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Effect of surface contact potential in atomic-size contacts

C. Rackson [a], A. Watt [a], W.J. Kim [a,b,*]

[a] *Department of Physics, Seattle University, 901 12th Ave, Seattle, WA 98122, United States*
[b] *Department of Physics, University of Washington, Seattle, WA 98195, United States*

A R T I C L E I N F O

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A B S T R A C T

We present a study of the effect of surface contact potential in a mechanical break junction experiment. Using amplitude-modulated Kelvin probe microscopy (KPM), we show that the surface potential of a real metal is highly non-uniform and is strongly distance-dependent. Based on our KPM results, we propose a model in which a current is induced from the capacitive coupling of the surface potential and accounts for much of the observed shifts of the conductance peaks from integer multiples. The significance of our results in other areas of physics is also discussed.

1. Introduction

The creation of atomic-size contacts via the mechanical break junction (MBJ) technique provides a simple experimental platform in which fundamental properties of nano-scale electron transport can be probed. According to the Landauer formula [1], the electrical conductance is quantized in units of $G_0 = 2e^2/h \sim 1/(12.9\ \text{k}\Omega)$ (with e and h being the magnitude of electric charge and Planck's constant, respectively), as the size of atomic constrictions becomes comparable to the Fermi wavelength of electrons. The physics of quantized conductance has received growing interest since the landmark demonstration of finite electrical conductances in two-dimensional electron gas (2DEG) in 1988 [2]. There, electrons were successfully confined on a lithographically defined quantum dot with precisely controlled dimensions. Later, J.L. Costa-Krämer et al. [3] demonstrated quantized conductance from a pair of bulk metallic wires as a table-top experiment at room temperature. Other experimental works include studies of quantized conductance using scanning tunneling microscopy (STM) [4–6], commercial electromechanical relays [7], and low temperature MBJs [8,9].

In most MBJ experiments, gold is a popular choice for creating atomic contacts because it is considered to be "clean" and is more immune to oxidation and corrosion than other common metals, such as silver and copper. Additionally, the interpretation of the conductance quantization in gold is rather straightforward since it has only one electron in its spherically symmetric valence shell (i.e., monovalent). Recent shot noise measurements on gold contacts suggest that the first peak of a conductance histogram originates from an almost fully-transparent single conductance channel, confirming that the step-like feature in the conductance data is likely to be the direct consequence of conductance quantization, rather than repeated creations of a preferred atomic configuration [10–13].

Common to many of the previous experiments involving atomic-sized point contacts is the apparent shift of conductance peaks in histograms below quantized values nG_0 (where $n = 1, 2, 3, \ldots$). To account for the observed shift, a "residual" resistance R_r is commonly introduced to position the observed conductance peaks at integer values. Although there is no definite theoretical justification for adding this *ad-hoc* resistance in series with an atomic contact, the resistance model serves a useful purpose by quantifying a degree of possible disorder arising from surface defects and imperfections at the banks of atomic-scale contacts leading to electron backscattering [14–19]. Typical values of the added resistance to account for the apparent shift range from 100 Ω to 1500 Ω [6–8,20]. To investigate the effect of disorder experimentally, Bakker et al. [20] demonstrated the shift of the conductance peaks in histograms upon addition of nickel impurities to pure copper. They found that the increase in nickel concentration directly led to the increase in series resistance needed to align the observed peaks at integer values, with the amount of resistance differing among different peaks. In the case of the $n = 3$ conductance peak, the applied "correction" was as large as 1.6 kΩ.

In this report, we suggest a realistic scenario in which electron conductions are modified due to strong capacitive coupling arising from the surface contact potential effect. Unlike a perfect conductor, the surface of a real metal is not equipotential, and its surface potential spatially fluctuates around the so-called contact potential difference (CPD), as routinely measured by Kelvin probe

* Corresponding author at: Department of Physics, Seattle University, 901 12th Ave, Seattle, WA 98122, United States.
E-mail address: kimw@seattleu.edu (W.J. Kim).

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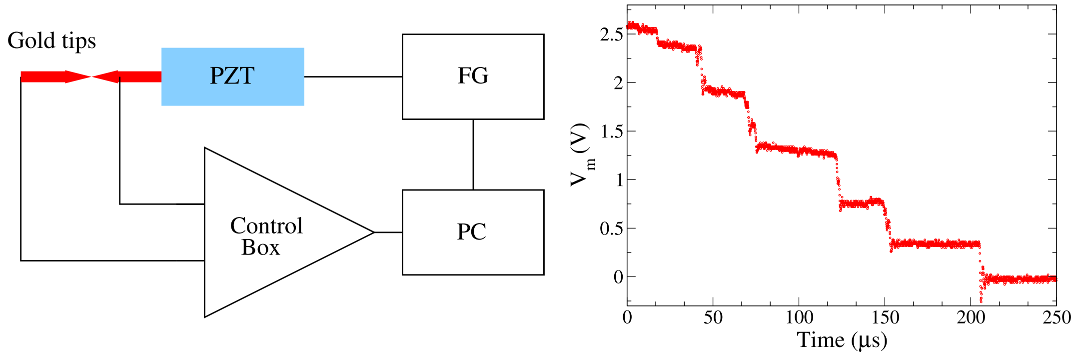

Fig. 1. Schematic of a mechanical break junction experiment (left) and a typical conductance trace (right). The piezoelectric transducer (PZT), driven by a function generator (FG), moves one of the gold tips in and out of contact with the other tip. The conductance is measured by an I–V converter inside the control box. All of the data collections, along with the PZT modulation, are automated in a MATLAB script.

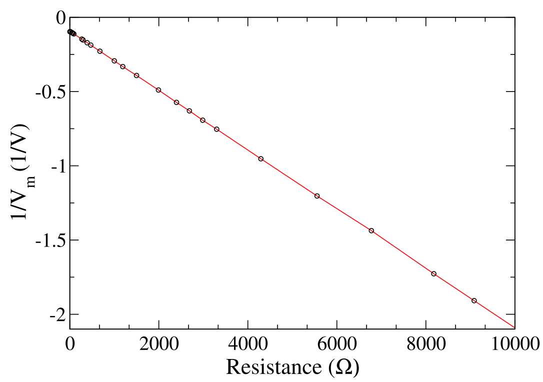

Fig. 2. Calibration of the I–V converter inside our electric control box: A linear fit (red, solid) is applied to calibration data (black, circle) and yields $R_0 = 470.4 \pm 0.5$ Ω and $R_{\text{gain}} = 1002 \pm 2$ Ω, as expected. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

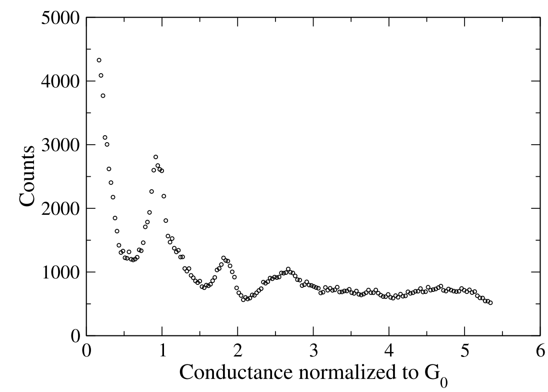

Fig. 3. A histogram of measured conductances representing over 200 traces of conductance steps similarly shown on the right of Fig. 1. Based on Gaussian fits, the first three peaks (widths) are 0.93 ± 0.08, 1.82 ± 0.15, and 2.64 ± 0.20 for $n = 1$, 2, and 3, respectively.

microscopy (KPM) [21]. As a consequence, when two imperfectly-conducting tips are brought into contact, surface charges are no longer free to move so as to keep the electrochemical potential constant on the surface [22,23]. Microscopically, the inherent process of repeated, physical indentations in an MBJ experiment — the making of atomic-sized contacts — causes the crystalline orientation of the surface atoms to change, thereby modifying the local electrical properties upon the formation of each atomic junction. We show that the induced current effected by the surface potential variation could account for the observed shift in the conductance peaks without having to add a large series resistance.

2. Experimental setup and results

Shown in Fig. 1 is a schematic of our mechanical break junction apparatus (left) and a typical conductance trace captured on an oscilloscope (right). Two gold wires are repeatedly brought in and out of contact by a piezoelectric transducer (PZT) connected to a function generator (FG). Typical modulation frequencies of the PZT translation range from 100 mHz to 10 Hz. Inside a home-built electric control box are a bias voltage source V_b, which is tunable from -1 V to $+1$ V in 10-μV-step resolution, and a current-to-voltage (I–V) converter with variable gain settings. Repeated contacts are made at room temperature in ambient pressure, with the entire apparatus sitting on a vibration-isolation table. The resulting conductance data are recorded in MATLAB installed on a PC. Most of our data acquisition took place overnight to minimize the noise associated with nearby human activity during the daytime.

In Fig. 2, we present a calibration result of our I–V converter, which enables us to convert the measured current to the actual conductance in units of G_0. For this, a number of precision resistors with known resistances (better than 1% tolerance) were employed to plot the current, measured in terms of the voltage output of the I–V converter V_{m}, against the known resistance R. The linear relationship between $1/V_{\text{m}}$ and R is evident from the calibration result shown in Fig. 2 and is given by

$$\frac{1}{V_{\text{m}}} = \frac{R + R_0}{V_{\text{b}} R_{\text{gain}}}, \tag{1}$$

where R_{gain} is the gain factor (10^3 Ω), and R_0 is the constant resistance mostly attributed to an internal resistor (470 Ω), which is connected in series with the gold junction. A bias voltage of $V_{\text{b}} = 500$ mV was applied throughout the calibration and during the conductance measurements. The calibration data are fit to Eq. (1), with the slope defined as $a \equiv 1/(V_{\text{b}} R_{\text{gain}})$ and the y-intercept by $b \equiv R_0/(V_{\text{b}} R_{\text{gain}})$. The obtained fit, indicated by the solid line in Fig. 2, gives excellent agreement with our calibration data. All of our subsequent conductance data are then directly obtained from the relation: $G = aV_{\text{m}}/(1 - bV_{\text{m}})$, with $G \equiv 1/R$.

Next, we collected over 200 conductance traces and created a histogram, as shown in Fig. 3. The horizontal axis of the histogram represents the normalized conductance in units of G_0. The first three peaks are well resolved, with the peak positions falling slightly below the integer indices: 0.93, 1.82, and 2.64 for $n = 1$, 2, and 3, respectively. In terms of the residual resistance R_{r} needed to position the peaks at integers, we obtain 903 Ω, 638 Ω, 586 Ω for $n = 1$, 2, and 3, respectively. Our result is consistent with the previous findings in which the experimental shifts were corrected by the extra resistance, with typical values being 400 Ω for a 2DEG [2] and 100 Ω–1500 Ω for STM and MBJ-style experiments [6–8,20]. Note that although our experimental results were