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Relationship between structure and conductance of nanometer-sized iridium contacts

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1. Introduction

Electron transport in nanometer-sized metallic contacts (NCs) has been studied in relation to quantized conductance, which was discovered in two-dimensional electron gases at semiconductor interfaces [1]. A major subject is to elucidate the variation in conductance of NCs as a function of their atomistic arrangement or structural factors, e.g. their cross-sectional area of constriction, opening angle of their connecting electrodes and interatomic distance. For gold (Au) NCs, histograms of conductance measured by mechanically controllable break junction and nanometer-tip manipulation methods showed broad peaks corresponding to integer multiples of a conductance quantum, G_0 ($G_0=2e^2/h$, where e is the charge of electron and h is the Plank constant)[2]. Conductance of an atomic-sized contact (ASC), i.e. a contact of single atom width, has been focused. The conductance of Au ASCs was deduced to be 1 G_0[3]. *In situ* transmission electron microscopy (TEM) with simultaneous measurement of conductance has been used to investigate directly the relationships between their atomistic configuration and conductance of Au NCs and ASCs during retraction procedures. For ASCs of other metallic elements, e.g. cobalt, palladium, platinum and iridium (Ir), the peaks did not appear at integer multiples of G_0 [4]. For structures of these metallic elements, the structures of their ASCs prepared by drilling using intense electron beams were observed by conventional TEM. In this report, we observed the *in situ* TEM of tensile deformation of Ir NCs and demonstrated the relationship between the cross-sectional area of constriction and conductance.

2. Experimental method

The experimental method in this study was developed based on *in situ* high-resolution TEM combined with conductance measurements using a two-terminal method as used in scanning tunneling microscopy [5]. First we prepared nanometer-sized Ir tips: Ir was evaporated and deposited on a Si cantilever with a nanometer-sized tip. The cantilever was attached to the front of a tube piezo on a cantilever holder of the transmission electron microscope. An Ir plate of 0.2 mm thickness was attached to a second sample holder. The cantilever and the plate holders were then inserted into the microscope. The tip of the cantilever was contacted with an edge of the opposing plate by piezo manipulation while applying a bias voltage of 75-200 mV between tip and plate. The tip was pressed into the plate to prepare NCs, and then retracted to elongate them and transform to ASCs. The structural dynamics of the sequence was observed *in situ* by lattice imaging of high-resolution TEM using a TV capture system. The high-resolution imaging and signal detection in this system were coincidentally recorded and analyzed for every image using our own software.

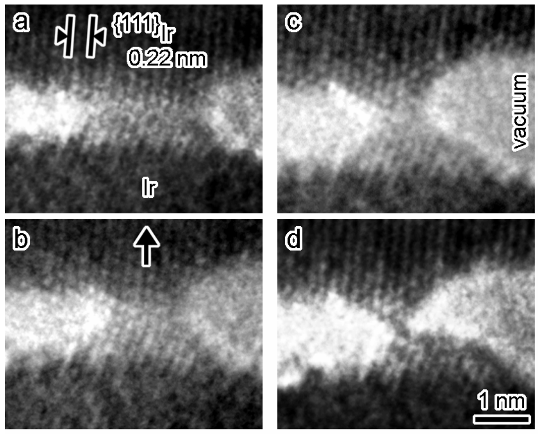

Fig. 1 Time-sequence series of high-resolution images of elongation of an Ir nanometer-sized contact (a - c) and successive growth of a wire of single atom width (d). The movement of the cantilever-tip as imaged with dark contrast (upper portion) is indicated by the bold

3. Results

Figure 1 shows a time sequence series of high-resolution images of the retraction of an Ir NC. The cantilever-tip and the plate are observed as dark contrast in the upper and the lower portions of Fig. 1(a), respectively. A contact between them is observed in the middle. The width is approximately 2 nm (Fig. 1a). As the cantilever-tip was retracted from the plate along direction indicated by an arrow, the width decreases by slip (Fig. 1b-c) on the {111} along the <110>.The width finally reaches to single atom (Fig. 1d). Figure 2 shows the variation in conductance of the NC during the procedure in Fig. 1 as a function of time. The bias voltage applied was 75 mV. The time associated with the triangles a ~ d (hereafter time a, b, c and d) corresponds to the time in which each image in Fig. 1(a) ~ (d) was observed. The conductance and area decrease similarly.

We assumed that the shape of the cross-section of the NC at a minimal constriction was circular, and measured the width from the images to estimate the cross-sectional area. Figures

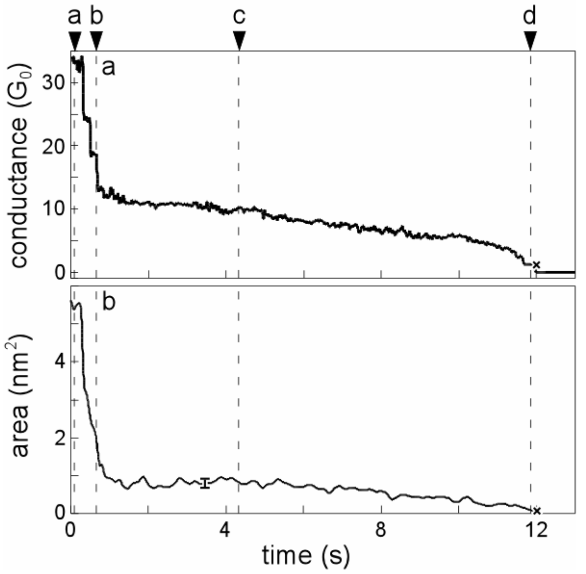

Fig. 2 Variation in conductance (a) and cross-sectional area (b) as a function of time for the procedure in Fig. 1. The time with the triangles a ~ d corresponds to the time at the recording of the images of a ~ d in Fig. 1.

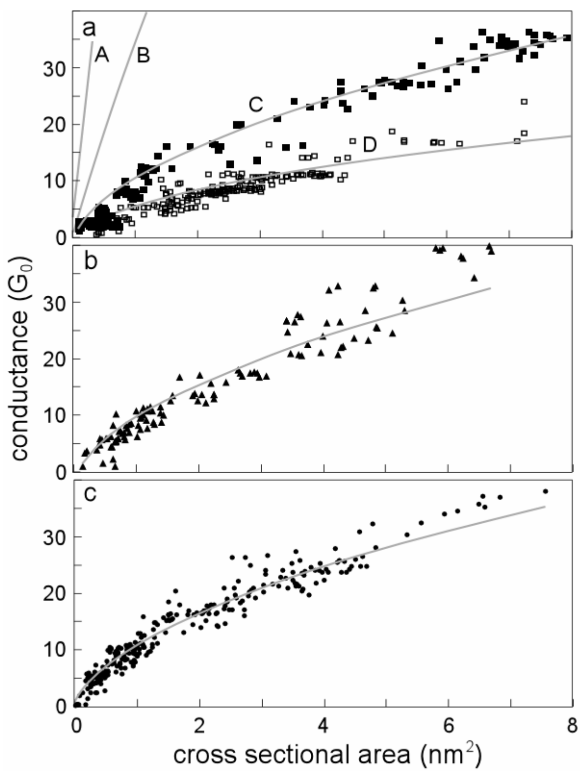

Fig. 3 Relationships between the minimal cross-sectional area of constriction and conductance of Ir NCs for bias voltages of 75 mV (a) filled squares, 200 mV (b) filled triangles and 300 mV (c) filled circle. Open squares represent conductance of Au NCs. Fitting curves (solid line) calculated based on the formulas according to Torres *et al.*(A), Ert *et al* (B). and Wexler for the Ir NC (C), Wexler for the Au NC (D) are inserted in (a).

3(a-c) show the relationships between the area and conductance measured with bias voltages of 75 mV (a), 200 mV (b) and 300 mV (c), respectively. Three relationships are similar; the dependence of bias voltage to conductance is hardly found in this range of bias voltage.

For comparison, we inserted an experimental conductance of an Au NC and theoretical fitting curves by Torres *et al.*[6]and by Ert *et al.*[7]in Fig. 3(a). The conductance of the Ir NC is higher than that of the Au NC for same cross-sectional area. This may be due to number of channels at Fermi levels. the number is 5 – 6 for Ir and 1 for Au, although we should consider that transmission probability of each channel contributes to total conductance. We then take electron scattering into consideration for fitting: semiclassical approach by Wexler based on the Boltzman formula regarding electron transport[8].

$$G_w = G_s\left(1+\frac{3\pi}{8}\Gamma(K)\frac{a}{l}\right) \qquad (1)$$

where G_S is Sharvin's conductance, a is the radius of the contact, l is the electron mean free path, $\Gamma(K)$ is a slowly varying function of order unity and $K= l/a$ is the Knudsen number.

The fitting curves for bias voltages of 75, 200 and 300 mV are inserted in Fig. 3(a-c) and agree with the experimental results.

4. Conclusion

The Ir NCs were observed by *in situ* transmission electron microscopy with simultaneous measurement of conductance. The Ir NCs were thinned to a width of single atom due to tensile deformation and then broke. The conductance decreased with their minimal cross-sectional area. The relationship between the cross-sectional area and conductance was compared with calculation based on theoretical models.

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