Conductance quantization in nanowires formed at the metal-semiconductor interface

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Abstract. We demonstrate that step-like conductance traces resulting from quantum effects such as the conductance quantization or formation of single-atom contacts are possible in the nanowires formed at the metal-semiconductor junction. In the macroscopic metal-semiconductor interfaces the Schottky barrier is usually risen. For the nanowires formed at the contact between the germanium surface and cobalt or gold tip, the conductance traces are characterized by a high reproducibility and long duration of the conductance plateaus. The current-voltage characteristics of these contacts are strongly nonlinear similarly to a junction with the Schottky barrier.

1. Introduction
In metallic nanowires, due to the formation of a quantum point contact (QPC), the conductance exhibits quantum effects. In future electronic circuits of nanometer dimensions it would be necessary to take these effects into account but it would be also possible to construct new devices with some unique functionality. A QPC occurs when the nanowire width at its neck is comparable to the Fermi wavelength $\lambda_F$. The value of Fermi wavelength in metals, $\lambda_F \sim 0.5 \text{ nm}$, is usually comparable to the diameter of a single atom. If, moreover, all the nanowire dimensions are below the electron mean free path $l_e$, the nanowire conductance can be calculated from the Landauer formula $G = G_0 \sum_{n=1}^{N} T_n$, where $G_0 = 2e^2/h$ is the conductance quantum and $T_n$ denotes the transmission coefficient for the channel $n$. In this range of the QPC the electrical conductance results from $N$ independent electron wave modes, referred to as conductance channels, contributing to the electron transport. When $T_n = 1$ in each conductance channel, the conductance of a nanowire with QPC is $G = NG_0$, where $N$ denotes the total number of open conductance channels. Typically fabricated by means of a scanning tunneling microscope (STM) [1, 2] and a mechanically controllable break junction (MCBJ) [3, 4], nanowires with a QPC have also been produced in relays [5] and between macroscopic wires [6]. In each case, the QPC is achieved by drawing a previously formed nanowire. Obtained while the nanowire is being drawn, conductance versus time plots (conductance traces), reveal steps, which result from the closing of consecutive conductance channels as the nanowire narrows down: quantized electronic levels pass through the Fermi level. As the process of nanowire drawing is by its
nature not fully reproducible, conductance histograms are constructed from a large number of conductance traces. In the case of gold [5, 6] and aluminium [7], histogram peaks tend to occur around values at integer values of $G_0$. Histograms built for copper and silver reveal one distinct peak slightly below $1G_0$. Moreover two extra peaks occur with a position and height depending on the measurement conditions. The method of mechanical fabrication of nanowires has also been used for conductance measurements of nanoscale metal-semiconductor contacts [8, 9] and semiconductor contacts [10].

Metal-semiconductor contacts are of such great importance since they are present in every semiconductor device. They can behave either as a Schottky barrier or as an ohmic contact depending on the characteristic of the interface, especially on the doping level in semiconductor region between the contact metal and the semiconductor. In this paper we report that conductance steps resulting from quantum effects can occur in nanowires formed at metal-semiconductor junction. The electronic properties of an interface result from the band structures of the materials in contact. Metal-semiconductor junctions are characterized by the Schottky barrier height [11], which is the energy distance between the Fermi level $E_F$ and the majority-carrier band edge. In an ideal junction of a metal and a p-type semiconductor the height of this barrier is $E_F - E_V = \Phi_{bp} - S_X(X_m - X_s)$, where $E_V$ is the valence band maximum at the interface, $\Phi_{bp}$ is the p-type branch point energy, $X_m$ is the electronegativity of the metal, $X_s$ is the electronegativity of the semiconductor, and $S_X$ is the slope parameter. Holes in the p-type semiconductors can lower their energy by traversing the junction. As the holes leave the semiconductor, a negative charge, due to the ionized acceptor atoms, remains behind. This charge creates a positive field and lowers the band edges of the semiconductor. Holes flow into metal until equilibrium characterized by a constant Fermi energy throughout the structure is reached. For the forward bias, the Fermi energy of the metal is lowered with respect to the Fermi energy in the semiconductor. This results in a smaller potential drop across the semiconductor that allows the large current. For the reverse bias, the Fermi energy of the metal is raised with respect to the Fermi energy in the semiconductor. The potential across the semiconductor now increases, yielding a larger depletion region and a larger electric field at the interface. The barrier that restricts the holes to the metal, is hardly changed so that the flow of holes is limited by that barrier irrespective of the applied voltage. It is considered that there are three dominant transport processes determining the current-voltage ($I$-$V$) characteristics due to diffusion, thermionic emission, and tunneling. It is interesting that it is possible to form a QPC at such an interface. Since the transport in QPCs is predominantly ballistic it is not obvious which physical mechanism leads to a strong nonlinear $I$-$V$ characteristic in that case.

2. Experimental setup
In order to investigate the transport properties of the metal-semiconductor interface we developed an experimental setup that allows to carry out the measurement of the $I$-$V$ characteristic in a very short time window, which ensures that a registration of a such a characteristic during a particular conductance plateau is stable. Figure 1 shows a block diagram of an experimental setup for conductance and $I$-$V$ measurements that was prepared on the basis of an earlier idea proposed by Hansen et al. [12]. Nanowires were formed between two electrodes labeled A (germanium) and B (metal). Our experiment was performed with the p-type polycrystalline germanium sample with resistivity of about 0.5 $\Omega$ cm at room temperature and tips made of gold (of purity 99.999%) and cobalt (of purity 99.997%). The electronegativity values of Ge, Au and Co were 2.01, 2.54 and 1.88, respectively, in the Pauling scale [11]. The germanium sample was cleaned by grinding the germanium surface. Next, surface regions with suitable cleanliness were searched for. The whole mechanical setup was placed on an antivibration table. In the diagram shown in Fig. 1 the tip-shaped electrode B is fixed to the head of a piezoelectric actuator (PI P250.20 HVPZT). The motion of the actuator head is controlled by
Figure 1. Block diagram of the experimental setup that allows for the registration of the current-voltage characteristic at a particular conductance plateau.

an Agilent 33220A function generator (labeled 1) and the generated voltage signal is amplified by a high-voltage amplifier (PI E-461). The function generator 1 is controlled from a PC through a GPIB interface, which allows the proper setup of the range and speed of the motion of electrode B. Measurements are initiated by triggering generator 1. The generated control signal is applied to the piezoelectric actuator, bringing electrodes A and B to collision and then retracting electrode B from electrode A. The nanowires produced during this retraction are drawn to break in turns, until a single one remains, forming a QPC just before breaking. Applied to the nanowire produced in this way, voltage $V_{DC} = 0.432$ V from the DC power supply unit (Agilent E3631) results in the generation of current $i_Q$. The current signal is converted by the I/V converter into a voltage signal $v_1$, entering through channel 1 the digital storage oscilloscope (DSO) where it is measured. The signal $v_1$ reading transferred through the GPIB interface to the PC is stored in a file. Conductance traces are calculated from data acquired for signal $v_1$. Conductance histograms were built from a large number of the conductance traces with correction of the analog-to-digital converter differential nonlinearity error [5, 13]. The measurement of the $I$-$V$ curves requires the employment of function generator 2. Before measurements, the $I$-$V$ curves of the oscilloscope trigger level must be set up at the value corresponding to the conductance level $kG_0$ ($k = 1, 2, ...$), at which the current-voltage curve is to be determined. Upon triggering the oscilloscope, it generates the external TTL TrigOut signal which is used to trigger the function generator 2 (not used in the conductance trace measurements). Added to $V_{DC}$, function generator 2 output signal, $v_{FG}$, alters the current $i_Q$ in the nanowire throughout the $I$-$V$ measurement range. Signal $v_2(t)$, or the sum of the DC supply signal $V_{DC}$ and the function generator signal $v_{FG}(t)$, enters the oscilloscope through channel 2. Channel 1 is reserved for the incoming I/V converter output signal $v_1(t)$. Transferred through the GPIB interface to the PC, the signals $v_1(t)$ and $v_2(t)$ reading are stored in a file. Using Ohm’s and Kirchhoff’s laws, the voltage drop $V$ across the QPC and current $I$ flow through the QPC are calculated from the data obtained for signals $v_1$ and $v_2$ [14]. The current-voltage curve of the nanowire with QPC is traced by plotting the values $(V, I)$ at the moment of the oscilloscope sampling in the $xy$ coordinate system.

3. Results and discussion
Conductance traces obtained from the measurements in nanowires formed between a gold tip and a gold surface are presented in Fig. 2(a), while those formed between a gold tip and a germanium surface in Fig. 2(b). In both cases the tip was brought towards the surface and
Figure 2. Conductance traces of nanowires formed between a gold tip and a gold surface (a) and between a gold tip and a germanium surface (b). Measurements were performed under ambient conditions, with the tip brought towards the surface and then retracted at 3 speeds 160 µm/s, 16 µm/s and 1.6 µm/s in both cases.

then retracted at 3 speeds 160 µm/s, 16 µm/s and 1.6 µm/s; its range of movement in the z direction was 16 µm. By comparing the conductance traces (a) and (b) in Figure 1 the duration of conductance plateaus in nanowires formed in the gold-germanium system is found to be approximately two orders of magnitude longer than in nanowires formed in the gold-gold system, despite the same value of retraction speed. For nanowires formed in the cobalt-germanium system the duration of conductance plateaus is found to be approximately from two to three orders of magnitude longer. This leads to an important practical conclusion as to the obtainment of conductance traces of nanowires formed between a metal tip and a Ge surface: in this case the time window should be longer than that used for a metal-metal system. The observed effect is a result of a complex interplay of unique mechanical and electronic properties of the metal-semiconductors interface. The Fermi energy in germanium, $E_F(\text{Ge}) \approx 0.34$ eV, is much smaller than in gold, $E_F(\text{Au}) \approx 5.5$ eV. However, once the Au tip is indented in the Ge surface the Fermi level $E_F(\text{Au−Ge})$ of the metal-semiconductor system shifts to an intermediate value. The corresponding Fermi wavelength values in Au and Ge are $\lambda_F(\text{Au}) \approx 0.52$ nm and $\lambda_F(\text{Ge}) \approx 2.1$ nm, respectively. Moreover, the mean free path $l_e$ will be longer than in metal due to the lower carrier density at the interface. Also mechanical properties of the nanowires formed between the flat clear crystalline germanium surface and amorphous metal define proper conditions for the formation of stable contacts. Further studies are required to elucidate the mechanism of attaining stable atomic arrangements at semiconductor interface. Such series of stable conductances due to electronic and atomic shell effects have been also observed for noble metals [15] and in alkali metals [16].

Figure 3(a) shows conductance traces of nanowires with QPC formed at the interface between a Co tip and a Ge surface (traces 1 to 3500, step 500). Additionally, traces 3000 to 3100, step 20, are shown in the dashed-line rectangle. The tip was brought towards the surface and then retracted at speed 32 µm/s, with z movement range 8 µm. The measurements were performed in ambient conditions, at bias voltage 400 mV. Figure 3(b) shows the conductance histogram built from all the 3500 conductance traces with peak conductance values specified, and, in the inset in the top left corner, the conductance histogram built from conductance traces 3000 to 3100 (encompassed by the dashed-line rectangle in Fig. 3(a)). Three long-duration plateaus of reproducible levels can be found in conductance traces 3000 to 3100, which proves that the process of nanowire forming and drawing was highly reproducible. These three stable conductance plateaus stem from the attainment of stable diameters, which are maintained much
Figure 3. Conductance measured in nanowires with QPC formed at the interface between a Ge surface and a Co tip: (a) conductance traces 1 to 3500, step 500; in the dashed-line rectangle: conductance traces 3000 to 3100, step 20; (b) conductance histogram built from all the conductance traces (1 to 3500); inset: conductance histogram built from conductance traces 3000 to 3100.

longer than other diameters of the nanowire neck. Note also that the range of tip movement in the z direction was 8 µm, which implies breaking of each nanowire formed. The high reproducibility of the conductance traces obtained from short series of measurements leads to very sharp peaks in the conductance histogram (Fig. 3(b), inset). For this reason, conductance histograms built from a large number of conductance traces will be irreproducible in both, shape and peak height. The peak maximums are clearly discernible, though. In the conductance histogram shown in Figure 2b peak maximums fall at conductance values: 3.51G0, 3.36G0, 2.99G0 (poorly visible in the overall histogram, this peak is more discernible in the histogram shown in the inset), 2.82G0, 2.58G0, 2.02G0, 1.66G0, 1.56G0 and 0.82G0.

We present conductance traces for QPCs in Fig. 4(a); they are characterized by the most stable in time atomic configurations, what corresponds to the longest duration of conductance plateaus in nanowires. The velocity of the Co tip retraction was the same as for measurements presented in Fig. 3, (32 µm/s). The average duration of conductance plateaus in the conductance traces is found to be approximately one order of magnitude longer. The measurements are performed for two different biases: forward and reverse bias at the Co-Ge junction. In the first case, the forward bias, the positive voltage VDC = +0.4V is applied to the Ge surface (Fig. 4(a), the conductance traces in the dotted-line rectangle), and in the second, the reverse bias, the positive voltage VDC = +0.4V is applied to the Co tip (Fig. 4(a), the conductance traces in the dashed-line rectangle). In Fig. 4(a), there are conductance traces 1 to 1000, step 250 for each direction of bias. There are depicted two conductance histograms built from all 1000 consecutive conductance traces for both bias directions in Fig. 4(b). One can observe a shift of the conductance plateaus values towards higher conductance after changing the bias from the reverse to forward direction. It is confirmed by the conductance histograms presented in Fig. 4(b), where after the change of bias direction the histogram maxima are shifted towards higher conductance values as well. Fig. 4(c), shows the I-V characteristics measured at the conductance plateaus corresponding to maxima a, b, and c of the conductance histograms from Fig. 4(b). These I-V characteristics have strong nonlinear character, which can indicate the formation of the Schottky barrier in the QPC at the Co-Ge interface.

4. Conclusion
In conclusion, we have set forth a method of nanowire fabrication at the semiconductor interface that occurs between a semiconductor and a metal. Conductance traces of the drawn nanowires
Figure 4. The effect of the forward and reverse bias of nanowires with the QPC formed at Ge-Co interface on the conductance quantization: (a) conductance traces for the forward and reverse bias (1 to 1000, step 250 for each type of bias); (b) conductance histogram built from all the conductance traces (1 to 1000) for both bias directions; (c) current-voltage characteristics recorded at the conductance plateau corresponding maxima a (dashed line), b (solid line), and c (dotted line) of the histogram from Fig. 4(b)

reveal highly reproducible conductance plateaus. This reproducibility is a result of stable diameters attained in the nanowires and leads to very sharp peaks in the histograms built from series of conductance traces. We developed a new experimental setup that allows the current-voltage characteristic measurements at a particular conductance plateau. We demonstrate that the $I$-$V$ characteristics are strongly nonlinear, which suggests a possibility of the Schottky barrier formation at the metal-semiconductor interface inside the QPC.

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