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Transport Properties of Ballistic Quantum Wire

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We investigate electronic properties of ballistic quantum wire with a stub by the tight-binding Green function method. It is shown that well-defined quasi-bound states are formed in this structure and that the dip structure in the conductance results from these states. A more realistic structure with round corners is also analyzed and there is no qualitative difference between the results for the two structures, especially in the single mode regime.

1. Introduction

The recent progress of microfabrication techniques has made it possible to create a nanometer-scale structure in semiconductors. The characteristics of this structure reflect the wave nature of electrons. Among these characteristics, the conductance of the quantum point contact in the modulation-doped heterostructure has been found to show step structure as a result of the quantization of the transverse momentum.[1)]

Using this quantum wire structure, many kinds of devices that utilize the interference effects have been proposed. Sols et al.[2),3)] proposed a quantum modulated transistor which is a quantum wire with a single stub. This device features a singly connected quantum wire and the current is modulated by a remote gate. This wire has a dip structure in the conductance and the current is modulated by controlling the position of the dips. However, as the physical picture of this dip structure remains unclear, analysis of experimental data relating to this effect is difficult.[4)] Moreover, it is not clear whether this effect remains when the abrupt corners are rounded, as the abrupt corners do not exist in the real nanometer-scale structures.

Similar dip structure has been reported by Bagwell[5)] and Tekman et al.[6)], both of whom analyzed a system in which attractive impurities were introduced in the wire. They suggested that the bound states splitting off from higher-lying confinement subband and the propagating states in the lower mode couple to become the quasibound states and totally reflecting states, and that these states are the source of the dip structures in the conductance. Kasai et al.[7)] investigated a similar structure with a slightly increased width, which when small enough has an effect similar to introducing attractive impurities. Recently, the authors investigated a structure similar to that of Kasai et al. and clarified that the quasibound states arise as a result of mode couplings and that these states are localized around the region of the width increase.[8)] All these pictures are restricted to the case when the propagating modes can be defined approximately throughout the wire.

In the present study, we investigate the transport characteristics of ballistic quantum wires with a single stub where the above pictures no longer hold true. In this case, the modes mix strongly and they cannot be defined throughout the wire. It is shown that the quasibound states also exist in these wires and these states are closely related to the transport properties of the wires in the structure with rounded corners, as well as in the structure with sharp corners.

2. Method

We employed the tight-binding Green function method, which is a slight modification of the recursive Green function method.[9)] Conductance and local density of states per unit length were calculated and compared. This approach has been recently proposed by the authors for the analyses of ballistic quantum wires. The transmission matrix can be determined by the Green function and the Landauer formula is used to evaluate the conductance. The local density of states per unit length of the wire at r_x, $D_w(r_x, E)$, and the local density of states per unit length for modes at r_x, $\rho_m(r_x, m_y, E)$, are defined as

$$D_W(r_x, E) = \sum_{r_y} \rho(\vec{r}, E) = \sum_{m_y} \rho_m(r_x, m_y, E), \quad (1)$$

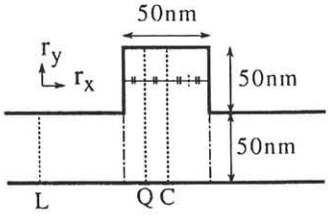

Fig. 1. Abrupt T-stub structure.

$$\rho_m(r_x, m_y, E) = \sum_n \delta(E - E_n)\cdot \varphi_n(r_x, m_y)\varphi^*_n(r_x, m_y) , \quad (2)$$

$$\varphi_n(r_x, m_y) = \sum_{r_y} f_{m_y}(r_y)\phi_n(r_x, r_y) , \quad (3)$$

where $\phi_n(\vec{r})$ and E_n are the complete set of orthonormal eigenfunctions and eigenvalues of the Hamiltonian H, respectively. $f_{m_y}(r_y)$ is the eigenfunction with respect to the transverse mode m_y and $\rho(\vec{r}, E)$ is the local density of states per unit area. In the tight-binding model,

$$f_{m_y}(r_y) = \sqrt{\frac{2}{N_w+1}} \sin\left(\frac{m_y \pi r_y}{N_w+1}\right), \quad (4)$$

where N_w is the number of sites in the transverse direction. $\rho_m(r_x, m_y, E)$ can be directly determined from the imaginary part of the diagonal element of the Green function. $\rho_m(r_x, m_y, E)$ can be considered to be the decomposition of the local density of states $D_w(r_x, E)$ for transverse momentum. The effective mass of GaAs ($0.067m_0$, where m_0 is the electron rest mass) is used and the lattice constant of the tight-binding lattice is taken to be 2.5nm throughout this study.

3. Results

First, the conductance g of abrupt structure as shown in Fig. 1 is plotted in Fig. 2 (a). The profile widely deviates from the conductance quantization profile, which implies that the modes mix strongly at the junction. The dip structure is seen in the profile. The local density of states $D_w(r_x, E)$ at C in Fig. 1 is plotted for (Fermi) energy in Fig. 2 (b). It is clearly seen that for each dip in the conductance profile, the local density of states has a clear sharp peak. The correspondence is especially clear for the dips in the single mode regime. As the peaks have small widths, they can be regarded as quasibound states. To clarify the origin of these peaks, $D_w(r_x, E)$ was decomposed to $\rho_m(r_x, m_y, E)$, which is plotted in Fig. 3 (a). It can be seen that most of the peaks have well-defined mode indices corresponding to the discrete levels of the quantum box in the stub region. The box is indicated by the dot-dashed lines in Fig. 1. The second, third, and fourth peak in Fig. 3 (a) correspond to the states which have the mode indices (m_x, m_y) = (1,3), (1,4), (1,5), respectively. The first peak corresponds to the state which is the combination of (1,1) and (1,2). The fifth peak corresponds to the state which is the combination of (3,1) and (3,2). The peak for $m_x = 2$ cannot be found in this profile, because $\rho_m(r_x, m_y, E)$ is plotted at C

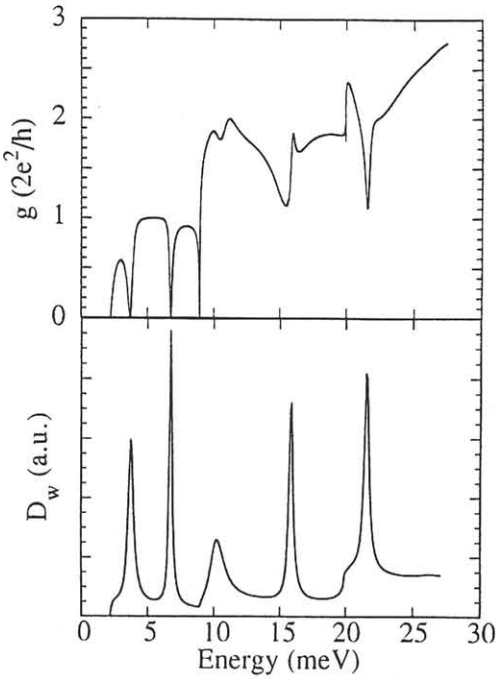

Fig. 2. (a) Conductance g, (b) local density of states per unit length $D_w(r_x, E)$ at C of the abrupt structure.

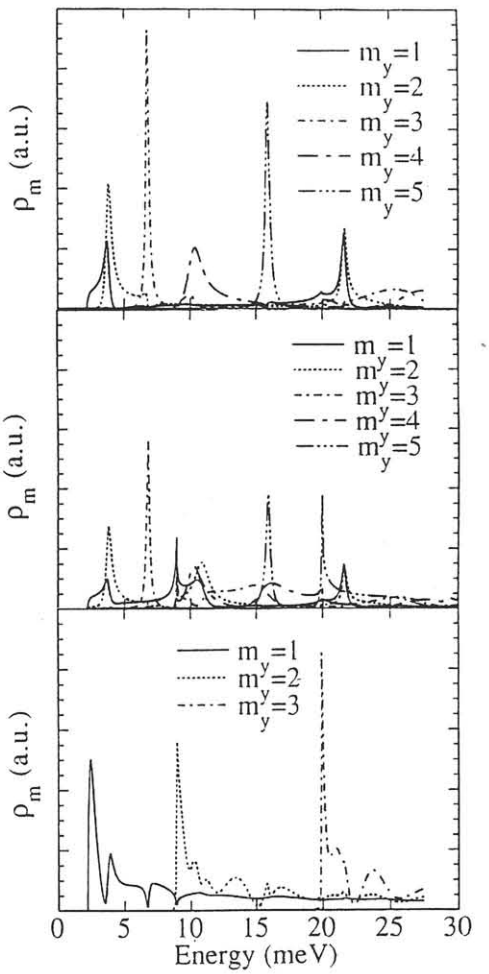

Fig. 3 Local density of states per unit length for modes $\rho_m(r_x, m_y, E)$ at (a) C, (b) Q, and (c) L of the abrupt structure.

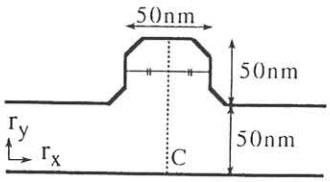

Fig. 4. T-stub structure with rounded corners.

where there is a node. This is confirmed by Fig. 3 (b), in which $\rho_m(r_x,m_y,E)$ at Q in Fig. 1 is plotted. A new peak appears at about E = 9 meV and this corresponds to the third dip in Fig. 2 (a).

As a result of attaching the leads, the discrete levels in the quantum box have finite probabilities of decaying outside the stub and they become the quasibound states. The positions of the peaks are slightly shifted from the discrete levels as a result of the couplings. The widths of these peaks can be related to the lifetime of these quasibound states by the uncertainty principle.

For comparison, $\rho_m(r_x,m_y,E)$ at L in Fig. 1 is plotted in Fig. 3 (c). Here a quasi-one dimensional subband spectrum can be seen and it is totally different from the spectrum in Fig. 3 (a) or (b). The oscillatory structure is the result of the interference effect.

Real systems fabricated by etching or the lift-off process never have the sharp corners as shown in Fig. 1. Accordingly, the four corners were rounded as shown in Fig. 4 to investigate the robustness of the results obtained above. The conductance g and the local density of states for modes $\rho_m(r_x,m_y,E)$ are plotted in Figs. 5 (a) and (b). The rounding causes no qualitative change in the result in the low energy region. Peaks in the local density of states are enhanced or reduced and slightly shifted. The peak at around E = 22meV disappears. It means that this rounding destructs only the quasi-bound state which has mode index m_x = 3. This is reasonable because the states which have small mode indices have large wavelengths and are not severely affected by the rounding of the corners. It is thus expected that this dip structure is not affected qualitatively as far as the well-defined quasibound states are formed in the stub region.

4. Conclusion

The electronic properties of a ballistic quantum wire with a single stub has been investigated by the tight-binding Green function method. The physical origin of the dip structure in the conductance profile was clarified; there are well-defined quasibound states and they correspond to the discrete levels of the quantum box. The conductance shows a dip structure at the energy corresponding to these quasi-bound states. A more realistic structure with rounded corners was also analyzed. No qualitative change in the results for the abrupt structure was found even after the corners were rounded, especially in the single mode regime. The characteristics of quantum interference device are closely connected with their structure, so our investigation gives an important insight into the designing of these devices.

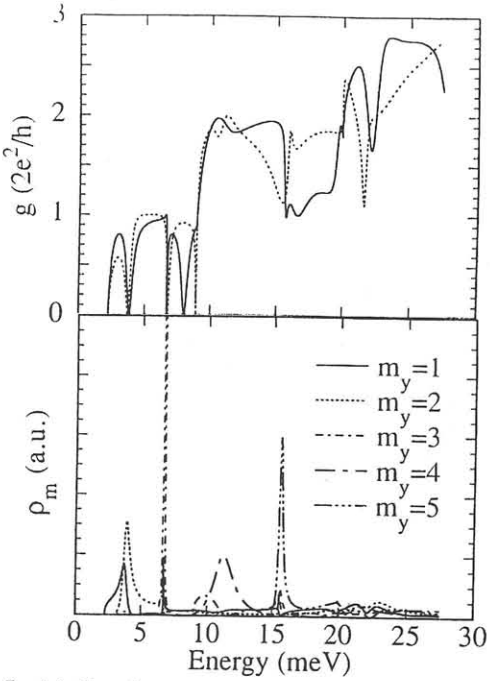

Fig. 5. (a) Conductance g of rounded (solid line) and abrupt structure (dotted line). (b) local density of states per unit length $\rho_m(r_x,m_y,E)$ of rounded structure.

Acknowledgments

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