Electrical Resistance of a Monatomic Step on a Crystal Surface

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We have succeeded in measuring the resistance across a single atomic step through a monatomic-layer metal on a crystal surface, Si(111)($\sqrt{3} \times \sqrt{3}$)-Ag, using three independent methods, which yielded consistent values of the resistance. Two of the methods were direct measurements with monolithic microscopic four-point probes and four-tip scanning tunneling microscope probes. The third method was the analysis of electron standing waves near step edges, combined with the Landauer formula for 2D conductors. The conductivity across a monatomic step was determined to be about $5 \times 10^3\ \Omega^{-1}\,\mathrm{m}^{-1}$. Electron transport across an atomic step is modeled as a tunneling process through an energy-barrier height approximately equal to the work function.

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Rapid progress in the miniaturization of microelectronics devices now forces signal currents to flow near the surface/interface region in semiconductor crystals, and ultimately, with continued miniaturization, will force the current through only one atomic layer. On an atomic (nanometer) scale, carriers strongly interact with localized scatterers. On crystal surfaces, atomic steps [1] are unavoidable defects, which become inevitable barriers for carrier transport through the topmost atomic layers in crystals. In this Letter, we report the measurement of the value of the conductance across a single atomic step per unit length and the transport processes involved.

A conductive metallic monolayer on a semiconductor crystal surface, Si(111)($\sqrt{3} \times \sqrt{3}$)-Ag surface superstructure, was employed as the sample. The surface has a parabolic electronic band crossing the Fermi level with a circular Fermi surface, indicating an isotropic two-dimensional free-electron like metal of monolayer thickness [2,3]. Recently, transport measurements with state-of-the-art monolithic micro-four-point probes (MFPP) and four-tip scanning tunneling microscope (STM) probes have been reported to be successful in obtaining (anisotropic) conductance values of atomic-scale structures on semiconductor surfaces, including the Si(111)($\sqrt{3} \times \sqrt{3}$)-Ag surface [4–9]. In the present study, two independent direct measurements of step resistance were performed with the same monolithic MFPP and four-tip STM techniques for surfaces with controlled step configurations. One was through measurements of anisotropy in sheet conductivity of a vicinal crystal surface where atomic steps were regularly aligned with almost equal spacing in one direction, and the other was through measurements across step-bunched regions where hundreds of monatomic steps were accumulated [10]. The results were then compared with that obtained using the "conventional" method of analyzing Friedel oscillations near step edges derived from microscopic surface images taken using scanning tunneling spectroscopy, dI/dV. At various values of the tip bias, standing waves near the steps were observed and the transmission probability was determined from the reflection phase shift. The Landauer formula relates conductance, σ, and the transmission probability, T. It varies with the dimensions. The conductance of 1D, 2D, and 3D conductors through 0D, 1D, and 2D potential barriers is generally expressed [11], respectively, by

$$\sigma_{1\mathrm{D}} = \frac{2e^2}{h} T\ [\Omega^{-1}], \tag{1}$$

$$\sigma_{2\mathrm{D}} = \frac{2e^2}{h} \frac{k_F}{\pi} T\ [\Omega^{-1}\,\mathrm{m}^{-1}], \tag{2}$$

$$\sigma_{3\mathrm{D}} = \frac{2e^2}{h} \frac{k_F^2}{4\pi} T\ [\Omega^{-1}\,\mathrm{m}^{-2}], \tag{3}$$

where e, h, and k_F are the elementary charge, Planck's constant, and Fermi wave number, respectively. $\sigma_{1\mathrm{D}}$ is a well-known formula for conductance quantization at nanowires and point contacts. $\sigma_{3\mathrm{D}}$ is also used for the analysis of tunneling devices. On the other hand, $\sigma_{2\mathrm{D}}$ has not been utilized much previously due to the lack of appropriate systems. The present case of 2D metallic monolayers (2D conductor) separated by a monatomic step (a 1D potential wall) is obviously suitable for such unusual research. Through the $\sigma_{2\mathrm{D}}$ analysis, we experimentally obtained the conductance or the conductivity across a step per unit length. All of these measurements, the four-tip STM, the monolithic MFPP, and dI/dV, gave consistent values of resistance. Electron transport across an atomic step is fairly modeled as a tunneling process through an energy-barrier height approximately equal to the work function. This is the first direct measurement of electrical resistance of a monatomic step.

For the first direct determination of conductivity across steps, we prepared the ($\sqrt{3} \times \sqrt{3}$)-Ag surface structure on a vicinal Si(111) crystal having a miscut angle of 0.9 ° or 1.8 ° toward the $[\bar{1}\,\bar{1}\,2]$ axis. The anisotropic conductivity was electrically measured by the so-called rotational square (RS) MFPP method [9] using the four-tip STM at room temperature. This is a four-point probe resistance measurement in a square arrangement of the four probes with several tens of μm probe spacing, as shown in Fig. 1, and the square is rotated with respect to the sample surface. On our sample surface, all the steps were aligned along the $[\bar{1}10]$ crystal axis and distributed uniformly with almost equal spacing (10–20 nm) over the surface, as judged from the STM observations (Fig. 1). On a micrometer scale, the vicinal surface can be regarded as an anisotropic 2D conductor because of the aligned step array; the conductivity in a direction perpendicular to the steps should be lower than that parallel to the steps. Therefore, any anisotropy in conductivity detected by the RS-MFPP measurement can be attributed to the steps and we can determine the resistance caused by atomic steps directly from the anisotropy. This is because any channel for electrical conduction near the surface (surface-state bands on the topmost atomic layers, bulk-state bands in a surface space-charge layer beneath the surface, and bulk-state bands in the inner crystal) is isotropic.

The resistance of the $(\sqrt{3}\times\sqrt{3})$-Ag surface on a 1.8 ° miscut wafer is shown in Fig. 2 as a function of the rotation angle of the square relative to the $[\bar{1}10]$ direction. By fitting the results with a formula derived from the Poisson equation [9], we obtained sheet conductivities parallel ($\sigma_{//}$) and perpendicular ($\sigma_{\perp}$) to the step direction separately; $\sigma_{//}$ and $\sigma_{\perp}$ are 23×10^{-6} and $14\times10^{-6}\ \Omega^{-1}\square^{-1}$, respectively, so that the anisotropy is $\sigma_{//}/\sigma_{\perp}\sim1.6$. For a sample with a smaller miscut angle on the crystal surface, we obtained a smaller anisotropy because of the lower step density.

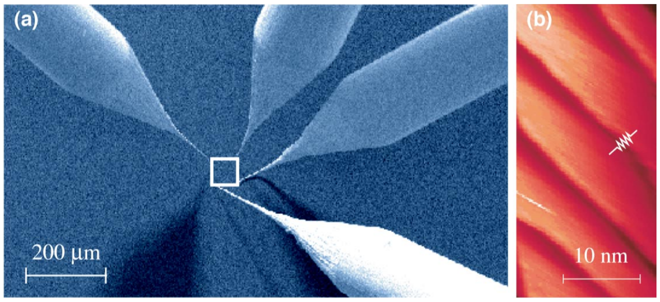

FIG. 1 (color online). (a) A scanning electron microscope (SEM) image of the four scanning tunneling microscope (STM) tips during direct transport measurement. (b) A topographic STM image of monatomic steps on Si(111)$(\sqrt{3}\times\sqrt{3})$-Ag on a vicinal Si(111) wafer taken with a tip bias, V_t, of −3.0 V. The schematic resistance of a step is depicted in the image.

As described above, the difference of sheet resistance between step-perpendicular, $1/\sigma_{\perp}$, and step-parallel, $1/\sigma_{//}$, directions is ascribed to the resistance associated with monatomic steps. The conductivity across a step of unit length σ_{step} ($\Omega^{-1}\,\text{m}^{-1}$) can be related to the sheet conductivities $\sigma_{//}$ and $\sigma_{\perp}$ by

$$N_{\text{step}}/\sigma_{\text{step}} = 1/\sigma_{\perp} - 1/\sigma_{//}, \tag{4}$$

where N_{step} (m^{-1}) is the step density on the sample surface. Our vicinal Si(111) wafer with a miscut angle of 1.8 ° has $N_{\text{step}}\sim10^{8}\ \text{m}^{-1}$. Therefore, we get $\sigma_{\text{step}}\sim3\times10^{3}\ \Omega^{-1}\,\text{m}^{-1}$.

For the second method of direct measurement of resistance across the steps, we have previously conducted linear MFPP measurements across a step-bunching region on the $(\sqrt{3}\times\sqrt{3})$-Ag surface at room temperature [10]. The measured resistance across the step-bunching region, which consists of ~300 monatomic steps with a step interval of several tens of nm, is higher by about 800 Ω when compared to the almost step-free terrace region. Through proper theoretical simulation [12], the resistance of the step-bunching region was determined to be about 1700 Ω. The relationship between resistance at a step-bunching region and that at a step can be written as

$$R_{\text{step bunching}} = B_{\text{step bunching}} R_{\text{step}} \tag{5}$$

$$= B_{\text{step bunching}}/(l_{\text{current}}\sigma_{\text{step}}), \tag{6}$$

where $R_{\text{step bunching}}$ and R_{step} are resistance (Ω) at a step-bunching region and a monatomic step, respectively.

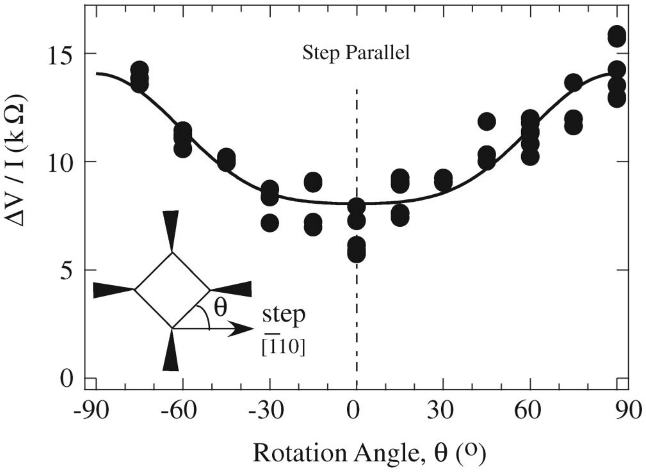

FIG. 2. Resistance measured as a function of the rotation angle in the rotational square micro-four-point probe (RS-MFPP) method for the $(\sqrt{3}\times\sqrt{3})$-Ag surface on a vicinal Si(111) wafer (n-type, 1–10 Ω cm) with a miscut angle of 1.8 ° at room temperature. The probe spacing (a side of the square) was 60 μm. Experimental data are fitted by a function described in Ref. [9].

$B_{\text{step bunching}}$ is the number of steps in a step-bunching region (~300) while l_{current} is the step length (m) through which the current passes. Solving a simple Poisson equation of the present probe arrangement indicated that almost 90% of the surface current was spread over twice the length of the current probe spacing in a direction perpendicular to the probe alignment. In the case of the present probe spacing of 8 μm, the two current probes are separated 24 μm from each other and l_{current} is estimated to be about 50 μm. Then, for $R_{\text{step bunching}} = 1700\ \Omega$, we find $\sigma_{\text{step}} \sim 4 \times 10^3\ \Omega^{-1}\,\text{m}^{-1}$. *This value shows good agreement with the result of the four-tip STM measurements.* It is to be noted that these values were measured at room temperature.

We next consider the experiments with the single-tip scanning tunneling spectroscope. Figure 3(a) shows the STM and spectroscopic dI/dV images of the $(\sqrt{3} \times \sqrt{3})$-Ag surface near an atomic step at 65 K [13,14]. It can be seen that the $(\sqrt{3} \times \sqrt{3})$-Ag surface superstructure almost extends up to the step edge [1]. In the dI/dV images, the modulation of the local density of states (LDOS) standing wave (Friedel oscillation) is caused by interference in the carrier scattering at a step. Its physical properties have been well studied on noble metal surfaces [15–19]. The wavelength varied with tip bias (not shown here) [15,16], and the energy versus wave number dispersion obtained through the bias-dependent standing waves showed a parabola with an effective mass equal to that obtained by angle-resolved photoemission spectroscopy (ARPES) [2,3,20,21].

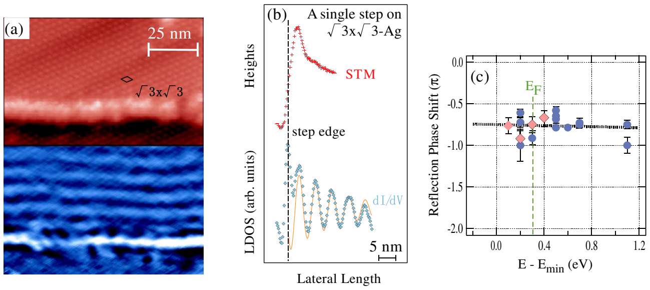

FIG. 3 (color online). (a) STM and LDOS (dI/dV) images near a monatomic step on the surface of a flat wafer acquired at $V_t = -0.9$ V. The dI/dV image is taken using lock-in detection. (b) Line profiles across a step in STM ($V_t = -0.9$ V) and dI/dV ($V_t = -0.7$ V) images. The step edge ($x = 0$) is indicated by a straight dashed line. The fitting function shown as a curve is described in the text. (c) Changes in the reflection phase shift with energy. Solid circles and diamonds are data points from the present work and the previous report [20], respectively. A least-squares fit is shown as a dotted line. The energy position on the horizontal axis is the bottom of the surface-state band, E_{min}. This is because energy positions with respect to the Fermi level (E_F) vary among the different STM/STS scanning regions on a semiconductor surface at low temperatures due to a tip-induced local band bending effect.

Figure 3(b) shows topographic STM and dI/dV profiles over a step. The damped oscillation in the LDOS along a direction perpendicular to the step edge (x axis) is fitted using a function, $\text{LDOS}(x) \propto \exp(-x/L)\cos(2kx - \eta)$, where L, k, and η are the decay length, wave vector, and reflection phase shift, respectively [18]. The reflection phase shift η is derived at each tip bias and plotted in Fig. 3(c). Within the experimental error, η is almost constant in the measured energy range. In the figure, the energy position on the horizontal axis is referred to as the bottom of the surface-state band, E_{min}. According to previous ARPES studies [2,3], E_{min} is located at a binding energy ~0.3 eV below E_F, so that E_F is located at ~0.3 eV in Fig. 3(c). The reflection phase shift around E_F is then determined to be about $-(0.8 \pm 0.05)\pi$.

Once the reflection phase shift at a step was determined, the transmission probability, T, was determined through the δ-potential model [19] and the conductance through a step could be derived from the Landauer formula [11]. The δ-potential model is suitable for the present system for the following reasons: (1) Since the surface state crosses E_F in the bulk band gap, no carrier scattering of surface-state electrons into bulk states occurs [17,19]. (2) The model gives more precise values for thinner potential widths; the step-edge potential barrier is as thin as an atom [11]. The transmission coefficient T and the reflection phase shift η are related by $T = 1 - [1 + \tan^2(\eta + \pi)]^{-1}$ [19]. Inserting the experimentally determined η into this equation, T was determined to be 0.3 ± 0.15. The conduction electrons in the $(\sqrt{3} \times \sqrt{3})$-Ag layer (surface state) pass through a step with a probability of about 30%. It should be noted that the transmission probability is the same for the step-up and step-down directions. This is supported by experimentally observed linear I-V curves in the present conductivity measurements and theoretically by the WKB tunneling regime typically used in STM theories [22]. Inserting T determined above and k_F (~0.1 Å^{-1}) determined in the previous ARPES measurements for the $(\sqrt{3} \times \sqrt{3})$-Ag surface [2,3,21] into Eq. (2), σ_{2D} at a monatomic step on this particular surface is determined to be $\sigma_{2D} = 9(\pm 4) \times 10^3\ \Omega^{-1}\,\text{m}^{-1}$. The σ_{2D} reasonably matches the σ_{step} obtained by the two independent methods of direct electrical measurements described earlier in the Letter. It should be noted that in the Landauer regime, the conductance is independent of temperature when the transmission coefficient (the reflection phase shift) is independent of energy [23]. The experimental result in Fig. 3(c) clearly supports this picture.

It is now obvious that conductance across a monatomic step on the $(\sqrt{3} \times \sqrt{3})$-Ag surface is about $5 \times 10^3\ \Omega^{-1}\ \text{m}^{-1}$. When electrical current flows through a step of 1 cm, 1 mm, 1 μm, and 1 nm length, the resistance across the step should be 0.02, 0.2, 200, and 2×10^5 Ω, respectively. *The resistance is negligible on a macroscopic scale, but large for nanometer length scales.*

The reasonable agreement among the three independent methods used indicates that *electron transport through a monatomic step on a crystal surface can be modeled as an electron tunneling process.* The δ potential adopted in the present study yields the product of potential barrier height and potential width, $V_0 a$, of the atomic step to be 10($\pm$6) eV Å. This value is similar to those reported on the vicinal Au surface estimated by ARPES data [24]. Assuming a as a bond length of the bulk Si crystal (2.35 Å), V_0 is 4.5($\pm$2.5) eV. This value roughly corresponds to the work function of the sample surface. This implies that, at a step, carrier electrons in metallic overlayers on semiconductor substrates tunnel through an energy barrier corresponding to the energy difference between the vacuum level and the Fermi level. The potential barrier height of the work function may be a good approximation to estimate conductance across an atomic step for other material systems.

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[1] M. Ueno, I. Matsuda, C. Liu, and S. Hasegawa, Jpn. J. Appl. Phys. **42**, 4894 (2003).

[2] J.N. Crain, K.N. Altmann, C. Bromberger, and F.J. Himpsel, Phys. Rev. B **66**, 205302 (2002).

[3] T. Hirahara, I. Matsuda, and S. Hasegawa, e-Journal of Surface Science and Nanotechnology **2**, 141 (2004); T. Hirahara, I. Matsuda, M. Ueno, and S. Hasegawa, Surf. Sci. **563**, 191 (2004).

[4] S. Hasegawa and F. Grey, Surf. Sci. **500**, 84 (2002).

[5] T. Tanikawa, K. Yoo, I. Matsuda, S. Hasegawa, and Y. Hasegawa, Phys. Rev. B **68**, 113303 (2003).

[6] T. Tanikawa, I. Matsuda, R. Hobara, and S. Hasegawa, e-Journal of Surface Science and Nanotechnology **1**, 50 (2003); T. Tanikawa, I. Matsuda, T. Kanagawa, and S. Hasegawa, Phys. Rev. Lett. **93**, 016801 (2004).

[7] I. Shiraki, F. Tanabe, R. Hobara, T. Nagao, and S. Hasegawa, Surf. Sci. **493**, 633 (2001).

[8] B. Velschow, Copenhagen Applied Research, http://www.capres.com/.

[9] T. Kanagawa, R. Hobara, I. Matsuda, T. Tanikawa, A. Natori, and S. Hasegawa, Phys. Rev. Lett. **91**, 036805 (2003).

[10] S. Hasegawa, I. Shiraki, T. Tanikawa, C.L. Petersen, T.M. Hansen, P. Boggild, and F. Grey, J. Phys. Condens. Matter **14**, 8379 (2002).

[11] J.H. Davies, *The Physics of Low -Dimensional Semiconductors* (Cambridge University Press, Cambridge, England, 1998).

[12] T.M. Hansen, K. Stokbro, O. Hansen, T. Hassenkam, I. Shiraki, S. Hasegawa, and P. Boggild, Rev. Sci. Instrum. **74**, 3701 (2003).

[13] H. Morikawa, I. Matsuda, and S. Hasegawa, Phys. Rev. B **65**, 201308 (2002).

[14] H. Aizawa, C.M. Tsukada, C.N. Sato, and S. Hasegawa, Surf. Sci. **429**, L509 (1999).

[15] M.F. Crommie, C.P. Lutz, and D.M. Eigler, Nature (London) **363**, 524 (1993).

[16] Y. Hasegawa and P. Avouris, Phys. Rev. Lett. **71**, 1071 (1993).

[17] M.F. Crommie, C.P. Lutz, D.M. Eigler, and E.J. Heller, Surf. Rev. Lett. **2**, 127 (1995).

[18] P. Avouris, I.-W. Lyo, R.E. Walkup, and Y. Hasegawa, J. Vac. Sci. Technol. B **12**, 1447 (1994).

[19] L. Bürgi, O. Jeandupeux, A. Hirstein, H. Brune, and K. Kern, Phys. Rev. Lett. **81**, 5370 (1998).

[20] N. Sato, T. Nagao, S. Takeda, and S. Hasegawa, Phys. Rev. B **59**, 2035 (1999).

[21] X. Tong, S. Ohuchi, N. Sato, T. Tanikawa, T. Nagao, I. Matsuda, Y. Aoyagi, and S. Hasegawa, Phys. Rev. B **64**, 205316 (2001).

[22] A. P. French and E. F. Taylor, *An Introduction to Quantum Physics*, (MIT, Cambridge, MA, 1978).

[23] S. Datta, *Electronic Transport in Mesoscopic Systems* (Cambridge University Press, Cambridge, England, 2002).

[24] A. Mugarza, A. Mascaxaque, V. Perez-Dieste, V. Repain, S. Rousset, F.J. GarciadeAbajo, and J.E. Ortega, Phys. Rev. Lett. **87**, 107601 (2001).