \ll \lambda_0$ [1,2].) The experimental results, which are presented in Refs. 1 and 2, clearly demonstrate the well pronounced variation of A along a QWI. We propose that this cross sectional variation has a serious effect on transport phenomena so our emphasis will be on transport properties related to the dependence of A on x in long 1-D samples (we are not interested in ballistic transport, which can occur in a short 1-D sample).

Proposed Model

In any theoretical calculation, the electron energy,

$$E_{ij}(k) = (\hbar k)^2/(2m) + E_{ij}; \quad E_{ij} = E_i + E_j; \quad i,j = 1,2,3., \quad (1)$$

is a function of the longitudinal electron wave vector $k = k_x$, and two quantum numbers, i and j. Here m is the effective mass of the electron, $\hbar$ is Planck's constant, and E_i and E_j are quantized levels corresponding to the confinement of the electron motion in the y- and z-directions, respectively.

Different theoretical models employ different assumptions about E_i and E_j. Practically all of them [3-6] assume that the QWI of thickness d_y is a part of a quantum well structure. The models for E_j are different. In this presentation we will emphasize one of them despite the fact that several models were exploited in our calculations. For the z-direction, a quantum well of thickness d_z is assumed [4], and for simplicity we consider a QWI with square cross section [7], $d_y = d_z = d$ and introduce [4]

$$E_{ij} = E_1(i^2 + j^2)/2; \quad E_1 = (\hbar\pi)^2/(md^2); \quad i,j = 1,2,3., \quad (2)$$

where E_1 is the energy position of the first subband at $i = j = 1$ (note, that for $i \neq j$ a subband has a two-fold degeneracy).

In this approach we have only one parameter, $d(x)$, which defines $E_1(x)$ and hence $E_{ij}(x)$. (It is necessary to stress that the approach $d_y = d_z = d$ does not change the major results we want to demonstrate. We considered, for example, the case when $d_y \ll d_z$, so that either d_y or d_z was x-dependent. The results were qualitatively the same, because a fluctuation in d_y or d_z produces a fluctuation of $E_{ij}(x)$.)

For each subband given in Eqs. 1 and 2 the spectrum is parabolic, so that the density of states (DOS) per unit length, $g(E)$, can be easily calculated [4-7]:

$$g(E) = \sqrt{m/(2\pi^2\hbar^2)} \sum_{ij} (E - E_{ij})^{-1/2}, \quad (3)$$

where the difference $E - E_{ij}$ should always be positive.

The energy E_{ij} depends on $d(x)$; so does $g(E)$. If E_{ij} varies smoothly with x (so that the characteristic size of the fluctuations of $d(x)$ along x is larger than λ_0), Eq. 3 defines the local DOS. The average over the sample DOS $< g(E) >$ can be determined by averaging Eq. 3 for a known distribution of d on x. We analyzed different functions of $d(x)$, starting from the simplest $d(x) = < d > (1 + a\sin(\gamma x))$, with $a \ll 1$ and $\gamma \ll \lambda_0$ as a parameters. We found that the results depend on the normalised-to-unity probability of having each value of d in the QWI. That is why for demonstrative purposes we use a Gaussian distribution of $d(x)$ around its average value $< d >$, with the characteristic half width Δ_d:

$$\Phi(d(x)) = \frac{1}{\Delta_d\sqrt{2\pi}} \exp\left(-\frac{(d(x) - < d >)^2}{2\Delta_d^2}\right), \quad (4)$$

where the probability $\Phi(d)$ is normalized to unity.

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Results and Discussion

Figure 1 demonstrates the dependence of the average DOS, $< g(E) >$ (in units of $m < d > /(\sqrt{2}\hbar^2\pi^2)$) versus energy (in units of $\hbar^2\pi^2/(m < d >^2)$) for $\Delta_d/ < d >$ equal to 0.005 (solid line), 0.05 (dashed line) and 0.15 (dotted line).

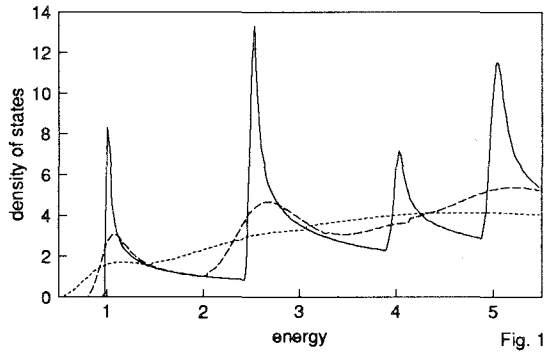

Fig. 1

The solid curve has very well pronounced peaks at energies equal E_{ij}. Due to the two-fold degeneracy of the second and fourth levels, the corresponding peaks have larger amplitudes than the other two. It is important to stress that even for a variation of QWI thickness as small as $\Delta_d/ < d > = 0.005$, there is no divergence of the average DOS appearing at $E = E_{ij}$; such a divergence would exist at these points for a perfect QWI [3-7] where $\Delta_d \equiv 0$ is assumed. In the current technology ($\Delta_d/ < d > \cong 0.05$) the observed maxima in the dependence of the average DOS on energy are reasonably pronounced only for the first two levels (dashed line). This is due to the fact that the increasing energy E does not result in an abrupt crossing of energy level E_{ij} by the level E, as in the idealized model. Now level E must go through all the fluctuations of E_{ij} in order to cross E_{ij}. For $\Delta_d/ < d > \cong 0.15$ we predict that the sharper features are almost completely absent (dotted line).

The nonmonotonic (up to peak-like) dependence of $< g >$ on E causes the nonmonotonic dependence of all transport coefficients of the sample on the Fermi energy in a degenerate semiconductor. The semiclassical Boltzmann transport equation can be written, and thus the transport phenomena can be studied by solving this equation [4-7] for known probabilities of scattering between states in different subbands (intersubband) and between different k states inside each subband (intrasubband). We consider the simplest case of gradual (see above) fluctuations of the QWI cross section, when spatial derivatives in the Boltzmann transport equation are negligible. We take into account elastic acoustic phonon scattering in the relaxation time approximation. The acoustic phonons were taken as in the bulk material in accordance with the model that the QWI is embedded into the material with the same coupling strength characteristic [8]. This approach allows us to calculate all local transport coefficients and hence their average over the sample.

Calculated in the same way as $< g(E) >$, the average resistivity $< \rho >$ (in units of $2kTm^2 < d >^2 \varepsilon^2/(\hbar^3 u^2 \pi \zeta)$, where ε is the deformation potential constant, u is the acoustic velocity and ζ is the material density) versus Fermi energy (in units of $\hbar^2\pi^2/(m < d >^2)$) is shown in Figure 2 for the same values of $\Delta_d/ < d >$ as in Figure 1.

The peaks of $< \rho >$ are well pronounced (solid line) at energies $E_F \cong E_{ij}$ for a QWI with almost no fluctuation of the cross section ($\Delta_d/ < d > \leq 0.005$). (The dependence of $< \rho >$ on the average electron concentration $< n >$ is analogous to the dependence of $< \rho >$ on E_F. Hence we reproduce it without any discussion as an example in the inset of Figure 2 for the same two out of three values of $\Delta_d/ < d >$, where the concentration per unit length is in units of $\sqrt{2}/ < d >$.) Only one quite broad maximum is seen in $< \rho > (E_F)$ for $\Delta_d/ < d > \cong 0.05$ (dashed line). There is a monotonic decrease of $< \rho >$ for $\Delta_d/ < d > \cong 0.15$. The smearing of the peaks with increasing $\Delta_d/ < d >$ is understandable from the previous discussion. Analogous smearing due to level broadening by scattering has been described previously (see e.g. [3,4]).

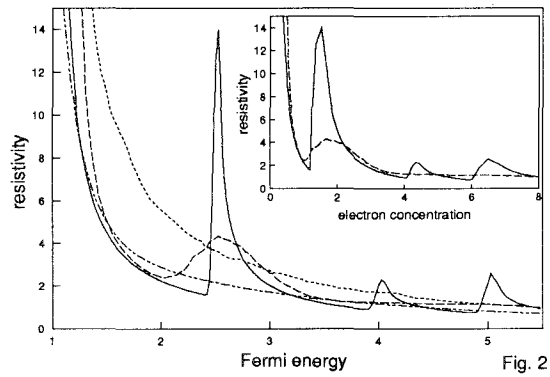

Fig. 2

There is another even more important result in the dependence of $< \rho >$ on $\Delta_d/ < d >$. The resistivity increases when the cross section fluctuation increases, and the most pronounced effect is in the range of small E_F, when only one,

$$E_{11}(< d >) < E_F < E_{12}(< d >) \quad (= E_{21}(< d >)), \quad (5)$$

or two,

$$E_{12}(< d >) < E_F < E_{22}(< d >), \quad (6)$$

levels are populated.

This phenomenon does not exist in the case when level broadening is due to scattering. For comparison we reproduce by a dotted-chain line in Figure 2 $< \rho > (E_F)$ for the case when the level broadening due to scattering in the perfect QWI ($\Delta_d \equiv 0$) results in the same dependence of the DOS on energy as shown by a dotted line in Figure 1. A huge difference in the resistivity (dotted and dotted-chain lines) at small E_F (5) for the same average DOS is due to the completely different cause and consequence of broadening in these two cases. The broadening due to scattering [3] is homogeneous along the QWI, and, in fact, introduces new channels for the current so that the conductivity is calculated as an average conductivity of these parallel channels. The channels with the largest conductivity give the major contribution to the average conductivity. That is why such

broadening practically does not change the resistivity if only one quantum level is filled (5). In our treatment the major increase of resistance with broadening occurs in this range (5) of E_F. This is because the local DOS as well as the conductivity fluctuates along the QWI; the system is analogous to the series connections of the resistors and the major contribution to $< \rho >$ comes from the high resistance part of the QWI. Hence the narrowest part of the QWI defines its resistivity and $< \rho >$ exceeds its values for the perfect QWI ($\Delta_d \equiv 0$). In previous calculations essential impurity scattering was introduced to increase the calculated resistivity to the measured values. Our calculation proves that an alternative mechanism exists. Instead of introducing an impurity scattering it is necessary to take into account the experimentally verified [1,2] cross sectional variation. Thus, we suggest that the importance of impurity scattering has been overestimated.

It is necessary to stress that the conclusions remain the same for a QWI confined in a manner different from that considered here. This is due to the fact that in our quasilocal approach the results depend only on the probability of having a particular energy level in the spectrum of energy levels allowed for a wire having a specific variation in its cross section (2,4).

Lastly, the best way to detect phenomena related to 1-D quantization is to average over several identical QWI connected in parallel. This avoids universal conductance fluctuations, which tend to obscure the peculiarities caused by subband quantization (see e.g. [3]), and allows us to deal in the theoretical calculations with one QWI without considering universal conductance fluctuations.

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References

1. H.I. Smith, K. Ismail, W.Chu, A. Yen, Y. C. Ku, M.L. Schattenberg, and D.A. Antoniadis, in Nanostructure Physics and Fabrication, ed. by M.A. Reed and P. Kirk, Academic Press, Boston, 1989, p. 57.
2. T. Fukui, H. Saito, Y. Tokura, K. Tsubaki, and N. Susa, 4th Int. Conf. Modulated Semiconductor Structures, July 17-21, 1989, Ann Arbor, MI, pp. 27-31.
3. S.Das Sarma, X.C.Xie, Phys. Rev., B35, 9875 (1987).
4. M.J. Kearney and P.N. Butcher, J. Phys. C: Solid State Phys. 19, 5429 (1986); 20, 47 (1987).
5. H. Ghosal, D. Chattopadhyay, and H. Bhattacharyya, J. Appl. Phys., 59, 2511 (1986).
6. S. Briggs and J.P. Leburton, Phys. Rev., B 39, 8025 (1989).
7. T. Yamada, and J. Sone, Phys. Rev., B40, 6265 (1989).
8. J. Lee and M.O. Vassell J. Phys. C: Sol. St. Phys., 17, 2525 (1984).