Quantum-constriction rectifier

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A simple quantum constriction (wide-narrow geometry) is found to act as a rectifier in the coherent transport regime if Fermi energy is between the propagation thresholds of the wide and narrow parts. Therefore a simple diode could consist of only two identical leads of different widths. The current-voltage characteristics of this structure are calculated for several temperatures and lead widths, and generalized to other cases by appropriate scaling rules. The rectification properties disappear as the temperature or the size of the system increase. This structure also exhibits regions of negative-differential resistance. [S0163-1829(96)02136-4]

The current rectification effect is achieved by elements with asymmetric internal potential barriers. A classic way for creating such barriers is by charge distributions (e.g., *p*-*n* junction) or with the Schottky barrier. However, alternative diode structures have been proposed, based on advanced fabrication techniques. In order to obtain a barrier shape independent of the carrier distribution, Allyn, Gossard, and Wiegmann[1] suggested a unipolar semiconductor rectification structure created by a molecular-beam-epitaxy (MBE)-grown $Al_xGa_{1-x}As/GaAs$ heterostructure. An asymmetric potential barrier has been produced by compositional grading, i.e., by linearly increasing the mole fraction of Al in the $Al_xGa_{1-x}As$ barrier in the space between layers of *n*-type GaAs. Recently, Papp *et al.*[2] proposed a similar resonant-tunneling diode. Instead of a resonant-tunneling diode based on a double-barrier quantum well,[3] they proposed a structure with a single indented barrier with two different Al concentrations, which operates on the same principle. Here we discuss the possibility of an alternative rectifying structure which operates in the world of mesoscopic devices.

We find that, for mesoscopic structures, a rectifying effect can be also achieved if devices have an asymmetric geometry, without compositional grading. In this case the transverse component of electron momentum (i.e., energy) is quantized, and the propagation threshold becomes dependent on the width of the element. A decrease of the width of the device has the same effect as an increase of Al in an $Al_xGa_{1-x}As$ barrier if the Fermi energy (E_F) has the appropriate value.[4] Similarly, the effect of an asymmetric potential barrier might be achieved for mesoscopic devices in the coherent transport regime by attaching asymmetric electrodes (i.e. leads of different widths) to an element. We examine the simplest of such structures: two perfect leads joined without any element between them [Fig. 1(a)], i.e., a quantum constriction. Electron transmission coefficients in this wide-narrow (WN) geometry were calculated by Szafer and Stone[5] on the basis of a linear model. Here we calculate the complete current-voltage characteristics of this element with a suggestion of a possible device application.

The asymmetric potential of an unbiased WN junction [Fig. 1(b)] is a consequence of different threshold levels in the leads. The offset of the threshold energies (Δ_T) is given in the tight-binding (TB) picture by

$$\Delta_T = E_N - E_W = 2|X|\left(\cos\frac{a\pi}{d_W} - \cos\frac{a\pi}{d_N}\right) \approx |X| a^2\pi^2\left(\frac{1}{d_N^2} - \frac{1}{d_W^2}\right), \tag{1}$$

where $X = -\hbar^2/(2m^*a^2)$ is the hopping matrix element, a is the lattice constant, and m^* is effective mass of an electron. Electron transport in the WN junction does not depend on the evanescent modes,[5] i.e., the electron transmission $T(E)$ sharply increases as the channels of narrow wire are filled.

A WN junction best works as a rectifier if the Fermi level is between the propagation thresholds of the wide and narrow wire (Fig. 1). We first discuss the zero-temperature case. When forward bias voltage V is less than Δ/e, Fig. 1(b), the propagation threshold of the narrow wire $E_N - eV$ is above the Fermi energy E_F, and the net electrical current is zero. The forward turn-on voltage is $V = \Delta/e$, Fig. 1(c). In the case

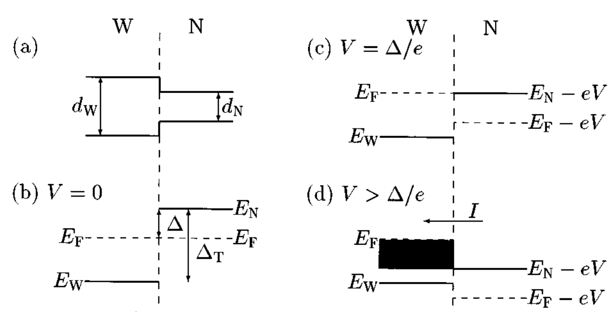

FIG. 1. (a) A quantum constriction—WN junction. (b) Unbiased system. The Fermi level in equilibrium is for Δ below the propagation threshold of the narrow wire ($\Delta = E_N - E_F$). E_W and E_N are the propagation thresholds in the leads. (c) Biased system: $V = \Delta/e$ ($V_W = 0$, $V_N = V$). (d) At $T = 0$ K, for $\Delta/e < V < \Delta_T/e$, only states from the range $E_N - eV < E < E_F$ (darkened part) contribute to the net electric current, whereas for $V > \Delta_T/e$ the relevant states are in the range $E_W < E < E_F$.

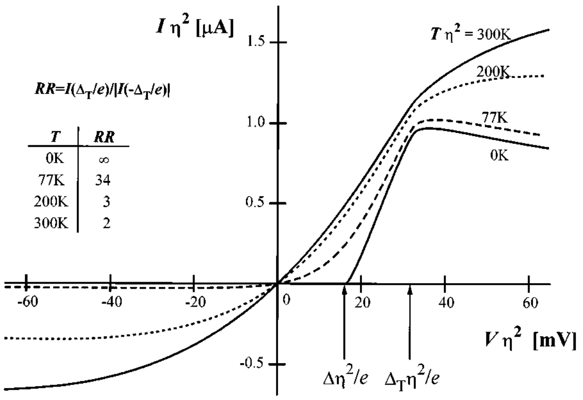

FIG. 2. I-V characteristics of a WN junction for various temperatures. For the widths of the wide and narrow leads we take $d_W/d_N(=\Delta_T/\Delta)=2$ and $d_N=20a$. The scaling factor is defined as $\eta=d_N/(20a)$. Values for the rectification ratio RR of this structure are given in the inset.

when $V>\Delta/e$ [Fig. 1(d)], electrons are transmitted from the wide to narrow wire, and conduction starts. Only electrons with energies between $E_{\rm F}-eV$ and $E_{\rm F}$ contribute to the current. When the bias polarization is reversed, then the propagation threshold in the narrow wire remains above the Fermi energy for all voltages, and therefore there is no current. Thus the I-V characteristic of this element will be asymmetric and rectifying. In our calculations we assume that the whole voltage drop V occurs at the abrupt constriction. Note that if the Fermi level is below E_W in equilibrium, then the current would be zero, at $T=0$ K, regardless on the voltage V, whereas for $E_F>E_N$ the nonzero current would exist regardless on the bias polarity. The current-voltage characteristic of a WN junction can be calculated from the formula[6]

$$I=\frac{2e}{h}\int_{-\infty}^{+\infty}[f(E)-f(E+eV)]T(E,V)\mathrm{d}E, \tag{2}$$

where $f(E)$ is the Fermi-Dirac distribution function. Electron states are described by a nearest-neighbor TB Hamiltonian on a square lattice. The total transmission $T(E,V)$ can be obtained from Ando's formula,[7] simplified for the case of zero magnetic field[8] and generalized for asymmetric leads:

$$T(E,V)=4X^2\sum_{\alpha,\beta}\mathrm{Im}\lambda_{\mathrm{N}\alpha}(E,V)\mathrm{Im}\lambda_{\mathrm{W}\beta}(E,0)$$
$$\times|[\mathbf{U}_{\mathrm{N}}^{-1}\mathbf{G}_{1,0}(E,V)\mathbf{U}_{\mathrm{W}}]_{\alpha,\beta}|^2, \tag{3}$$

where $\mathbf{U}$ and λ matrices are rightgoing (from W to N) eigenvectors and eigenvalues of the Schrödinger equation for an electron in the perfect lead. $\mathbf{G}_{1,0}$ is the Green's function which couples the leads in the system.[7,9] Summations in (3) go only over the open channels (α, β) in the leads. Formula (3) is valid for a coherent transport.

In Fig. 2 are shown the calculated I-V characteristics of a WN junction. We assume that only one channel is open in the wide lead. At zero temperature, the increase of the voltage V above Δ/e (i.e., $\Delta\eta^2/e$) causes an increase of the electric current $[I\sim(2e^2/h)(V-\Delta/e)]$, since the number of electron states contributing to the current increases. The maximum current is achieved when the propagation threshold in the wider lead (E_W) levels with the threshold in the narrower lead (E_N-eV), i.e., when $V=\Delta_T/e$, because then the largest number of states contributes to the current. For $V>\Delta_T/e$ the number of propagation states (they are in the range $E_W<E<E_F$) does not change, but the transmission decreases due to the increase of electron reflection on the potential jump at the constriction. Therefore the current decreases, and the characteristics of the WN junction enters the region of negative differential resistance (NDR).

As the temperature increases, the number of states that contribute to the net electric current becomes greater, and therefore the current also increases for the same bias. However, at higher temperatures the forward turn-on voltage for the diode is not well defined (at zero temperature it is at $V=\Delta/e$), and for $V<0$ the rectifying feature of this system gradually disappears.

A similar effect on the I-V characteristics has the increase of the size of the system as the rise of temperature. If the system dimensions increase (e.g., $d'=\eta d$, $\lambda'_{\rm F}=\eta\lambda_{\rm F}$, etc.—where $\lambda_{\rm F}$ is the Fermi wavelength), then the same I-V characteristics are obtained but with scaled voltage, current, and temperature in the problem, according to the rules[10,11] $V'=V/\eta^2$, $I'=I/\eta^2$, and $T'=T/\eta^2$. Hence raising the temperature η^2 times, for the fixed size of the system, yields current-voltage characteristics which are identical with ($\eta^2 I$-$\eta^2 V$) characteristics in the case when the width of the system is η times larger at the fixed temperature. For example, the dc characteristics for $d_N=20a$ (which means $d_N=11.2$ nm for $a=0.56$ nm and therefore $X=-1.8$ eV for GaAs) and temperature $T=300$ K in Fig. 2 ($\eta=1$) also correspond to the case, say, $d_N=40a$ ($\eta=2$) and the temperature $T=300\ \mathrm{K}/\eta^2\approx77$ K.

In order to assess the quality of the rectification, one can use a rectification ratio, which we define as the ratio of the current at forward bias $V=\Delta_{\rm T}/e$ (when the zero-temperature current is at a maximum), and current at the same but reverse bias. Values for the rectification ratio are given in Fig. 2. The ratio decreases with temperature as the rectification feature of this element disappears, due to the thermal activation of electrons around the subband bottom.

A possible deviation from the ideal geometry in Fig. 1 is that one of the leads is moved up or down, i.e., that the axis of symmetry is not the same for both leads. In this case we find that the current will decrease in proportion to the offset of the two leads. The reason for this is the following. Transmission through the element is proportional to the overlap integral of the transverse wave functions of a particle in the wide and narrow leads.[5] Above the turn-on voltage both leads are in the single-mode regime, while for transverse wave functions we have $\varphi(y_i)\sim\sin\pi y_i/d_i$, where y_i is the lateral coordinate, and d_i, $i=W,N$ is the width of the wide or narrow lead. Now it is obvious that the overlap is greatest when leads are centered. Note that this deviation does not change the effect qualitatively.

At $T=0$K in the OFF state ($V<\Delta/e$) the total transmission is zero due to the mutual positions of the Fermi level and propagation thresholds in the leads. Therefore disorder should have no effect on the OFF state. However, in the ON state (the conducting state of a rectifier) defects will cause an overall decrease of current (except for the case of short-range attractive impurities[4]). Resistance in the ON state is very high $[R_{\mathrm{ON}} \geqslant h/(2e^2) \approx 13\mathrm{k}\Omega]$ regardless on the presence of disorder, which limits an efficient application of the device in fast switching circuits.[12]

This type of theoretical consideration usually assumes different lateral confinements in an otherwise homogenous structure along one direction. Therefore the Fermi energies in two quantum wires would be the same if they were separated. However, it is possible that either intentionally, or due to fabrication imperfections, the Fermi levels in two wires would not be the same. In this case charge transfer will occur $(T>0\mathrm{K})$ at the junction, which causes band bending. For electron transfer from the N to W wire (then $E_{FW}<E_{FN}$), the Schottky barrier will form on the N side. The barrier impedes electron transmission through the junction. This will cause an increase of the turn-on voltage and an overall decrease of the current for the forward bias. For the reverse bias, the current will also globally decrease due to the barrier, in comparison to the case with no barrier. However, it is possible that the increase of the reverse bias will lower the barrier, and that therefore the current will increase faster than in the no-barrier case. For higher temperatures and high barriers it is even possible that the diode function is completely reversed. Furthermore, with appropriate band engineering it could be possible to design a rectifier with the desired characteristics.

In conclusion, we propose a WN junction as a mesoscopic rectifier, which shows features of an ideal rectifying barrier at zero temperature. The value of the forward turn-on voltage for this diode can be controlled by changing the width of the electrodes, independent of the carrier distribution (which is a traditional way of creating a rectifying barrier).

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