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Evidence of metallic nature of the surface bands of Au/Si(557)

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We have studied temperature dependence of the two proximal bands, S1 and S2, from the one-dimensional (1D) Au/Si(557) system using angle-resolved photoemission spectroscopy with synchrotron photons. The intriguing feature of these bands reported earlier, metallic S1 and insulating S2 at room temperature [J. R. Ahn, H. W. Yeom, H. S. Yoon, and I. W. Lyo, Phys. Rev. Lett. **91**, 196403 (2003)], has neither been reproduced nor understood properly yet. Our band images, however, unambiguously reveal that both bands behave nearly identically with temperature and remain metallic for $83\ \mathrm{K} \leq T \leq 300\ \mathrm{K}$ as seen by the well-defined Fermi-Dirac edges. We thus exclude the presence of a Peierls-type metal-insulator transition claimed earlier and discuss possible causes for the difference. The metallic nature of these bands is further illustrated by the presence of a satellite peak in the Au $4f_{7/2}$ core level reflecting the 1D plasmon excitation.

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Enhanced correlation interaction of electrons restricted to one-dimensional (1D) systems has long been predicted to cause novel non-Fermi-liquid properties such as the uncoupled low-energy collective excitations of spin (spinon) and charge (holon) degrees of freedom of electrons depending essentially on the interaction itself.[1–4] There have been continued efforts to find the presence of such behavior in various 1D interacting electron systems including the metallic 1D systems formed on vicinal silicon surfaces, Au/Si(557),[5–22] Au/Si(553),[22–30] and Au/(5512).[31] Among these, the nature of the two metallic surface bands of the quasi-1D Au/Si(557) system, where the 1D system is not completely isolated from its supporting substrate, has been extensively studied. It has initially been triggered by angle-resolved photoemission (ARP) study interpreting these bands as the spinon and holon excitations in Luttinger liquid.[5] Although this interpretation has been denied by the subsequent ARP works by revealing the well split two surface bands, S1 and S2, at Fermi level E_F instead of recombining these excitations into an electron at E_F as theory predicts.[3,4] Because the Au/Si(557) system was found to be quite close to an ideal 1D metallic system[5,6] to study electron correlation effect, the study on the precise nature of these surface bands has been continued characterizing its atomic structure by x-ray measurement[7] followed by first-principle density-functional theory (DFT) calculations.[8,9]

The Peierls instabilities characteristic of 1D metallic system has also been invoked to this 1D metallic system.[5,6,10,24,33] Ahn *et al.*[10] reported, however, that only S1 is metallic at room temperature (RT), which undergoes a Peierls-type metal-insulator transition (MIT) with a transition temperature $T_c = 120\ \mathrm{K}$ while S2 appears to be nonmetallic with an energy gap of about 100 meV nearly independent of T. They also observed period doubling below T_c for the step-edge Si atoms associated with the S1 band in their scanning tunneling microscope (STM) images. Meanwhile from their DFT calculations, Sánchez-Portal *et al.*[9,18] showed that the splitting of a surface band into two S1 and S2 bands near E_F stems from the spin-orbit coupling of the Si-Au band. The period doubling was also reproduced by their simulated STM image of the ground-state configuration with two-step-edge atoms of different heights rather than from a Peierls-type lattice modulation. They, however, suggested a possibility for a Peierls-type MIT in terms of the fluctuation of the step-edge band when its spectral weight at E_F varies with T. Despite these continued efforts, the nature of the two proximal surface bands, especially regarding to their different behavior on temperature, has not been properly explained yet. Here we show that both bands, S1 and S2, appear to be metallic and exhibit the same behavior on temperature from RT down to 83 K, well below T_c. They remain metallic at all temperatures and do not show any Peierls-type MIT in this temperature range in sharp conflict with previous ARP study.[10] We provide a plausible explanation for the discrepancy. The persistent metallic character of the surface bands is found to produce a satellite peak in the Au $4f$ core level at a binding energy 1.0 eV higher than that of the Au $4f_{7/2}$ peak.

The experiments were performed at the 3A2 beamline of the Pohang Accelerator Laboratory. Our ARP measurements using Synchrotron photons were collected by using Scienta R4000 analyzer in an ultrahigh vacuum system maintained at a base pressure below 1×10^{-10} Torr. The optimum energy resolution of the beamline is below 50 meV. We used a rectangular-shape *n*-doped Si(557) wafer of resistivity 1–10 Ohm cm purchased from Siltronix. The Si(557) sample was cleaned by repeatedly flashing up to 1250 °C until we find the 17×2 low-energy electron-diffraction (LEED) pattern. We have deposited Au on thus cleaned sample maintained at 600 °C while monitoring the exposure with a thickness monitor up to an optimum coverage of 0.2 monolayers. We then annealed the sample at 850 °C to obtain a well-defined 5×2 LEED pattern. We have repeated ARP measurements several times by using either synchrotron photons at the synchrotron site or a He lamp at home laboratory using PHOIBOS analyzer with an energy resolution about 50 meV.

Figure 1(a) shows the band image in the second Brillouin zone (BZ) for momentum $k_\parallel \geq \pi/a = 0.82\ \text{Å}^{-1}$ obtained by using synchrotron photons of energy 34 eV. One finds the surface band which becomes well split into two proximal

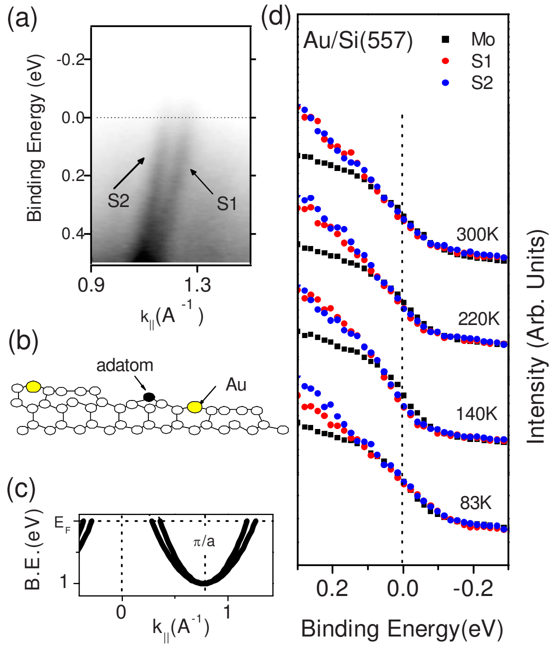

FIG. 1. (Color online) (a) Band dispersion image in the second BZ showing the two proximal bands S1 and S2 obtained with synchrotron photons of energy 34 eV at RT. (b) Schematic side view of the atomic structure and (c) band diagram of the Au/Si(557) structure. Note that the zone boundary locates at $k_{\parallel}=\frac{\pi}{a}=0.82$ Å^{-1}. (d) Change in the EDCs near Fermi level (E_F) with temperature T. Both bands appear to behave the same way with T maintaining their Fermi edges almost identical with that of the metallic molybdenum for $83\ \text{K} \leq T \leq 300\ \text{K}$.

bands S1 and S2 near E_F. Several previous ARP data also showed that these bands are well split and cross E_F at two different momentum values separated by $\Delta k_{\parallel}=0.06$ Å^{-1}.[6,9,11] Such observation clearly rules out the possibility of the spinon-holon excitations predicted for a Luttinger liquid. Meanwhile *ab initio* calculations revealed that both bands are metallic and split off essentially from a single band of Au 6*p* and Si 3*p* mixed orbitals by the spin-orbit coupling.[9,18] The electronic nature of these bands has been relatively well characterized to date except the observation that S1 crosses E_F but not S2 at RT, and the metallic S1 undergoes a Peierls-type MIT upon cooling while insulating S2 remains unaltered.[10]

Our energy distribution curves (EDCs) for these bands are presented in Fig. 1(d) for several temperatures in the range $83\ \text{K} \leq T \leq 300\ \text{K}$. One immediately finds that both bands definitely cross E_F and reveal almost identical behavior with temperature. Note that the Fermi edges of the bands at $T=83$ K nicely overlap with that of molybdenum taken as a reference metal. These Fermi edges appear to accurately describe the Fermi-Dirac distribution function when our EDCs are fitted. Such observations completely deny the claim of observing a Peierls-type MIT from the S1 band reported earlier.[10] It is a challenging subject to understand, however, how the Au atomic chains of the Au/Si(557) surface known as one of the most ideal self-assembled 1D systems[23] remains stable at least down to 83 K overcoming the intrinsic Peierls instabilities. It would still be possible to find a Peierls-type MIT, if any, with T_c lower than 83 K as long as the substrate plays no crucial role in the transition.

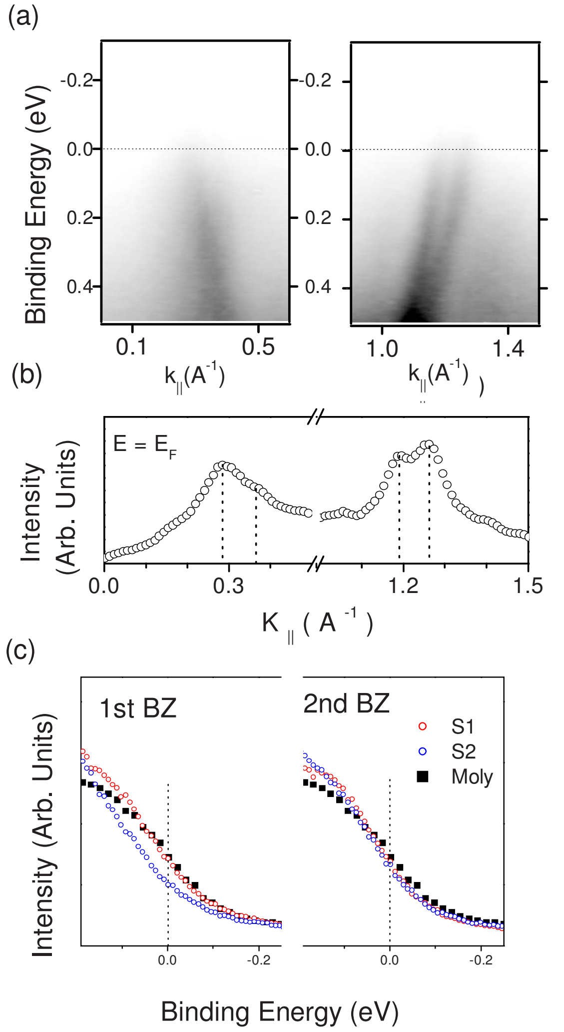

FIG. 2. (Color online) (a) Band dispersion images in the first (left) and in the second (right) BZ acquired at RT. Note that the splitting is more prominent in the second zone as seen in momentum distribution curve at E_F in (b). (c) The Fermi edges of the bands S1 and S2 obtained from the first (left) and from the second (right) Brillouin zone. The metallic nature of both bands is apparent from their Fermi edges of both bands nearly identical to that of molybdenum despite the slightly reduced but finite intensity at E_F especially for S2 even in the first BZ.

Why such conflicting data from the same Au/Si(557) system? One may think of several causes for the difference. First, Ahn *et al.* measured the bands in the first BZ with a He I lamp as a photon source of energy 21.2 eV. In Fig. 2(a) we also present our band image in the first BZ (left) acquired with synchrotron photons of energy 34 eV as well as the one in the second BZ (right) at RT. One notices that the spectral intensity, especially near E_F, is much weaker in the first BZ crossing E_F near $k_{\parallel}=0.30$ Å^{-1} than in the second BZ around $k_{\parallel}=1.20$ Å^{-1}. We believe that the weaker intensity in the first BZ simply reflects the matrix element effect from the k dependence of the transition probability. Previous work regarding to this point also showed such bands of different

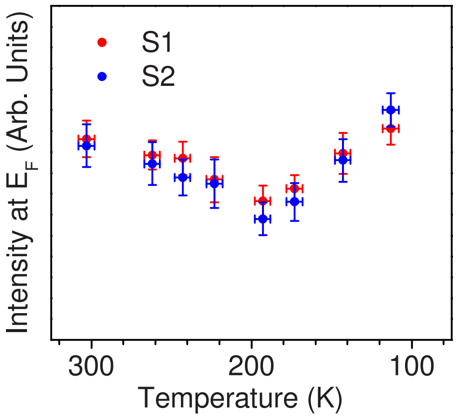

FIG. 3. (Color online) Variation in spectral intensity at Fermi level for the two proximal bands S1 and S2 as a function of temperature. The two bands appear to behave almost identically with temperature.

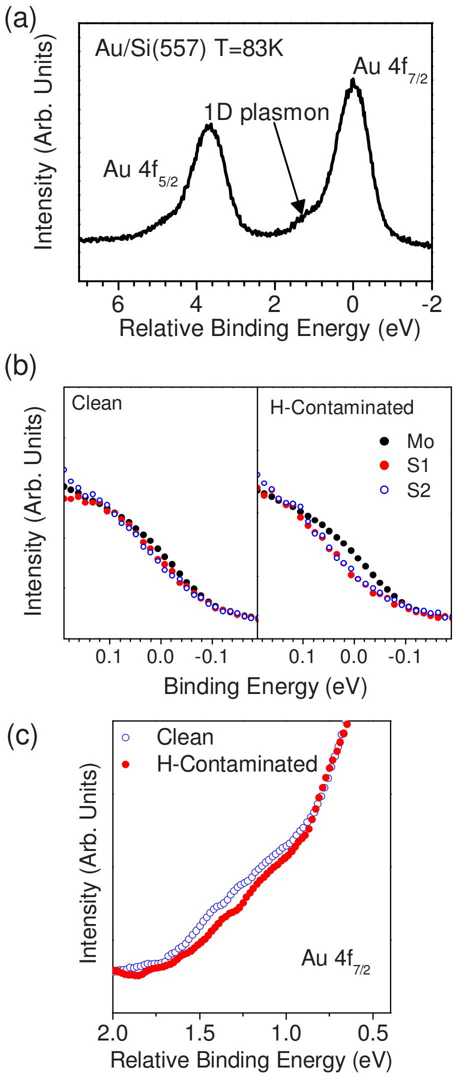

FIG. 4. (Color online) (a) Au 4f core-level spectrum taken at $T=83$ K. The satellite peak (marked by arrow) appearing on the higher binding-energy side of the bulk $4f_{7/2}$ peak is attributed to the 1D plasmon of the Au-Si metallic chains. (b) Changes in spectral intensity of S1 and S2 by hydrogen contamination. (c) Corresponding change on the shoulder of Au $4f_{7/2}$ peak.

intensities.[12,22] The two bands are much better resolved in the second BZ as seen in the momentum distribution curves in Fig. 2(b). As pointed out by Losio *et al.*,[6] the situation becomes worse with a He I lamp producing much reduced spectral intensity with a deteriorated resolution. We also noticed this from our band image especially in the first BZ obtained with a He I lamp (not shown).

Figure 2(c) compares the Fermi edges of the bands in the first (left) and the second (right) BZ. The spectral intensity of S2 in the first BZ is noticeably reduced but still remains significant, indicating the metallic nature of the band. We, thus, observe that both bands apparently cross E_F and are metallic at RT. Since the surface photovoltage effect should affect equally on both bands, it cannot be a factor to explain the insulating S2 at RT reported earlier.[10] As proposed by Sánchez-Portal *et al.*, there is still a possibility of producing different spectral intensity for the two bands as a result of the coupling with the weak step-edge band narrowly distributed near the Fermi level.[9,18] This is not the case, however, as seen in Fig. 3 where no remarkable gap in spectral intensity for the two bands is found. The slight increase in intensity upon cooling below 200 K is typical in ARP measurements due to the reduced phonon scattering. With no Peierls-type MIT observed, the origin of the periodicity doubling observed for the step-edge atoms in Ref. 10 becomes an important question to ask. From the STM images taken from our sample, we find well-resolved doubled periodicity not only along the adatom rows but also along the step-edge atoms, not hampered by the presence of defects.[32] The doubled periodicity clearly observed along the step-edge atoms may reflect the buckled feature of the step edges. We, therefore, conclude that the two split bands S1 and S2 are metallic at all temperatures in the range $83 \text{ K} \leq T \leq 300 \text{ K}$. Although the theoretical model by Riikonen and Sánchez-Portal[18] showing the changes in the proximal bands due to thermal fluctuations (see Figs. 9 and 10 of Ref. 18) suggests a possibility for the persistent metallic nature of this system upon cooling temperature down to 83 K (Fig. 1), the buckled nature of the step-edge atoms observed in our STM images may provide another experimental explanation in terms of charge redistribution due to the buckling. Details of the STM study will be published elsewhere.[32]

In order to examine how the metallic surface bands affect the Au atomic chains, we have measured Au 4f core level shown in Fig. 4(a). When compared to the bulk Au 4f core level, one finds a weak satellite peak at a binding energy 1.0 eV higher from that of the bulk Au $4f_{7/2}$ peak. This satellite peak appears reproducibly whenever the Au/Si(557) is prepared with almost the same spectral weight and binding energy. Although one may first invoke the presence of metallic Au islands as a possible source of the satellite peak, the absence of any valence bands associated with bulk Au safely excludes this possibility. The atomic structure of the Au/Si(557) surface determined by x-ray diffraction shows that there is only one kind of Au atoms in the unit cell containing $5\frac{1}{2}$ silicon chains. Therefore the satellite peak is not from the second kind of Au atoms, if any. Since earlier high-resolution electron energy-loss spectroscopy study[15,33] as well as theoretical calculations[25] have shown the presence of a 1D plasmon excitation from this system with an excitation energy ranging from 0.8 to 1.0 eV, the satellite peak of the Au $4f_{7/2}$ may reflect the plasmon excitation in the Au-Si metallic chains. This assignment becomes more plausible when one finds the remarkably weakened satellite when the surface becomes less metallic by contamination. Figure 4(b) shows such a change in the valence-band edge when the surface is exposed intentionally to hydrogen contamination from the ambient pressure of the chamber ($\leq 1\times 10^{-10}$ Torr) for an extended period of time. One finds that the two split bands react almost identically to contamination resulting in the much reduced spectral intensities in the vicinity of the Fermi level. Also the reduced intensity of the 1D plasmon satellite peak in Fig. 4(c) indicates the less metallic feature of the contaminated surface.

In summary, we have studied temperature dependence of the two proximal bands S1 and S2 of the Au/Si(557) surface. We observe the two surface bands metallic for a temperature range 83 $\text{K} \leq T \leq 300$ K as seen by their significant spectral weights at Fermi level and also by their Fermi edges accurately describing the Fermi-Dirac distribution function for all temperatures. Despite the ideal 1D character of the Au chains of this surface, we observe no Peierls-type metal-insulator transition in sharp contradiction to the earlier report claiming such a transition from the metallic band S1.[10] We discussed several possible causes for the confliction of data including the much reduced spectral weight especially in the first Brillouin zone of the split bands near Fermi level when a He I lamp is adopted, coupling with the weak step-edge band distributed near Fermi level and the contamination effect. The metallic character of the proximal split bands also explains the presence of a satellite peak near the Au $4f_{7/2}$ core level invoking the 1D plasmon excitation in the Au-Si metallic chains of the surface.

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[1] Thierry Giamarchi, *Quantum Physics in One Dimension* (Clarendon, Oxford, 2004).
[2] J. M. Luttinger, J. Math. Phys. **4**, 1154 (1963).
[3] J. Voit, J. Phys.: Condens. Matter **5**, 8305 (1993).
[4] J. Voit, J. Electron Spectrosc. Relat. Phenom. **117-118**, 469 (2001).
[5] P. Segovia, D. Purdie, M. Hengsberger, and Y. Baer, Nature (London) **402**, 504 (1999).
[6] R. Losio, K. N. Altmann, A. Kirakosian, J. L. Lin, D. Y. Petrovykh, and F. J. Himpsel, Phys. Rev. Lett. **86**, 4632 (2001).
[7] I. K. Robinson, P. A. Bennett, and F. J. Himpsel, Phys. Rev. Lett. **88**, 096104 (2002).
[8] D. Sánchez-Portal and R. M. Martin, Surf. Sci. **532-535**, 655 (2003).
[9] D. Sánchez-Portal, S. Riikonen, and R. M. Martin, Phys. Rev. Lett. **93**, 146803 (2004).
[10] J. R. Ahn, H. W. Yeom, H. S. Yoon, and I. W. Lyo, Phys. Rev. Lett. **91**, 196403 (2003).
[11] D. Sánchez-Portal, J. D. Gale, A. García, and R. M. Martin, Phys. Rev. B **65**, 081401(R) (2002).
[12] K. N. Altmann, J. N. Crain, A. Kirakosian, J. L. Lin, D. Y. Petrovykh, F. J. Himpsel, and R. Losio, Phys. Rev. B **64**, 035406 (2001).
[13] H. W. Yeom, J. R. Ahn, H. S. Yoon, I. W. Lyo, H. Jeong, and S. Jeong, Phys. Rev. B **72**, 035323 (2005).
[14] J. A. Lipton-Duffin, J. M. MacLeod, and A. B. McLean, Phys. Rev. B **73**, 245418 (2006).
[15] T. Nagao, S. Yaginuma, T. Inaoka, and T. Sakurai, Phys. Rev. Lett. **97**, 116802 (2006).
[16] I. Barke, F. Zheng, T. K. Rugheimer, and F. J. Himpsel, Phys. Rev. Lett. **97**, 226405 (2006).
[17] T. K. Rugheimer, T. Fauster, and F. J. Himpsel, Phys. Rev. B **75**, 121401(R) (2007).
[18] S. Riikonen and D. Sánchez-Portal, Phys. Rev. B **76**, 035410 (2007).
[19] I. Barke, F. Zheng, S. Bockenhauer, K. Sell, V. v. Oeynhausen, K. H. Meiwes-Broer, S. C. Erwin, and F. J. Himpsel, Phys. Rev. B **79**, 155301 (2009).
[20] C. Tegenkamp, T. Ohta, J. L. McChesney, H. Dil, E. Rotenberg, H. Pfnur, and K. Horn, Phys. Rev. Lett. **100**, 076802 (2008).
[21] J. A. Lipton-Duffin, A. G. Mark, J. M. MacLeod, and A. B. McLean, Phys. Rev. B **77**, 125419 (2008).
[22] J. N. Crain, A. Kirakosian, K. N. Altmann, C. Bromberger, S. C. Erwin, J. L. McChesney, J. L. Lin, and F. J. Himpsel, Phys. Rev. Lett. **90**, 176805 (2003).
[23] P. Starowicz, O. Gallus, Th. Pillo, and Y. Baer, Phys. Rev. Lett. **89**, 256402 (2002).
[24] P. C. Snijders, S. Rogge, and H. H. Weitering, Phys. Rev. Lett. **96**, 076801 (2006).
[25] Takeshi Inaoka and Tadaaki Nagao, Mater. Trans. **48**, 718 (2007).
[26] J. R. Ahn, P. G. Kang, K. D. Ryang, and H. W. Yeom, Phys. Rev. Lett. **95**, 196402 (2005).
[27] J. N. Crain, J. L. McChesney, Fan Zheng, M. C. Gallagher, P. C. Snijders, M. Bissen, C. Gundelach, S. C. Erwin, and F. J. Himpsel, Phys. Rev. B **69**, 125401 (2004).
[28] J. N. Crain, M. D. Stiles, J. A. Stroscio, and D. T. Pierce, Phys. Rev. Lett. **96**, 156801 (2006).
[29] H. Okino, I. Matsuda, R. Hobara, S. Hasegawa, Y. Kim, and G. Lee, Phys. Rev. B **76**, 195418 (2007).
[30] S. Riikonen and D. Sánchez-Portal, Phys. Rev. B **77**, 165418 (2008).
[31] J. R. Ahn, H. W. Yeom, E. S. Cho, and C. Y. Park, Phys. Rev. B **69**, 233311 (2004).
[32] J. H. Han, H. S. Kim, H. N. Hwang, B. Kim, S. Chung, J. W. Chung, and C. C. Hwang (unpublished).
[33] C. G. Hwang, N. D. Kim, S. Y. Shin, and J. W. Chung, New J. Phys. **9**, 249 (2007).