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IMAGE QUALITY OF STM AND APEX PROFILE OF A SCANNING TIP

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Abstract - Variations of the topographic images by scanning tunneling microscopy (STM) and dual-polarity tunneling imaging (DPTI) and the current images of current imaging tunneling spectroscopy (CITS) with bias voltages were examined. While DPTI shows the normal image depicted by a single apex atom for the specimen voltage of -2V, the image at +2V is occasionally a double tip image. Furthermore, the current image by CITS for -2V often exhibits the reversed contrast grey-scale images with bright corner holes of the unit cell of the Si(111)-(7x7) reconstructed structure. The observed variation of the images with bias voltages is explained as a result of the difference in the effective tunneling barrier and the surface state density of the tip apex and specimen, and also as the effect of the atomic arrangement and composition and profile of the tip apex.

1 - INTRODUCTION

Application of the scanning tunneling microscopy (STM) has been extended to the scanning tunneling spectroscopy (STS) to investigate the electronic states of an individual surface atom. Becker et al. studied the variation of the surface states with the atomic positions of the Si(111)-(7x7) surface2/ and Hamers et al. exhibited the directly interpretable images of the electronic structure of the Si(111)-(7x7) surface and developed a new STS method called current imaging tunneling spectroscopy (CITS)/3,4/. An interesting finding is the reversed contrast image with the bright corner holes and is explained as the result of the tunneling current from the exposed dangling bonds in the corner holes. The variation of the current image by the polarity of the bias voltages, known as dual-polarity tunneling imaging (DPTI), was also examined/5, 6/ but no reversed image was observed. Accordingly, the purpose of this study is to clarify the cause of image variation with bias voltages utilizing CITS and DPTI techniques.

2 - EXPERIMENTAL

An ultrahigh vacuum STM was employed./7/ The STM was operated in the vacuum of 1~2X10^-10 Torr. A (111)-oriented W single crystal filament was electrochemically polished to form a scanning tip. The sharpness and cleanliness of the tip apex were inspected by observing field emission images projected on the screen installed in the STM chamber. The tips were heated and cleaned by electron bombardment and sharpened by the build-up effect of the W(111) plane./8/ A P-doped n-Si(111) wafer with the resistivity of ~0.01Ω cm was cut into rectangular pieces ~5mm X 15 mm as a specimen, etched by the Shiraki method.
/, and then resistively heated at 500-600°C for several hours and finally flashed at ~1100°C in the STM.

Topographic STM images were depicted passing a constant tunneling current in the range of 0.2~1 nA and applying +2V to the specimen. One frame of the image was formed by 256×128 pixels and a grey-scale image was obtained by expressing the vertical position of each pixel with 256 grey steps. The scanning time of one frame was 30~60 sec.

DPTI images were obtained by the constant current mode and each raster line was scanned twice successively switching the specimen bias voltage from +2V to -2V and vice versa. The feedback signal monitoring the tip position was held while the voltage switching to avoid a tip-specimen contact. The dual scanning for DPTI requires the scanning time twice that of the STM scanning.

In the case of CITS the tip scanned over the specimen surface, keeping the tunneling current constant, and I-V curves were obtained at each pixel varying the sampling voltages 128 steps from +2V to -2~3V while fixing the tip-specimen separation. One frame of the CITS image was formed by 64×64 pixels and took ~90 sec to acquire ~1 MB of data. The electronic state density of a specimen surface was obtained by calculating \((dI/dV)/(I/V)\) from the I-V curve.

3 - RESULTS

Since the tunneling current is constant for DPTI, the depicted images of the Si(111)-(7×7) surface applying the bias specimen voltages with respect to the tip \(V_s=+2V\) and -2V are topographic and both images are fundamentally identical, exhibiting the bright Si adatoms of the reconstructed structure and the dark corner holes of the unit cell of the (7×7) structure/10/. However, the DPTI image \(V_s=-2V\) exhibited adatoms in the faulted half of the unit cell slightly brighter and the net of the dimer lines is darker and wider than the other half reflecting the electronic state of the Si surface. An interesting finding is the difference in the specimen-tip gaps for \(V_s=+2V\) and -2V. The tip for \(V_s=-2V\) scans closer to the specimen surface by about 0.9A than for \(V_s=+2V\) indicating a larger tunneling barrier and a lower electronic state density for the Si surface.

The current image of CITS at the bias voltage for scanning is monotonous and no grey-scale image is exhibited because the tunneling current is monitored at a constant level. Thus, the CITS image at the bias voltage of the specimen \(V_s=+2V\), Fig. 1(a), is topographic and quite similar to the DPTI images. The current image at \(V_s=-1.9V\), Fig. 1(b), is also very similar to the topo-

![Fig. 1 - CITS images of Si(111)-(7×7) surface. (a) Topographic constant current image at \(V_s=+2V\). \(I_t=0.2nA\). (b) Current image for \(V_s=-1.9V\).](image)

graphic DPTI image at $V_s = -2V$. The confusing point of CITS is the frequent appearance of misleading current images, as shown in Figs. 2(a) and (b). The images were obtained using the same tip and specimen under experimental conditions identical to those used for obtaining Fig. 1. While Fig. 2(a) exhibits the normal $(7 \times 7)$ structure as Fig. 1(a), Fig. 2(b) is the completely reversed grey-scale image of Fig. 2(a) with bright corner holes. Hamers et al. observed the similar reversed grey-scale image and explained it as the result of tunneling from the dangling bond in the corner hole and the regions surrounding the adatoms where Si-Si backbonds and additional Si-Si bonds exposed to the vacuum/4/.

![Fig. 2 - CITS images of Si(111)-(7x7) structure. (a) Topographic constant current image at $V_s = +2V$. $I_t = 0.5$ nA. (b) Current image for $V_s = -2V$. The image contrast is the reversal of (a). The probed depth of the corner holes 0.8Å on the average is slightly deeper than that for Fig. 1(a), 0.7Å.]

4 - DISCUSSION

The observed normal, Fig. 1(b), and reversed, Fig. 2(b), CITS current images are very contradictory because the images are obtained through experiments repeated under identical conditions. The contradictory images also imply that the reversed image can not be attributed to the tunneling from the exposed Si atoms of the atomic layers lower than the adatom layer. Stroscio et al. explained the image reversibility of the Si(111)-(2x1) surface as the result of the exponential variation of the tunneling current with bias voltage/11/. Although their explanation is fairly persuasive, their experiment was conducted in a rather narrow voltage range from $V_s = +1.5V$ to $+0.34V$ and no inverted voltage was examined. Accordingly, the study revealed only the tunneling characteristics from the tip apex to the specimen surface and might not be appropriate for clarifying the reason for the image reversal caused by the reversed tunneling direction.

Reversed image contrast was also observed for the Si(111)-($\sqrt{3} \times \sqrt{3}$)Ag structure and explained as the effect of adsorption of a strongly electronegative atom at the tip apex/12/. Although the proposed model explains the reversed contrast successfully, the model is not applicable for the present DPTI study in which no reversed image has been observed.

One probable explanation is the difference in the degree of corrugation depicted by a scanning tip apex for positive and negative bias voltages reflecting the surface electronic state density of the tip apex and specimen. One evidence to support this explanation is the grey-scale image of the Si(111)-$(7 \times 7)$ surface with bright and dark half unit cells for $V_s = -2V$ due to the difference in the electronic states of the faulted and unfaulted halves.
Figure 3 illustrates the traces of the scanning tip for $V_s = 2V$ and the contours which give constant tunneling currents from the Si surface for $V_s = -2V$. Since the peaks and valleys of the traces and contours coincide well, the grey-scale DPTI images of either voltage polarities are very similar. Note that the constant current contours, solid lines in Fig. 3, represent the trace for DPTI at $-2V$. Accordingly, the trace of the scanning tip of DPTI is different depending on the polarity of the bias voltage. In the case of CITS, the tip follows the trace of the DPTI bias voltage $V_s = 2V$ and the variation of tunneling current with bias voltages is recorded at each pixel while holding the tip position on the trace.

The solid lines in Fig. 3 represent the contours of the tunneling current from the Si surface which decreases exponentially and becomes flatter as the distance from the Si surface increases in the order from $I_1$ to $I_4$. Then, the tunneling current for $V_s = -2V$ flows from the Si surface and is smaller at the corrugation peak of the trace A-A of Fig. 3 than at the valley because the peak of the trace is higher than the contour $I_2$ and the valley is closer to the specimen surface than $I_3$ and the tunneling current there is larger than $I_2$. Consequently, the grey-scale CITS current image for $V_s = -2V$ is the reversed image of the constant current image at $V_s = +2V$.

When a single apex atom is sitting on a wide, flat substrate layer, the cone angle of the tip apex is large and the trace of the constant current is less corrugated, as indicated by the trace B-B of Fig. 3, and flatter than the constant current contours $I_2$. Then, the tunneling current from the specimen is large at the peak of the trace B-B and small in the valley because the trace B-B is lower than $I_2$ at the peak and higher in the valley. Accordingly, the CITS current image for $V_s = -2V$ exhibits the same image contrast as the DPTI image for $V_s = +2V$. Consequently, the reversed image of Fig. 2(b), Fig. 4, is very similar to Fig. 2(a). This implies that the reversed contrast image, Fig. 2(a) is not formed by the tunneling electrons from the dangling bond in the corner hole and the regions where Si-Si bonds exposed to the vacuum.

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Fig. 3 - Schematic representation of the traces of a scanning tip apex for constant current imaging at $V_s = +2V$, dashed lines A-A and B-B, and the contours of the constant current tunneling from the specimen Si surface, solid lines $I_1$, $I_2$, $I_3$, and $I_4$, for $V_s = -2V$. $I_1 > I_2 > I_3 > I_4$.

DPTI images are also affected by the apex profile, occasionally exhibiting the image which is very similar to the image depicted by two apex atoms 4.5 Å apart/13/ for $V_s = 2V$, Fig. 5(a). Peculiarly the regular reconstructed structure was imaged for $V_s = -2V$, Fig. 5(b). The superposition of Fig. 5(a) on Fig. 5(b) clearly indicates that only one apex atom is participating in the
depiction of Fig. 5(b) and the trace for $V_s = -2V$ is about 0.8Å closer to the specimen surface. Park et al. also observed the polarity dependent DPTI images and interpreted the observed images as the result of two protruding chemically different apex atoms\cite{14}. In their case, the double tip image was observed for $V_s = -2V$ and explained as the result of an adsorbed Si atom which had a high density of states above the Fermi level $E_F$ and participated in the tunneling as one of the two apex atoms. On the contrary, the double tip image was observed at $V_s = 2V$ for the present study implying that one of the apex atoms had the filled states below $E_F$. Such a situation can be realized by the adsorption of a hydrogen atom to one of two W apex atoms separated by 4.5Å, the nearest W atom distance on the W(111) plane. Then, both W atoms participated in tunneling for $V_s = 2V$, depicting the double tip image because adsorbed hydrogen provides the energy state of $\sim$1 eV below $E_F$ around a nearby W atom\cite{15} and only the hydrogen-free W apex atom receives the tunneling electrons from the specimen Si surface for $V_s = -2V$ showing the regular reconstructed structure.
5 - CONCLUSION

The double tip image and no reversed contrast image for DPTI and the bright faulted half of the unit cell of the Si(7x7) structure and the reversed image for CITS clearly indicate that the constant current images by DPTI and the current images by CITS strongly depend on the electronic state of the uppermost atomic layer of the specimen, the arrangement and composition of the apex atoms and the profile of the tip end. The observed images also imply that the tunneling electrons from the specimen surface are emitted from the Si adatoms forming the uppermost surface layer and the contribution of the Si atoms exposed to the vacuum below the adatoms and the dangling bonds in the corner holes is negligibly small. The observed variation of DPTI and CITS images with the atomic arrangement and chemical composition of the tip apex strongly recommends to inspect the apex with a field ion microscope/16,17/and the analyzing of the apex composition with an atom-probe/18,19/. Characterization of the apex geometry and chemical property would greatly improves the reliability of the STS study and the reproducibility of the STM observation.