Real-Space Observation of Screened Potential and Friedel Oscillation by Scanning Tunneling Spectroscopy

Y Hasegawa1,2, M Ono1,3, Y Nishigata1, T Nishio1, and T Eguchi1

1Institute for Solid State Physics, The University of Tokyo, Kashiwa, 277-8581 Japan
2PRESTO, Japan Science and Technology Agency, Japan
corresponding e-mail address: hasegawa@issp.u-tokyo.ac.jp

Abstract. Using scanning tunneling spectroscopy at 5K electrostatic potential profile on the Si(111)$\sqrt{3}$x$\sqrt{3}$Ag surface has been obtained with high spatial and energy resolutions. The potential profile measured around a step edge was explained with the Coulomb potential screened by a two-dimensional electron system which intrinsically exists on the surface. Friedel oscillation, which is characteristic to the screening, was also observed in the potential images. Its shape and phase were discussed in comparison with those of standing waves.

1. Introduction

When an electrical charge is situated in an electron gas, Coulomb potential originating from the charge is modified and reduced by the electrons in the gas. The effect called screening is one of the fundamental phenomena in condensed matter physics, playing an important role in various electronic behaviors in materials [1]. In metals, the original long-range $1/r$ potential is modified into short-range $\exp(-r/\lambda)$ by the screening, where the decay length $\lambda$ is $\approx 0.1$ nm. The short decay of the potential is the reason why valence electrons in metals can behave like free electrons. On the Si(111)$\sqrt{3}$Ag surface (hereafter we call $\sqrt{3}$Ag surface), which has a two-dimensional electron system (2DES) in an energy gap of the semiconductor substrate, the screening effect is weaker than metals since electrons are mobile only in a 2D plane. It reduces the Coulomb potential into $1/r^3$, still long-range [2]. It is, therefore, possible to observe the screened potential using scanning probe microscopy. In this paper, we first explain a method for measuring electrostatic potential profiles on the surface using scanning tunneling spectroscopy (STS) and then demonstrate a real-space observation of the screened potential and Friedel oscillation [3]. The oscillation in the potential is intrinsic to the screening and has a period of the half Fermi wavelength of the 2DES on the surface.

2. Results and discussion

2.1 surface potential measurement

When the electrostatic potential changes on a surface, energy levels of all surface electronic states shift accordingly. Therefore, by measuring an energy level of one of the states we can measure the surface potential [4]. In fact, on the $\sqrt{3}$Ag surface, the potential change was measured by photoemission spectroscopy (PES) [5]. The PES study reported that a small amount of Ag deposition (< 0.02ML) on the surface shifts energy levels of the whole surface states to the higher binding energy side and that...
the shift can be explained with the potential shift due to the charge transfer from the deposited Ag atoms to the surface. While PES provides us the potential change averaged over the surface, STS on the surface states allows us to measure the potential locally and to make its images with high spatial resolution. It should be noted here that Morgenstern et al. [6] also successfully obtained a potential mapping on cleaved InAs(110) surface. They measured the potential variation from an energy level of the confined states in the tip-induced quantum dot.

The STS measurements were performed with an ultrahigh vacuum low-temperature scanning tunneling microscope (LT-STM) with the tip and sample cooled at 5K [5, 7]. Two-dimensional tunneling spectroscopy (2DTS), namely, a measurement of a tunneling spectrum at every point during the STM scanning, was carried out for the potential mapping. The sample was prepared by a deposition of 1ML Ag on the clean Si(111) 7x7 surface and anneal at ~ 600 °C. It was characterized with STM observation as shown in Fig. 1(a).

2.2 a potential profile near a step edge
In Fig. 1, (a) STM image on the √3 Ag surface and (b) simultaneously obtained differential tunneling conductance (dI/dV) image are presented. The dI/dV image clearly shows standing wave pattern originating from the 2DES on the surface. In its Fourier transformed (FFT) image (Fig. 1(c)), a circular pattern is observed, as well as the hexagonal √3×√3 spots, indicating an isotropic energy dispersion of the 2DES. The sequential FFT patterns of the dI/dV images taken at various energy levels reveal that the states have a parabolic dispersion (Fig. 1(d)), implying a free-electron-like nature of the 2DES. We found that the binding energy of the 2DES depends on the sample preparation method, ranging from +0.1 eV to -0.3 eV with respect to the Fermi energy. In an analysis of the screened potential, therefore, the values of the binding energy and Fermi wavelength measured for each surface were used. In the case of Fig. 1, the

Fig. 1: (a) STM image on the √3 Ag surface and (b) dI/dV image. sample bias voltage Vs: 0.8V, tunneling current It: 200pA, area: 30nm×30nm, temperature: 5K. (c) A FFT mapping of (b). A ring located at the center originates from the standing wave pattern. Six spots arise from periodicity of the √3Ag structure. (d) A cross-sectional image of a stack of the FFT mappings. From fitting with a parabolic curve shown in a red line the effective mass (0.13 m_e) and the binding energy (0.1eV above the Fermi energy) were obtained.

Fig. 2. (a): an STM image (40×40nm²) on the √3Ag surface. (b) A series of tunneling spectra taken in the rectangular area of (a) are shown in a color-coded manner. (c): the peak energy shift as a function of distance from the step edge (black dots). It can be fitted well by the calculated screened potential (red solid line). Blue dotted line depicts topograph indicating the step position.
energy level of the states is above the Fermi level and therefore 2DES is not formed.

We measured the potential around a step edge, at which excess Ag atoms are accumulated and thus one-dimensional positively-charged array is formed. In Fig. 2(b), color-coded tunneling spectra (normalized \(dl/dV\)) are drawn in an order of distance from the step edge. In the differential spectra, a strong peak is found at a binding energy of 0.85 eV, which corresponds to S\(_2\)/S\(_3\) states observed by PES [5]. As the measured site approaches to the step edge, the peak energy shifts downwards to the higher binding energy side. In fact, not only the main peak, another peak around 0.5 eV and other small features observed in the spectra also shift with the distance keeping energy separations rigidly. This is due to the potential variation induced by the charges at the step edge.

On the 0.85 eV peaks, a small modulation is found in its intensity. This is due to a modulation of density of states within a unit cell of the \(\sqrt{3}\)Ag structure. In fact, in the potential measurement the peak energy level should be compared at the same site of the unit cell since the peak energy and intensity may change depending on a site in the unit cell. This means that the spatial resolution of this potential measurement is limited by the size of the unit cell.

The potential profile measured from the main surface states (0.85 eV) is drawn with black dots in Fig. 2(c). We first noticed that the profile does not look like a simple Coulomb potential and then found a small wiggling in the profile, whose wavelength is similar to that of the standing waves at the Fermi level. Based on these findings we presumed this is due to the screening by the 2DES on the surface. In order to confirm the presumption, we calculated a profile of the screened potential using a linear response theory proposed by Lindhard and compared it with the experimental result.

### 2.3 screened potential

In order to calculated the screened potential it is necessary to obtain a dielectric function of 2DES [2, 8]. The static dielectric function \(\varepsilon(q)\) at zero temperature was obtained from a polarization function of 2DES; a response function of charge density to external electrical field. The polarization function can be calculated by a perturbation theory assuming a linear response of the charge density to the field. According to a formulation of Lindhard, the dielectric function of the 2DES can be written as following [8]:

\[
\varepsilon(q) = \left\{ \begin{array}{ll}
1 + \frac{q\pi}{q} & q \leq 2k_F, \\
1 + \frac{q\pi}{q} \left\{ 1 - \left[ 1 - \left( \frac{2k_F}{q} \right) \right]^{1/2} \right\} & q > 2k_F,
\end{array} \right.
\]

where \(q_{TF}=m^*/2\pi\varepsilon_0\), \(k_F\) is the Fermi wavenumber of the 2DES, and \(m^*\) is an effective mass of the 2DES electrons.

The Fourier transform of the screened potential \(V_{SCR}(q)\) is then given by dividing the Fourier transformed Coulomb potential \(v_{2D}(q)=e^2/2\varepsilon_0\varepsilon_0q\) by \(\varepsilon(q)\). The screened potential can, then, be calculated by the inverse Fourier transformation of \(V_{SCR}(q)=v_{2D}(q)/\varepsilon(q)\). By integrating it in the cylindrical coordinates the potential becomes [2]

\[
\phi(r) = \frac{1}{4\pi} \int_0^{2\pi} d\theta \int_0^\infty e^{iqr \cos \theta} V_{SCR}(q) dq = \frac{1}{2\pi} \int_0^\infty q V_{SCR}(q) J_0(qr) dq
\]

using the zeroth-order Bessel function \(J_0\), which satisfies the following equation:

\[
\int_0^{2\pi} e^{iqr \cos \theta} d\theta = 2\pi J_0(qr).
\]

Since the last formula cannot be solved analytically, we numerically calculated to obtain the screened potential around a single charge, and then integrated the single-charge potential to obtain a potential profile around the linearly charged step edge. The result is drawn with a solid line in Fig. 2(c), in good agreement with the experimental result. The only fitting parameter is a scaling factor of the potential, which is proportional to the linear charge density at the step edge. The estimated value of the charge density was obtained from the fitting.
2.4 potential images and the Friedel oscillation

From the energy level of the S_{2}/S_{3} states, we can make a mapping of the potential variation over the surface. An example of the potential image is shown in Fig. 3(b). The image clearly demonstrates the lowered potential not only near step edges but also around Ag adsorbates (dark triangles found in the corresponding STM image shown in Fig. 3(a)). A weak oscillatory pattern, whose period is equal to the half Fermi wavelength of the 2DES, is visible in the potential image. This is the Friedel oscillation, which originates from a sharp cutoff at $2k_F$ in the 2DES dielectric function. It should be mentioned here that the image does not render the potential correctly inside the island since extra states, probably states due to confinement by the island, are found there, making the peak energy measurement difficult.

The Friedel oscillation is often mixed up with the standing waves, which are also observed on the surface (see Fig. 1(b)). After the first observation of the standing waves [9, 10], they are also called energy-resolved Friedel oscillation since the sum of the standing waves from the bottom energy to the Fermi level should be equal to the Friedel oscillation [11]. As shown in Fig. 3(c), however, the shape and peak positions (phase) are different between the two oscillations. In fact, various surface phenomena, such as the surface-state-mediated adatom-adatom or adatom-step interactions [12–15], were discussed in relation to the standing waves since their characteristic distances seem to be related to the Fermi wavelength. Obviously the modulated potential affects the interactions and thus should be included in their analyses. The potential should also play an important role in electrical conductance at surface steps, which was recently reported on the $\sqrt{3}$Ag surface [16]. Investigation of the surface potential and its real-space imaging are therefore quite important to understand these nanoscale and atomistic phenomena on the surfaces.

3. Conclusion

In this paper, we have demonstrated that the surface potential of the $\sqrt{3}$Ag surface can be measured with 2DTS from the peak energy of surface states. From the potential mapping, we found that the potential was lowered around step edges. The reduced potential is explained with the screening by the 2DES on the surface. The Friedel oscillation was, for the first time, observed in the potential mapping. The sub-nanometer scale measurement of surface potential is quite important to understand the behaviors of the surface 2DES and various surface phenomena affected by the potential.
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