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ELECTRICAL AND THERMAL PROPERTIES OF NANOWIRES IN QUANTUM REGIME

Waldemar Nawrocki

Poznan University of Technology, ul. Piotrowo 3A, 60-965 Poznan, Poland

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Abstract. Problems concerning electron transport in mesoscopic structures and nanostructures are considered in the paper. The electrical conductance of nanowires has been measured in a simple experimental system. Investigations have been performed in air at room temperature measuring the conductance between two vibrating metal wires with a standard oscilloscope. The conductance quantization in units of $G_0 = 2e^2/h = (12.9\ k\Omega)^{-1}$ up to five quanta of conductance has been observed for nanowires formed in many metals. The explanation of this universal phenomena is the formation of a nanometer-sized wire (nanowire) between macroscopic metallic contacts which have induced, in accordance with the theory proposed by Landauer, the quantization of conductance. The thermal problems in nanowires are also discussed in the papers.

1. INTRODUCTION

In the last 20 years considerable attention has been focused on the quantization of both electrical and thermal conductance in nanostructures. It should be underlined that electrical and thermal conductance of a nanostructure describe the same process: the electron transport in a nanostructure. Therefore, there are several analogues between the two physical quantities. The theoretical quantum unit of electrical conductance $G_0 = 2e^2/h$ has predicted by Landauer [1] in his new theory of electrical conductance. In 1987 Gimzewski and Moller [2] published the results on measurements of the quantization of conductance in metals at room temperature observed with a scanning tunnelling microscope. In 1988 two groups [3,4] reported the discovery of conductance quantization in a controllable two-dimensional electron gas (2DEG) in the GaAs constriction at liquid He temperature. Formation of nanowires in the process of breaking the contact between ordinary metallic wires at room temperature was proposed by Costa-Kramer et al. [5] in 1995.

Heat exchange is very important for integrated circuits, as well. It is generally known that limits for speeding-up digital circuits, especially microprocessors, are determined by thermal problems. Therefore, many groups investigate the heat exchange and thermal conductance in nanostructures. The first theoretical analyses of thermal conductance in structures in the ballistic regime were made by P. Streda [6]. Next papers on a quantization of thermal conductance came from several groups, e.g. [7, 8].

In this paper, electrical conductance and thermal conductance in nanostructures are considered, e.g. in such structures as integrated circuits. However, the measurements presented in this paper concern electrical conductance only.

2. THEORY OF CONDUCTANCE QUANTIZATION

Transport of electrons can be described classically by the Boltzmann transport equation (the Drude model) which introduces a mean free path Λ. At relatively low temperatures some considerable con-

Corresponding author: W. Nawrocki, e-mail: nawrocki@et.put.poznan.pl

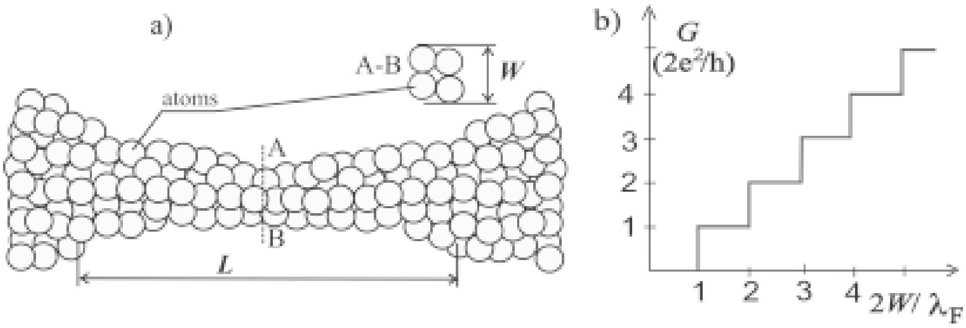

Fig. 1. Conductance quantization in a nanowire (a conductor with length $L < \Lambda$ and width W comparable with Fermi wave length λ_F): (a) nanowire outline (the third dimension is not considered); (b) conductance quantization G versus width W.

tribution to conductivity is given by electrons with the energy close to the Fermi surface. Hence, conductivity is given by:

$$\sigma = \frac{ne^2\tau}{m^*}, \tag{1}$$

where n is the concentration of the carriers, m^* – the effective mass of the electron, τ – the relaxation time.

Another parameter characterizing the system is Fermi wavelength $\lambda_F = 2\pi/k_F$, where k_F is the Fermi wavevector. For metals like copper or gold, $\lambda_F \approx 0.5$ nm is much less than the free electron path Λ ($\Lambda_{Au} = 14$ nm). If the system dimensions are less than a free electron path, the impurity scattering is negligible, so the electrons transport can be regarded as ballistic. If the outside diameter of a metal wire is W, comparable with Fermi wavelength λ_F, and the length L is less than Λ, the system can be regarded as one-dimensional (1D), the electron – as a wave, and quantum effects can be expected.

Let us consider a perfect conductor with diameter W and length L (Fig. 1) connecting two wide contacts (reservoirs of electrons) between which conductivity is measured.

Assuming that the wide contacts are infinitely large, the electrons are in a thermodynamic equilibrium described by the Fermi-Dirac statistics. When the electrons enter a 1D conductor, nonequilibrium states occur with negative and positive velocities. If there is a resultant current, the states with positive velocities correspond to higher energies [1]. According to the Büttiker model [9], the Hamiltonian of the perfect conductor can be expressed as follows:

$$H = \frac{1}{2m^*}\left(\eta^2 k_x^2 + \eta^2 k_y^2\right) + V(x), \tag{2}$$

where y is a coordinate (a dimension along the wire), x is in the transverse direction, m^* is the effective mass, $V(x)$ denotes the potential well of width W, k_y is a wavevector along y, and k_x is a wavevector along x. Because of the narrowness of potential well $V(x)$ the energy for transverse propagation is quantized:

$$E_{Tj} = \frac{\eta^2 k_x^2}{2m^*} = \frac{\eta^2}{2m^*}\left(\frac{j\pi}{W}\right)^2. \tag{3}$$

The formula (3) is valid if the potential energy tends to infinity at the quantum well boundary.

For the Fermi level $E_F = E_j$ there is a number $N \sim 2W/\lambda_F$ of states E_{Tj} below the Fermi surface. Let us assume that thermal energy k_BT is much smaller then the energy gap between levels, and that the wide contacts are characterized by chemical potentials μ_1 and μ_2 with ($\mu_1 > \mu_2$). Then, the current of electrons in j^{th} state is equal to:

$$I_j = e\nu_j \left(\frac{dn}{dE}\right)_j \Delta\mu, \tag{4}$$

where ν_j is the velocity along y and $(dn/dE)_j$ is the density of states at the Fermi level for state j^{th}. The density of states for 1D conductor is

$$\frac{dn}{dk} = \frac{1}{2\pi} \quad \text{and} \quad \left(\frac{dn}{dE}\right)_j = \left(\frac{dn}{dk}\frac{dk}{dE}\right)_j = \frac{2}{h\nu_j}. \tag{5}$$

The factor of 2 results from spin degeneracy. Hence, the current for j^{th} state $I_j = V(2e^2/h)$ does not depend on j (where the voltage difference $V = \Delta\mu/e$). The total current $I = \sum_{j=1}^{N} I_j$. , hence conductivity is expressed as

$$G = \frac{2e^2}{h}N, \tag{6}$$

where N depends on the wire width (Fig. 1).

However, defects, impurities and irregularities of the conductor shape can induce scattering, in such event conductivity is given by the Landauer equation:

$$G = \frac{2e^2}{h}\sum_{i,j=1}^{N} t_{ij}, \tag{7}$$

where t_{ij} denotes the probability of transition from state j^{th} to i^{th}. Thus Eq. (7) is reduced to Eq. (6) in the absence of scattering $t_{ij} = \delta_{ij}$.

The measurements of electrical resistance (or conductance) of a sample of the size about Λ mesoscopic range) show that the Landauer theory better describes electrical conductance in samples than the Drude model.

3. TECHNOLOGY OF SEMICONDUCTOR DEVICES

All silicons and gallium arsenides are used first of all as the material for manufacturing fast digital integrated circuits (IC). The greatest compaction of electronic elements in IC is obtained in monolithic VLSI circuits using the CMOS technology. The degree of miniaturization of components in the integrated circuit is determined by a linear dimension (given in micrometers or nanometers). This dimension means the channel length in the MOS transistor. In 2008 the best parameters of commercial ICs are the following: the processor clock frequency is 4, 7 GHz (IBM microprocessor) and the number of transistors in one chip is 2×10^9 (4-core Tukwila microprocessor, Intel). The clock frequency (on chip) and the number of transistors in one chip have their physical limits. There are two essential limitations one physical and one technological, on any further miniaturization of integrated circuits and on enlarging the speed of signal processing. The physical limitations include: the speed c of the electromagnetic wave in a vacuum (e.g. the speed of light) and the quantum effects in electron transport in conductors and semiconductors.

The forecasts of the semiconductor industry development foresee that the size of electronic components in integrated circuits will be smaller than 10 nm within several years, it will even be 4 nm in 2022 – see Report of the International Technology Roadmap for Semiconductors, 2007 Edition (www.itrs.net). For this and many other reasons, it is necessary to study the electric and thermal proprieties of nanostructures. Electric and thermal proprieties of electronic components of nanometer sizes are not better described by the classical theory of conductance and by the Boltzmann transport equation than by quantum theories. The classical theories of electrical and thermal conductance assume a huge number of atoms and free electrons. However, the number of atoms and free electrons in a nanostructure is not sufficient for statistical processing of their behaviour.

Let us assume a silicon cube with one side dimension of a and with a common doping of 10^{16} cm^{-3}. There are 5×10^7 atoms and 50 free electrons in the a n-doped silicon cube 100 nm^3 in size, however, there are 5×10^4 atoms and a chance of only 5% to find **one** free electron in the Si cube 10 nm^3 in size.

4. MEASUREMENTS OF ELECTRICAL CONDUCTANCE

The experimental setup consisted of a pair of metallic wires (forming a nanowire), a digital oscilloscope, a motion control system (not shown on the picture) and a PC (see Fig. 2). The instruments were connected into one system using an IEEE-488 interface. Resistor R_p = 1 kΩ was in series to the connected wires. The circuit was fed by constant voltage V_s and measurements of current $I(t)$ were taken. The conductance was determined by current I according to:

$$G = I\frac{1}{V_s - IR_p}. \tag{8}$$

The transient effects of making or breaking the contact gave the time dependent current. Voltage V_p on resistor R_p was measured with a computer controlled oscilloscope. A piezoelectric device was used to control the backward and forward movement of the macroscopic wires between which nanowires occur (QPC – quantum point contact). A high voltage amplifier controlled by a digital function generator supplied the piezoelectric device. Both the QPC electrodes (see Fig. 2) were made of wire 0.5 mm in diameter or of small pieces of metal. The conductance was measured between two metallic electrodes, moved to contact by the piezoelectric tube actuator. The oscilloscope was triggered by a single pulse. All experiments were performed at room temperature and at ambient pressure.

In order to compare our results with those published before by other groups, the first experiment was performed for gold wires. Even if quantization of conductivity by $G_0 = 2e^2/h$ did not depend on the metal and on the temperature, the purpose of studying the quantization for different metals was to ob-

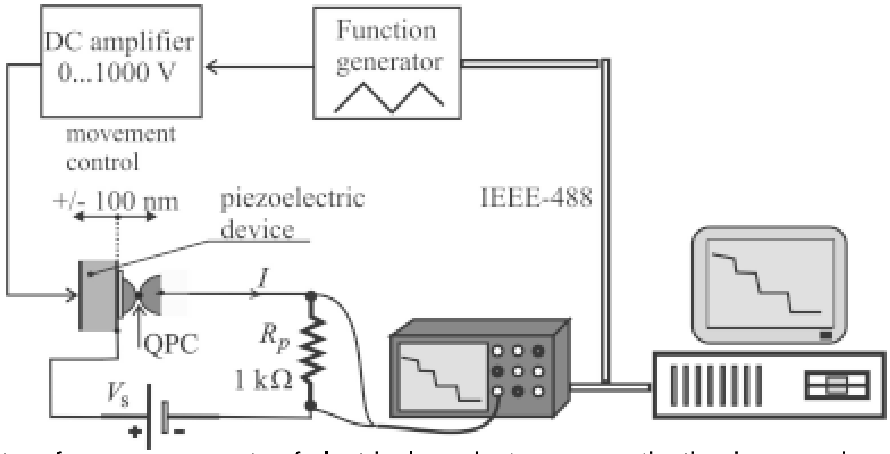

Fig. 2. A system for measurements of electrical conductance quantization in nanowires (QPC) formed between two macroscopic wires.

serve how the metal properties affected the contact between wires. Therefore, we investigated the conductance quantization in nanowires for three nonmagnetic metals (gold, copper and tungsten) and for magnetic metals (cobalt and nickel). We measured the quantization of electrical conductance for nanowires formed between a semiconductor plate (Ge) and a metallic tip (Co), as well.

The quantization of electric conductance depended neither on the metal type nor on the temperature. The conductance quantization for nonmagnetic metals in units of $G_0 = 2e^2/h = 7.75\times10^{-5}$ [A/V] $= (12.9\ \text{k}\Omega)^{-1}$ had been previously observed for the following nanowires: Au-Au, Cu-Cu, Au-Cu, W-W, W-Au, W-Cu. The quantization of conductance in our experiment was evident. All characteristics showed the same steps equal to $2e^2/h$. We observed two phenomena: quantization occurred when breaking the contact between two wires, and quantization occurred when establishing contact between the wires. The characteristics are only partially reproducible; they differ in terms of the number and height of steps, and the time length. The steps can correspond to 1, 2, 3 or 4 quanta. It should be emphasised that the quantum effects were observed only for some of the characteristics recorded. The conductance quantization has been so far more pronouncedly observable for gold contacts (see Fig. 3a).

Then, we measured the electrical conductance quantization in nanocontacts formed mechanically between a cobalt tip and a germanium sample (plate) using the "making contact – breaking contact" method. We have measured 1700 nanowires, consecutively formed between Co and Ge [10]. The data processing has shown that the clear quantization steps occur at $2.1G_0$, which may indicate that either the corresponding apex is not of one-atomic shape, or the atomic structure of the apex is such that it permits contribution from both s and d electrons. It may be expected that s electrons would contribute to the plateaus at nG_0 with a roughly integer n, whereas the d electrons may give contributions differing from those corresponding to a perfect transmission, as the d electrons of Co atoms must couple to Ge atoms which have a different electronic structure. In turn, the higher conductance plateaus, $G = 2.8G_0$ and $G = 3.5G_0$, may indicate the role of d electrons and the presence of spin polarized conductance channels. After 1442 cycles of "making contact – breaking contact" operations an inner atomic structure of the Co-Ge contact altered. We suppose that a material (both Co and Ge) in a junction region degenerated because of many mechanical and thermal processes. Thermal processes are induced by electrical current during measurements. The main conductance plateau is shifted from $2G_0$ $1.5G_0$. Traces of conductance before and after the degeneration can be seen- Fig. 3b.

5. THERMAL PROBLEMS IN NANOWIRES

Electron transport in nanostructures is described by electrical G_E and thermal G_T conductance. Therefore, there are several analogues between the two physical quantities. In addition to the observations of electrical conductance quantization in nanowires,

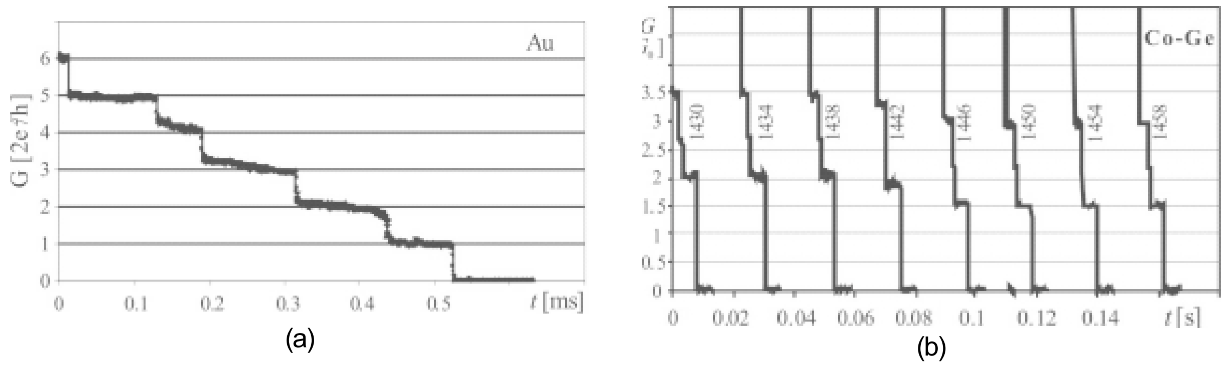

Fig. 3. Quantization of electrical conductance in nanowires in air at room temperature: (a) in a nanowire formed by contact between a gold macrowires; (b) in nanowires formed between Co tip and Ge plate. (Measurements made by M. Wawrzyniak).

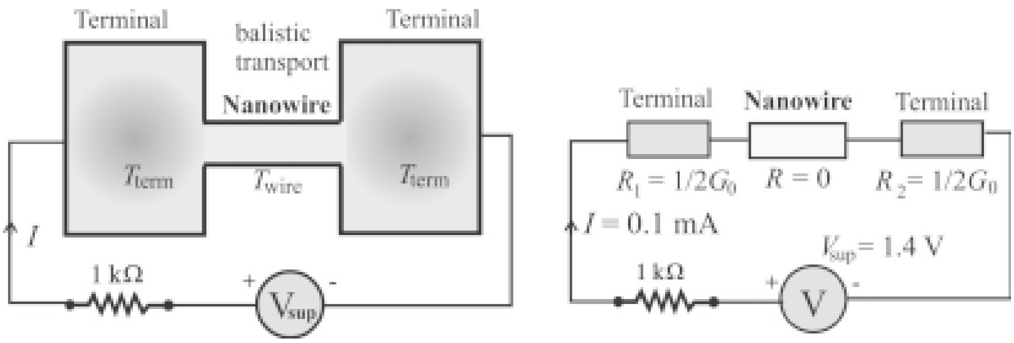

Fig. 4. Conductance distribution in a nanowire with ballistic transport.

thermal conductance quantization can be expected, as well. Electron transport in a nanowire causes two effects: electrical current $I = G_E \times \Delta V$ and heat flux density $Q_D = G_T \times \Delta T$, where G_E – the electrical conductance of a sample, ΔV – the difference of electrical potentials, G_T – the thermal conductance of a sample, ΔT – the temperature difference.

$$G_E = \sigma \times A / l, \ G_T = \lambda \times A / l, \qquad (9)$$

where σ – the electrical conductivity, λ – the thermal conductivity, l – the length of a sample (e.g. nanowire), A – the cross-section area of a sample.

However, an analysis of thermal conductance is more complex than an analysis of electrical conductance because of the contribution of either phonons or electrons in the heat exchange. Quantized thermal conductance in one-dimensional systems has been predicted theoretically by Greiner [11] for the ballistic transport of electrons and by Rego [12] for the ballistic transport of phonons. The thermal conductance is considered in a similar way as the electrical conductance. Conductive channels are formed in one-dimensional systems. Each channel contributes to the total thermal conductance with the quantum of thermal conductance G_{T0}.

Quantized thermal conductance (caused by ballistic transport of phonons) and its quantum (unit) G_{T0} has been confirmed experimentally by Schwab [8]. The universal quantum G_{T0} of thermal conductance

$$G_{T0}\,[W/K] = \left(\pi^2 k_B^2 / 3h\right) T = 9.5 \times 10^{-13} T \qquad (10)$$

depends on the temperature. At T = 300K the value of $G_{T0} = 2.8\times10^{-10}$ [W/K]. This value is determined for ideal ballistic transport (without scattering) in a nanowire, with the transmission coefficient t_{ij} = 100%. It means that the thermal conductance is below the limit given by formula (10) in all practical cases (t_{ij} < 100%).

A single nanowire (metallic or semiconductor) should be considered together with its terminals (Fig. 4). They are called reservoirs of electrons. The electron transport in the nanowire is ballistic, it means transport without any scattering of electrons and without energy dissipation. The energy dissipation occurs partly in terminals. Due to the energy dissipation the local temperature T_{term} in terminals is higher than the temperature T_{wire} of nanowires (Fig. 4). The temperature distribution in terminals of a nanostructure should be analyzed.

Dissipated energy is quite large in small structures. $G_E = G_{E0} = 7.75\times10^{-5}$ [A/V] for the first step of conductance quantization, and the current in the circuit I = 100 μA at the supply voltage V_s = 1,4 V (I = 190 μA for the second step of quantization). The power dissipation in nanowire terminals is $P = I^2/G_{E0}$ = 130 μW for the first step and P = 230 μW for the second step. It should be noticed that the electric current density in nanowires is extremely high. The gold nanowire diameter on the first step of quantization can be estimated as D = 0.4 nm, hence the current density $J \approx 8\times10^{10}$ [A/cm^2] for I = 100 μA.

6. CONCLUSIONS

The influence of quantum occurrences must be taken into account for objects of about a nanometer size. The miniaturization of devices and paths in integrated circuits and transducers has its limits. The electric and thermal parameters of electronic devices of the 10 nm technology would change dramatically. It is the quantization of the electrical and thermal conductance that becomes particularly essential for nanostructures. In our measurements the quantization of electrical conductance has proved to be observable in a simple experimental setup. The energy dissipation in nanowires takes part in their terminals. The local temperature in terminals is higher than the nanowire temperature due to the energy dissipation.

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