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Structure, strength and conductance of palladium wires of single atom width

Tomoko Matsuda[1] and Tokushi Kizuka[1,2,3]

[1]Institute of Materials Science, University of Tsukuba, Tsukuba 305-8573, Japan.
[2]Special Research Project of Nanoscience, University of Tsukuba, Tsukuba 305-8573, Japan.
[3]Precursory Research for Embryonic Science and Technology, JST, Tsukuba 305-8573, Japan.
E-mail: kizuka@ims.tsukuba.ac.jp

1. Introduction

The presence of one-dimensional arrays of single atoms (atomic-sized wires, ASWs) was envisaged in the studies on nanometer-sized contacts (NCs) of metallic elements [1-3]. NCs are thinned during retraction of their two connecting electrodes; their minimal cross-sectional area finally reduces to the cross-sectional area of single atom. The conductance and force of ASWs have been deduced in relation to quantized conductance of NCs. Various structural models of ASWs, i.e. atomistic configuration and interatomic distance, were proposed based on calculation. Transmission electron microscopy (TEM) has been performed to analyze their atomistic arrangements. Two types of preparation methods of ASWs for TEM have been used: drilling of thin films by intense electron beams [4-6,7,8] and *in situ* tensile deformation [9]. In this letter, we used latter method for Pd ASWs in order to investigate relationships between their atomic arrangements, strength and conductance.

2. Experimental method

The experimental method in this study was developed based on *in situ* high-resolution TEM combined with sub nanonewton force measurements as used in atomic force microscopy (AFM) and electronic conductance measurements as used in scanning tunneling microscopy [9]. First we prepared nanometer-sized Pd tips: Pd was evaporated and deposited on a Si cantilever with a nanometer-sized tip, as used in AFM in a vacuum chamber. The cantilever was attached to the front of a tube piezo on a cantilever holder of the transmission electron microscope in University of Tsukuba. A Pd plate of 0.2 mm thickness was attached to a second sample holder. The thickness of the contact edge of the plate was reduced to 5 - 20 nm by argon ion milling. 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 100 mV between the tip and plate. The tip was pressed into the plate to prepare NCs, and then retracted to elongate them and transform to ASWs. A series of these manipulations were performed at room temperature in a vacuum of 1 x 10^{-5} Pa. The structural variation of the sequence was observed *in situ* by lattice imaging of high-resolution TEM using a TV capture system. The time-resolution of the image observations was 17 ms. The force applied between tip and plate were simultaneously measured by optical detection of the cantilever deflection. The conductance was measured using a two-terminal method. The high-resolution imaging and signal detection in this system were coincidentally recorded and analyzed for every image using our own software.

3. Results and Discussion

Figure 1a shows a high-resolution image of a Pd ASW. Fig. 1b corresponds to the image in Fig. 1a. This wire is composed of three atoms. Each atom is lined straight. The interatomic distance is 0.30 $\pm$ 0.1 nm. Figure 2 shows current and force measured for the ASW in Fig. 1 until fracture. The force acting on the Pd wires was 0.5 $\pm$ 0.2 nN. For the estimation of stress applied to the ASW, we assumed the cross-sectional area of Pd single atom using a hard-sphere model for atoms; the area is $S \sim 0.059$ nm^2. The corresponding strength σ is 15 $\pm$ 5 GPa. According to Matuda *et al*. Young's modulus of Pd NCs of a few atoms width was ~ 100 GPa [10]. We applied this value of Young's modulus E and estimated strain of the present ASW ε from the formula $\sigma = E\varepsilon$: Then ε is ~ 0.15. When we take into account this elongation, the interatomic distance of ASW at a strain of zero is estimated to be 0.26 $\pm$ 0.1 nm. Concerning interatomic distance of ASWs of single metallic elements, we could refer the interatomic distance of their dimmers and the nearest neighbor distance of atoms in their bulk. For Pd, former is reported by Seongbok *et al*. [11] as 0.25 nm, and the latter is 0.27 nm [12]. The present interatomic distance estimated for a strain of zero, 0.26 $\pm$ 0.1 nm, is intermediate in the interatomic distance of the dimmer and the nearest neighbor distance of bulk. Such interatomic distance in the intermediate levels was reported for Au ASWs [6]. The current through the Pd wires was measured to be 0.4 μA at a bias voltage of 100 mV; conductance was 0.05 G_0 (where $G_0=2e^2/h$, with e as the charge of electron and h as the Plank constant). This conductance is ~ 5 % of that proposed for Au ASWs, approximately 1 G_0, however, is clearly much larger than tunneling current in scanning probe microscopy. On the other hand, using the cross-sectional area S, the current density was estimated to be 3 TA/m^2. This current density is 10^7 times as large as that of coarse-grained Pd crystals [12].

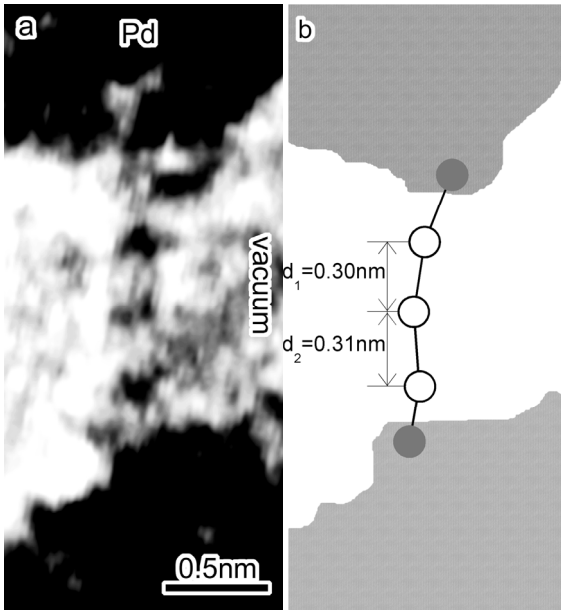

Fig.1 High-resolution image of a Pd wire of single atom width. The image in a is illustrated in b.

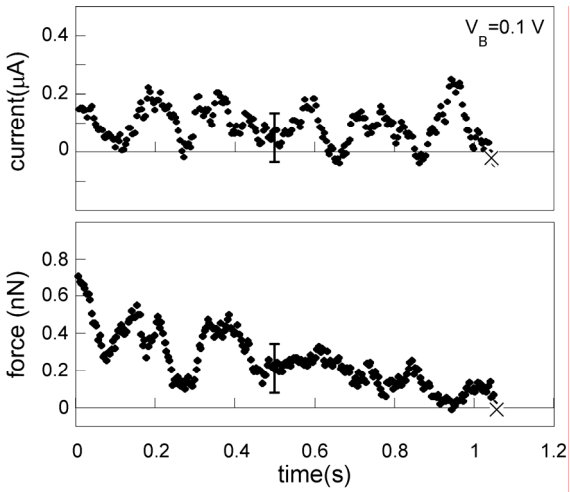

Fig.2 Current and force measured around fracture of the ASW in Fig. 1. The time at fracture is represented as a cross. Both current and force fluctuate due to vibration of the tips connecting to the ASW.

4. Conclusion

The Pd ASWs prepared by contact and successive retraction of two Pd nanometer-tips, were observed by *in situ* transmission electron microscopy with simultaneous measurements of force and conductance. The Pd wires composed of three atoms grew straight along the retraction direction of the tip. The interatomic distance was 0.30 $\pm$ 0.1 nm. The force acting on the Pd wires was 0.5 $\pm$ 0.2 nN, corresponding to a strength of 15 $\pm$ 5 GPa according to estimation of the cross-sectional area using a hard-sphere model for atoms $S \sim 0.059$ nm^2. The current through the Pd wires is 0.2 μA at a bias voltage of 100 mV; conductance was 0.05 G_0. Using the cross-sectional area S, the current density was estimated to be 3 TA/m^2.

Acknowledgment

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Reference

[1] A. Yazdani, D. M. Eigler and N. D. Lang, Science **272** (1996) 1921.

[2] T. Junno, S. -B. Carlsson, H. Xu, L. Montelius and L. Samuelson, Appl. Phys. Lett. **72** (1998) 548.

[3] C. Z. Li, A. Bogozi, W. Huang and N. J. Tao, Nanotechnology **10** (1999) 221.

[4] H. Ohnishi, Y. Kondo and K. Takayanagi, Nature **395** (1998) 780.

[5] V.Rodorigues and D. Ugarte, Phys. Rev. B **63** (2001) 073405.

[6] Y. Takai, T. Kawasaki, Y. Kimura, T. Ikuta and R. Shimizu, Phys. Rev. Lett. **87** (2001) 106105.

[7] V.Rodorigues, J. Bettini, A. R. Rocha, L. G. C. Rego and D. Ugarte, Phys. Rev. B **65** (2002) 153402.

[8] V.Rodorigues, J. Bettini, P. C. Silva and D. Ugarte, Phys. Rev. Lett. **91** (2003) 096801.

[9] T. Kizuka, S. Umehara and S. Fujisawa, Jpn. J. Appl. **40** (2001) L71.

[10] T. Matsuda and T. Kizuka, to be published.

[11] S. Lee, D. M. Bylander and L. Kleinman, Phys. Rev. B **39** (1989) 4916.

[12] W. F. Gale and T. C. Totemeire (eds.), *Smithells Metals Reference Book*, Elsevier (2004)