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Mesoscopic diode

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Abstract

Here we discuss the possibility of an alternative rectifying structure which operates in the world of mesoscopic devices. 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. Also a quantum structure is proposed which is predicted to operate as a rectifier at room temperatures. This diode for the nanostructures is a quantum wire with an asymmetric quantum constriction (AQC) which works in the coherent transport regime. Structurally imperfect mesoscopic diodes retain rectifying features, although the actual *I–V* characteristics are different in comparison to the perfect devices.

Keywords: Nanoelectronic device; A new quantum rectifier

1. Introduction

The miniaturization of integrated circuits and components approaches nearly atomic-scale dimensions. Therefore there is a need for developing new basic electronic components for nanoelectronics, with the device physics based on the quantum mechanics. For example, a T-shaped waveguide-like structure is proposed as a possible way for exploiting quantum interference effect for realizing device functions such as switching or amplification [1,2] or analog-to-digital conversion [3]. Alternative diode structures have been also proposed, based on advanced fabrication techniques [4,5].

The current rectification effect is achieved by elements with asymmetric internal potential barrier. A classic way for creating such barriers is by charge distributions (e.g. p–n junction) or with the Schottky barrier. However, we find that, for mesoscopic structures, a rectifying effect can be also achieved if devices have an asymmetric geometry [6], 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. 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. The simplest of such structures is

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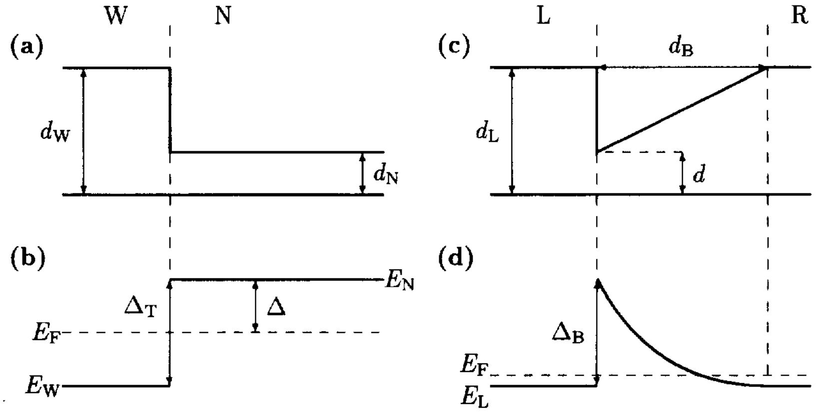

Fig. 1. (a) A quantum constriction Wide–Narrow (WN) junction. (b) The energy diagram of a WN junction in the thermodynamic equilibrium. E_W and E_N are the propagation thresholds in the leads. (c) Asymmetric quantum constriction (AQC). (d) The energy diagram for an AQC junction in the equilibrium.

wide–narrow junction (WN): two perfect leads (of different widths) joined without any element between them, i.e. a quantum constriction, Fig. 1(a). The complete current–voltage characteristics of this element, and a discussion of possible device application are presented in the next sections. However, predicted rectifying properties of a WN junction degrade rapidly as temperature increases from zero to room temperature. The ultimate goal is fabrication of a reliable diode which operates at room temperatures. Here we propose a possible structure which could be an answer to this problem, for the case of coherent transport, i.e. when all phase-breaking processes can be neglected.

2. Wide–narrow (WN) junction

A WN junction best works as a rectifier if the Fermi level is between the propagation thresholds of the wide (E_W) and narrow wire (E_N), Fig. 1(b). The asymmetric potential of an unbiased WN junction is a consequence of different threshold levels in the leads. Let the Fermi level in equilibrium is for Δ below the propagation threshold of the narrow wire ($\Delta = E_N - E_F$). When forward bias voltage V is less than Δ/e, the propagation threshold of the narrow wire $E_N - eV$ is above Fermi energy E_F} and net electrical current is zero, for the zero-temperature. The forward turn-on voltage is $V = \Delta/e$, Fig. 2. When $V > \Delta/e$ electrons are transmitted from the wide to narrow wire, and conduction starts. When the bias polarisation 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. For $V > \Delta_T/e$ (where $\Delta_T = E_N - E_W$) the characteristics of the WN junction can enter the region of negative differential resistance.

The current–voltage characteristic of a WN junction, Fig. 2, can be calculated from the formula [7]:

$$I(V) = \frac{2e}{h} \int_{-\infty}^{\infty} [f(E) - f(E + eV)] T(E, V) \, \mathrm{d}E, \tag{1}$$

where $f(E)$ is the Fermi-Dirac distribution function. Electron states are described by a nearest-

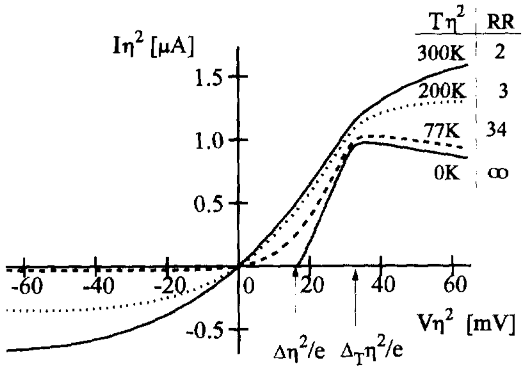

Fig. 2. I–V characteristics of a WN junction for various temperatures. The scaling factor is defined as $\eta = d_N/(20a)$, where d_N is the width of the narrow lead and a is the lattice constant.

neighbour TB Hamiltonian on a square lattice. The total transmission $T(E,V)$ one can obtain by using the Green's function iterative method [8,9], simplified for the case of zero magnetic field and generalized for asymmetric leads [10]. Coherent transport is assumed for all considered temperatures. Although at room temperatures electrons experience frequent phonon scattering, the use of the phase coherent model is justified on the assumption that the device size is still smaller than the inelastic scattering length in the material. The population threshold in the narrow wire is above the Fermi energy, so the narrow wire is nonconducting for small applied voltages (zero-temperature case). Therefore, the voltage should drop in the whole of the narrow wire segment. But, when applied bias is higher than the forward turn-on voltage, the charge transfer will occur (from W to N wire). Then in our calculations we assume that the whole voltage drop V occurs at the abrupt constriction.

At higher temperatures the forward turn-on voltage for the diode is not well defined, and for $V<0$ the rectifying feature of this system gradually disappears, Fig. 2. 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 ($d=\eta d$, $\lambda_F' = \eta\lambda_F$, etc. – where λ_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: $V' = V/\eta^2$, $I' = I/\eta^2$, and $T' = T/\eta^2$. Hence raising the temperature η^2 times, for the fixed size of the system, yields the 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 bigger at the fixed temperature.

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 $V=\Delta_T/e$ (when the zero-temperature current is at a maximum), and current at the same but reverse bias. Values for the rectification ratio (RR) 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.

3. Asymmetric quantum constriction

A WN diode does not work as a rectifier at room temperatures. The inverse current is of the same order of magnitude as the forward current. However, we find that the current rectification might be possible with an asymmetric quantum constriction (AQC), shown in Fig. 1(c), which has two electrodes, right (R) and left (L), of the same widths ($d_R = d_L$), and an asymmetric narrow constriction between them. The energy diagram of an unbiased AQC is presented in Fig. 1(d), and it is similar to the diagram obtained for the system proposed by Allyn et al. [4]. Although this diagram is a qualitative one (which can be obtained from the dependences of the propagation threshold on the wire width [11]) it could well serve as a guide for understanding how this device works. The current–voltage characteristics are shown in Fig. 3. In the case of forward bias the propagation threshold of the R-wire ($E_R + eV$) moves towards higher energies, and thus lowers the barrier for electron transfer from the R to L wire and increases the forward current. On the other side, when the diode is inversely biased, the propagation threshold of the R wire is shifted towards lower energies, and if the inverse current depends only on the thermal excitations and Δ_B is big enough (e.g. $\Delta_B > 10k_BT$), the inverse current will be negligible. For the considered system we get $RR = 2 \times 10^3$ in the middle of the voltage bias range. Therefore, a very small value for the inverse current is controlled by narrowing the quantum wire at only one point. It is interesting that the same energy diagram has the Schottky junction, and that is why the AQC junction is its geometrical realization in the coherent transport regime.

To determine the transport properties of the system it is essential to consider how the applied voltage is dropped between the contacts. Firstly we assume that the voltage drop on the perfect leads is small and expect that the voltage is dropped predominantly across the constriction. The fraction of the dc voltage that is dropped between contact and narrowest part of the constriction is β, where $\beta \approx 0.5$ (except for gate voltages close to and beyond pinchoff, where $\beta \approx 0.2$) from the experiments of Kouwenhoven et al. [12], and the theoretical predictions of Glazman and Khaetskii [13]. This non-linear potential distribution was confirmed also by Patel et al. [14,15].

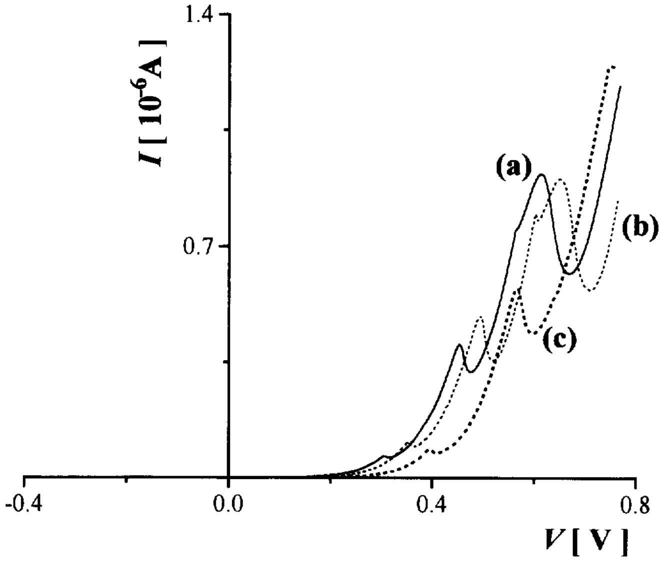

Fig. 3. I–V characteristics of an AQC rectifier – the influence of the structural disorder on the conducting state of the AQC rectifier of the dimensions $d_W = 8d$, $d_B = 7d$, $d = 5a$ and $T = 300$ K. The system is: (a) without defects, (b) with repulsive impurities $E_{imp} = |X|$, (X is the hopping matrix element, for GaAs $X = -1.8$ eV) $p = 5\%$, and (c) with edge roughness of the deviation $\sigma = 30\%$.

In Fig. 3 one can notice that the dc characteristics of an AQC structure, unlike WN junction, has several regions of negative differential resistance (NDR). The reason for this is the barrier region in an AQC structure where quasi-bound states are forming [16], which do not exist in a WN junction. As the forward bias is raising, the energy of a quasi-bound state is lowering, approaching the propagation threshold E_R. As the energy of a quasi-bound state E_{qb_s} comes closer to the propagation threshold E_R, the electron transmission $T(E_{qb_s})$ increases, and therefore the current I increases as well. When E_{qb_s} levels with E_R, then $T(E_{qb_s})$ has maximum and the current is in a local maximum. Further increase of the bias voltage will push E_{qb_s} below the propagation threshold, the transmission probability decreases, as well as the current and the region of NDR forms. When forward bias further increases, next quasi-bound state is approaching the propagation threshold, and the current raises again, and the whole cycle repeats.

We have also considered influence of the compositional disorder in an AQC structure, Fig. 3. For such small systems one should be always aware of possible influence of imperfections, generated during the fabrication, on the device characteristics. Defects in the structure, such as neutral impurities and edge roughness localized in the region of the constriction, are treated. In our calculations both types of disorder are modelled in the same way – by random replacement of the host atoms (in a 2D tight-binding lattice [10]) by the impurity atoms (concentration p) or hard-wall atoms (simulating rough boundaries, i.e. nonspecular reflections from the edges). The edge roughness is generated by increasing or decreasing the width of the constriction by adding n-atoms, where n is a random number. These numbers have Gaussian (discrete) distribution of mean zero and deviation σ. The peculiar shape of the I–V characteristics (multiple peaks and NDR regions) is preserved in the presence of disordered, only the positions of the current peaks are shifted. The repulsive impurities in the structure increase the energies of quasi-bound states [16], and higher biases are needed in order to E_{qb_s} and $E_R(=E_L)$ are levelled, Fig. 3(b). Hence, in the presence of the repulsive impurities the current maximums are achieved for higher biases in comparison to the case of an ideal diode. On the contrary, if attractive impurities are in the structure, the current maximums are shifted towards lower voltages. The boundary roughness type of disorder has a significant effect on the I–V characteristics only for a very strong edge fluctuations ($\sigma > 10\%$). The reason for this is that the transport is dominated by the electrons with energies just above the propagation threshold E_R, i.e. the long-wavelength electrons, which are unaffected by the small-scale edge roughness [10]. Therefore, the uneven barrier is effectively narrower than the ideal one, so the energy of the quasi-bound states increases and the whole I–V characteristic is shifted towards higher voltages (as in the case of repulsive impurities), Fig. 3(c). If both types of defects exist in the system, their effects on the device characteristics are simply combined [10]. In the case of the reverse bias, the repulsive impurities and the edge roughness only effectively increase the barrier and therefore decrease the intensity of the electric current. The attractive impurities have the opposite effect, but the current increase is not significant, and the device remains unconducting for the inverse biases regardless whether any defects are in the structure or not.

4. Conclusion

A WN junction 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 on the carrier distribution (what is a traditional way of creating rectifying barrier). However, the rectification properties of this structure depend on the temperature, and at the room temperatures the rectification almost disappears. Hence a simple quantum structure is proposed which is predicted to operate as a rectifier at room temperatures. This diode for the nanostructures is a quantum wire with the modulated width, i.e. AQC which works in the coherent transport regime. We find that an AQC structure acts like a Schottky barrier. The device geometry creates an asymmetric barrier which could enable the forward currents three orders of magnitude higher than the reverse currents, at $T=300$ K. This structure is a potential candidate for the role of a diode in the nanoelectronic circuits.

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