Electrical and thermal conductance quantization in nanostructures

Waldemar Nawrocki
Poznan University of Technology, Faculty of Electronics and Telecommunications, ul. Piotrowo 3A, PL 60965 Poznan, Poland
E-mail: nawrocki@et.put.poznan.pl

Abstract. In the paper problems of electron transport in mesoscopic structures and nanostructures are considered. The electrical conductance of nanowires was measured in a simple experimental system. Investigations have been performed in air at room temperature measuring the conductance between two vibrating metal wires with standard oscilloscope. Conductance quantization in units of $G_0 = \frac{2e^2}{h} = \frac{12.9}{k\Omega}$ 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 induced, due to theory proposed by Landauer, the quantization of conductance. Thermal problems in nanowires are also discussed in the paper.

1. Introduction
In last 20 years considerable attention has been focused on the quantization of both electrical and thermal conductance in nanostructures. It is to underline that the electrical and the thermal conductance of a nanostructure describe the same process: the electron transport in the nanostructure. Therefore there are several analogues between the two physical quantities. The theoretical quantum unit of electrical conductance $G_0 = \frac{2e^2}{h}$ was predicted by Landauer [1] in his new theory of electrical conductance. In 1987 Gimzewski and Moller [2] published 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 the conductance quantization in controllable two-dimensional electron gas (2DEG) in the GaAs constriction at the temperatures less than several kelvin. Formation of nanowires in the process of breaking contact between ordinary metallic wires was published by Costa-Kramer [5] in 1995.

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

2. Ballistic electron transport
Transport of electrons can be described classically by the Boltzmann transport equation (Drude model) which introduces mean free path $\Lambda$. At relatively low temperatures the considerable contribution to conductivity is given by electrons with energy close to Fermi surface. Hence, conductivity is given by:
\[ \sigma = \frac{n e^2 \tau}{m^*} \]  

(1)

where \( n \) is the concentration of the carriers, \( m^* \) – the effective mass of the electron, \( \tau \) – relaxation time.

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

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

![Figure 1](image_url)

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

Assuming that the wide contacts are infinitely large, the electrons moves are in the thermodynamic equilibrium described by Fermi-Dirac statistic. When the electrons enter 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 [2]. According to the Büttiker [9] model the hamiltonian of the perfect conductor can be expressed as follows:

\[ H = \frac{1}{2m^*} \left( \hbar^2 k_y^2 + \hbar k_y^2 \right) + V(x) \]  

(2)

where \( y \) is a dimension along the wire, \( x \) is in the transverse direction, \( m^* \) is the effective mass, \( V(x) \) denotes the potential well of the width \( W \), \( k_y \) is a wave vector along \( y \) and \( k_x \) is a wave vector along \( x \).

Because of the narrowness of the potential wall \( V(x) \) the energy for the transverse propagation is quantized:

\[ E_{jy} = \frac{\hbar^2 k_y^2}{2m^*} = \frac{\hbar^2}{2m^*} \left( \frac{j\pi}{W} \right)^2 \]  

(3)

For the Fermi level \( E_F = E_j \) there is a number \( N \sim 2W/\lambda_F \) of states \( E_{jy} \) below Fermi surface. Let us assume that thermal energy \( k_B T \) is much smaller then the energy gap between levels, and that the wide contacts are characterized by chemical potentials \( \mu_1 \) and \( \mu_2 \) with \( (\mu_1 > \mu_2) \).

Then current of electrons in \( j^{th} \) state equals to:
\[ I_j = e v_j \left( \frac{dn}{dE} \right)_j \Delta \mu, \]  

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

\[
\frac{dn}{dk} = \frac{1}{2\pi} \quad \text{and} \quad \left( \frac{dn}{dE} \right)_j = \left( \frac{dn}{dk} \frac{dk}{dE} \right)_j = \frac{2}{\hbar v_j} \tag{5}
\]

The factor of 2 results from spin degeneracy. Hence, the current for \( j^{th} \) state \( I_j = \frac{2e^2}{h} V \) does not depend on \( j \) (where the voltage difference \( V = \Delta \mu/e \)). 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 width of the wire (Fig. 1).

However, defects, impurities and irregularities of the shape of the conductor can induce scattering, then 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 probability of the transition from \( j^{th} \) to \( i^{th} \) state. In the absence of scattering \( t_{ij} = \delta_{ij} \) thus Eq. (7) is reduced to Eq. (6).

Figure 2 presents a resistance of a gold cube sample versus the dimension \( W \) (\( W \) is a cube side). Resistance has been calculated according to the Drude theory (\( W \) from 14 nm to 10 \( \mu \)m) and to the Landauer theory (\( W \) from 0.56 nm to 14 nm). For the size of the cube \( W \) equal to \( A_{\text{Au}} \) (\( A_{\text{Au}} \) is the mean free path for gold at 295 K, \( A_{\text{Au}} = 14 \) nm) one can compare results from this two theories: \( R_D = 1.6 \Omega \) (Drude theory) and \( R_L = 240 \Omega \) (Landauer theory).

![Figure 2](image-url)  

**Figure 2.** Resistance of a gold cube with a side \( W \): from the Drude theory (right line, up 10 \( \mu \)m) and the Landauer theory (link curve, from 0.56 nm to 14 nm). \( W = 14 \) nm = \( A_{\text{Au}} \) is a length of the mean free path for gold at 295 K.

Measurements of electrical resistance (or conductance) of a sample of the size about \( A \) (mesoscopic range) show that the Landauer theory better describes real parameters of the sample.
3. Technology of semiconductor devices

For manufacturing of fast digital integrated circuits (IC) are used semiconductor materials, mostly the silicon and the gallium arsenide. The greatest compaction of elements one obtains in monolithic VLSI circuits in the CMOS technology. The degree of the miniaturization of components in the integrated circuit is determined by a lineal dimension (given in micrometers or nanometers). This dimension means the length of the channel in the MOS transistor. In 2008 best parameters of commercial ICs are: the clock frequency of the processor 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 exist two essential limitations physical and one technological in the further miniaturization of integrated circuits and in enlarging of the speed of signal processing. Physical limitations are: the speed c of the electromagnetic wave in the vacuum (e.g. speed of the light) and quantum effects in the electron transport in conductors and semiconductors.

Prognoses of the development of the semiconductor industry (ITRS) foresee that sizes of electronic components in integrated circuits will be smaller than 10 nm in the course several years, in the year 2022 will even amount 4 nm (table 1). From this reason and many others it is necessary to study of electric and thermal proprieties of nanostructures. Electric and thermal proprieties of electronic components about nanometer sizes are not more described by the classical theory of conductance and by the Boltzmann transport equation, but by quantum theories. Classical theories of electrical and thermal conductance assume a huge number of atoms and free electrons. However number of atoms and free electrons in a nanostructure is not sufficient for a statistical processing of their behaviour.

| Table 1. Data of integrated circuits (IC) according to the Report of The International Technology Roadmap for Semiconductors (Edition 2007) |
|--------------------------------------------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| Year                | 2007         | 2010         | 2013         | 2016         | 2022         |
| Clock frequency (on chip, MPU) (GHz) | 4.7         | 5.9         | 7.3         | 9.2         | 14.3         |
| Functionality of IC (number of transistors) (mln) | 1106       | 2212        | 4424        | 8848        | 35391        |
| Supply voltage (V) | 1.1         | 1.0         | 0.9         | 0.8         | 0.65         |
| Dissipated power (cooling on) (W) | 189        | 198         | 198         | 198         | 198          |
| Gate length in CMOS transistors in an integrated circuit (MPU) (nm) | 25          | 18          | 13          | 9           | 4            |

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

4. Measurements of electrical conductance

The experimental setup consisted of a pair of metallic wires (they formed a nanowire), a digital oscilloscope, a motion control system (doesn’t show on the picture) and a PC (Fig. 3). Instruments are connected in one system using the IEEE-488 interface. There was the resistor \( R_p = 1 \text{ k}\Omega \) in series to the connected wires. The circuit was fed by the constant voltage \( V_t \) and measurements of current \( I(t) \) have been performed. Conductance was determined by current \( I \) accordingly to:

\[
G = I \frac{1}{V_t - IR_p}
\]

(8)

Transient effects of making contact or breaking the contact give time dependent current. The voltage \( V_t \) on the resistor \( R_p \) was measured with computer controlled oscilloscope. The piezoelectric device is used to control the backward and forward movement of the macroscopic wires between which nanowires occur. A high voltage amplifier controlled by a digital function generator supplies the piezoelectric device. Both electrodes (macroscopic wires) are made of wire 0.5 mm in diameter.
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.

Figure 3. A system for measurements of conductance quantization in nanowires formed between two macroscopic wires (e.g. Au and Cu wires).

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 \( G_0 = \frac{2e^2}{h} \) does not depend on the metal and on temperature, the purpose of studying quantization for different metals was to see how properties of the metal affect the contacts between wires. Therefore, we have investigated the conductance quantization of nanowires for three nonmagnetic metals (gold, copper and tungsten) and for magnetic metals (cobalt and nickel).

The quantization of electric conductance depends neither on the kind of metal nor on temperature. However, the purpose of studying the quantization for different metals was to observe how the metal properties affect the contacts between wires. For nonmagnetic metals, the conductance quantization in units of \( G_0 = \frac{2e^2}{h} = 7.75 \times 10^{-5} \) [A/V] = (12.9 kΩ)\(^{-1}\) was 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 the contact between the wires. The characteristics are only partially reproducible; they differ in number and height of steps, and in the time length. The steps can correspond to 1, 2, 3 or 4 quanta. It should be emphasised that quantum effects were observed only for some of the characteristics recorded. The conductance quantization has been so far more pronouncedly observable for gold contacts. Figure 4 and 5a shows example plots of conductance vs. time during the process of drawing Au- and Cu-nanowire, respectively, for the bias voltage \( V_s = 0.42 \) V [10].

Figure 4. Conductance quantization in metallic nanowires: golden nanowires (left) and copper nanowires (right). The characteristics presented are chosen from 20000 consecutive measurements for both metals.
Figure 5b show the conductance histogram obtained from 6000 consecutive characteristics in the conductance range from 0.5$G_0$ to 4 $G_0$.

**Figure 5.** Conductance quantization in gold nanowires: a time plot (left) and a histogram from 6000 consecutive formations of a nanowire.

### 4. Thermal problems in nanowires

Both electrical $G_E$ and thermal $G_T$ conductance of a nanostructure describe the same process: electron transport in nanostructures. Therefore there are several analogues between the two physical quantities. Beside observations of electrical conductance quantization in nanowires one can expect the thermal conductance quantization as well. Electron transport in a nanowire does two effects: an electrical current $I = G_E \times \Delta V$ and a heat flux density $Q_D = G_T \times \Delta T$, where $G_E$ – electrical conductance of a sample, $\Delta V$ – difference of electrical potentials, $G_T$ – thermal conductance of a sample, $\Delta T$ – temperature difference.

$$G_E = \sigma \times A/l, \quad G_T = \lambda \times A/l$$  

(9)

where $\sigma$ – electrical conductivity, $\lambda$ – thermal conductivity, $l$ – length of a sample (e.g. nanowire), $A$ – area of a cross-section of a sample.

Quantized thermal conductance in one-dimensional systems (e.g. nanowires) was predicted theoretically by Rego [11] using the Landauer theory. The thermal conductance is considered in a similar way like the electrical conductance. In one-dimension systems are formed conductive channels. Each channel contributes to a total thermal conductance with the quantum of thermal conductance $G_{T0}$.

Quantized thermal conductance and its quantum (unit) $G_{T0}$ was confirmed experimentally by Schwab [7]. The quantum $G_{T0}$ of thermal conductance

$$G_{T0} [W/K] = \left(\frac{\pi k_B^2}{3h}\right) T = 9.5 \times 10^{-11} T$$  

(10)

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

A single nanowire should be considered together with its terminals. They are called reservoirs of electrons. Electron transport in the nanowire itself is ballistic, it means the transport without scattering of electrons and without energy dissipation. The energy dissipation takes part in terminals. Because of the energy dissipation the local temperature $T_{\text{term}}$ in terminals is higher then the temperature $T_{\text{wire}}$ of nanowires itself Fig. (6). A heat distribution in terminals of a nanostructre should be analyzed.

In small structures a dissipated energy is quite large. For the first step of conductance quantization, $G_E = G_{ EO} = 7.75 \times 10^{-5}$ [A/V], and at the supply voltage $V_s = 1.4$ V the current in the circuit $I = 100\ \mu$A ($I = 190\ \mu$A for the second step of quantization). The power dissipation in terminals of nanowires is $P = \dot{I}/G_{E0} = 130\ \mu$W for the first step and $P = 230\ \mu$W for the second step. One ought to notice that the
density of electric current in nanowires is extremely high. The diameter of the gold nanowire on the first step of quantization can be estimated to \( D = 0.4 \) nm, so for \( I = 100 \, \mu \text{A} \) the current density \( J \approx 8 \times 10^{10} \, \text{[A/cm}^2\text{]} \).

5. Conclusions
Conductance quantization has proved to be observable in a simple experimental setup, giving opportunity to investigate subtle quantum effects in electrical conductivity. The energy dissipation in nanowires takes part in their terminals. Because of the energy dissipation the local temperature in terminals is higher then the temperature of a nanowire itself.

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