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Spin-polarized scanning tunneling microscopy and spectroscopy study of $c(2\times2)$ reconstructed Cr(001) thin film surfaces

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Spin dependent electronic properties of $c(2\times2)$ Cr(001) thin film surfaces grown on MgO(001) substrates are investigated by means of spin-polarized scanning tunneling microscopy and spectroscopy. An averaged dI/dV spectrum obtained on the $c(2\times2)$ Cr(001) thin film surfaces exhibits a surface state around +0.1 eV above the Fermi level. The intensity of the surface state peak in the spectra measured on (001) terraces is alternately varied whenever a monatomic step is crossed. Therefore, the shifted surface state as well as an original one on (1×1) Cr(001) surfaces has spin-polarized feature. © *2006 American Institute of Physics*. [DOI: 10.1063/1.2173634]

I. INTRODUCTION

Now spin-polarized scanning tunneling microscopy and spectroscopy (SP-STM/STS) with magnetic tips were well established as techniques for investigation of surface magnetism with nanoscale.[1] SP-STM/STS make it possible to reveal correlation between topographic, electronic, and magnetic properties using spin-polarized surface states.[2–5] A bcc-Cr(001) surface with a (1×1) structure exhibits a surface state at 0.05 eV below the Fermi level.[6] Furthermore, band structure calculations predicted that the surface state is highly spin polarized due to its origin from minority spin band.[6] Kleiber *et al.* revealed that tunneling current via the surface state is spin polarized by means of SP-STM/STS and that the clean Cr(001) surfaces show topological antiferromagnetism, which means that adjacent (001) terraces separated by a monatomic step are magnetized antiferromagnetically.[7]

However, many results with SP-STM/STS are obtained on the only clean surface. The surface state is easily modified by surface structures, e.g., steps, adsorbed atoms, defects, and surface reconstructions. Therefore, it is a very interesting issue to investigate how the spin-polarized surface states are influenced by the surface structures. Recently, we have demonstrated that $c(2\times2)$ reconstructed Cr(001) thin film surfaces grown on MgO(001) substrates exhibit a surface state at 0.1 eV above the Fermi level.[8]

In this paper, we report on spin dependent electronic properties of the surface state observed on the $c(2\times2)$ reconstructed Cr(001) thin film surfaces with SP-STM/STS.

II. EXPERIMENTAL PROCEDURE

As a substrate of the Cr(001) thin films, a commercially available MgO(001) single crystal (Furuuchi Chemical, purity: 99.9%) was used. Soon after cleavage, the MgO(001) substrate was introduced into an ultrahigh vacuum (UHV) system.[9] In vacuum the cleaved MgO(001) substrate was degassed at 600 K for more than 3 h. And then the substrate was flashed at 1200 K for 1 min in order to remove surface contaminants. Preparation procedure of the cleaved MgO(001) substrate has been described in Ref. 8 in detail.

The Cr thin films were grown on the cleaved MgO(001) substrates at room temperature (RT) and at a growth rate of 0.1 nm/min up to 10 nm in thickness. During the deposition, reflection high energy electron diffraction (RHEED) patterns of the thin films have never indicated halo ones. Furthermore, the RHEED observations revealed that the Cr thin films grew on the cleaved MgO(001) substrates with an epitaxial relationship of [110](001)bcc-Cr//[100](001)MgO.[10] Following the deposition, the Cr(001) thin films were annealed at 600 K for 1 h. Figures 1(a) and 1(b) show RHEED patterns of the Cr(001) thin films obtained in the MgO[100] and MgO[110] directions, respectively. The RHEED pattern of the annealed Cr(001) thin films taken in the MgO[100] direction showed a twofold periodicity as shown in Fig. 1(a). On the other hand, the RHEED pattern in the MgO[110] direction in Fig. 1(b) did not show any periodicities except for the onefold one. Moreover, a low energy electron diffraction pattern of the Cr(001) thin films demonstrably indicated a $c(2\times2)$ reconstruction.[8]

STM/STS measurements were performed in a constant current mode at RT with electrochemically etched W tips. Preparation and cleaning procedures of the W tips have been described in detail elsewhere.[11] SP-STM/STS measurements were carried out at RT with Fe-coated W tips. After electron-beam bombardment of a W tip under UHV, Fe thin films were deposited on the tip up to 4 nm at RT. Subsequently the

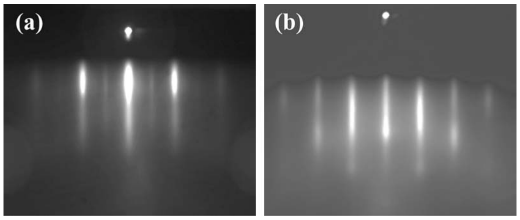

FIG. 1. RHEED patterns of the Cr(001) thin films. (a) and (b) were taken in the MgO[100] and MgO[110] directions, respectively.

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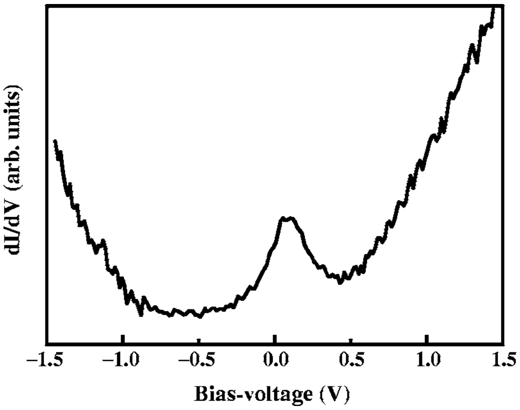

FIG. 2. Averaged dI/dV spectrum taken on the $c(2\times2)$ Cr(001) thin film surfaces with the W tip.

Fe-coated W tip was annealed at 600 K for 30 min. Differential conductivity (dI/dV) spectra were obtained by means of the phase-sensitive detection technique with an ac modulation voltage of 20 mV at frequencies of 8–12 kHz applied to the gap voltage.

III. RESULTS AND DISCUSSION

Figure 2 shows an averaged dI/dV spectrum taken on the $c(2\times2)$ reconstructed Cr(001) thin film surfaces with the W tip. In the dI/dV spectrum, an intense peak corresponding to the surface state was observed around +0.1 eV above the Fermi level. However, surface state energy observed on the $c(2\times2)$ Cr(001) thin film surfaces is higher than that on the (1×1) Cr(001) surfaces, which is about −0.05 eV.[6,7,12,13]

Many groups reported on the origins of the surface state shift. Impurity atoms, e.g., carbon and oxygen, included in bcc-(001) surfaces shift the surface state energy.[14,15] Other origin is that confinement effect induced by surface atomic arrangements gives rise to the surface state shift. Biedermann *et al.* showed that one-dimensional localization of Fe atoms, which was surrounded by Si atoms on FeSi(001) surfaces, induced surface state shift from 0.3 to 0.6 eV above the Fermi level.[16] Schmid *et al.* revealed that the surface state at about −0.06 eV shifted upward to about +0.1 eV on $c(2\times2)$N/Cr(001) surfaces.[12] We demonstrated that energy shift of the surface state from +0.17 to +0.43 eV was observed on $c(2\times2)$ Fe(001) thin film surfaces.[17]

To investigate chemical species making the $c(2\times2)$ structure on the Cr(001) thin film surfaces, Auger electron spectroscopy (AES) measurements were performed. An AES spectrum (not shown here) indicated existence of carbon and oxygen atoms in addition to Cr atoms. Since there is a possibility that both of the carbon and oxygen atoms make the $c(2\times2)$ structure on the Cr(001) surfaces,[18,19] the $c(2\times2)$ structure on the Cr(001) thin film surfaces would be composed by carbon and/or oxygen atoms.

Two dI/dV spectra taken on the $c(2\times2)$ Cr(001) thin film surfaces using the Fe/W tip are shown in Fig. 3. Each black and gray spectrum was measured on each adjacent terrace separated by a monatomic high step. Both dI/dV spectra exhibited a distinct peak around +0.1 eV above the Fermi level, which is the almost same energy level as the peak position observed with the W tips shown in Fig. 2. However, the intensity of the peaks in Fig. 3 was apparently different. One possibility is to assume that the different intensity results from spin-polarized tunneling between the magnetically in-plane sensitive Fe/W tip and antiferromagnetic coupling Cr(001) terraces.[7] Another possibility is that it originates from different chemical species, carbon or oxygen atoms.[15] However, the latter one is excluded since the difference of the chemical species must lead to that of the surface state energy as well as the peak intensity.

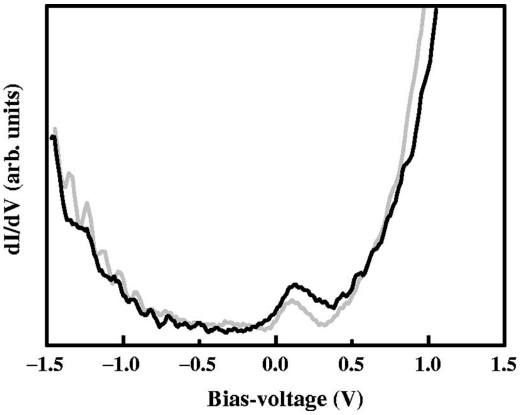

FIG. 3. Averaged dI/dV spectra taken with the Fe/W tip. The two spectra were taken on different terraces separated by a monatomic high step at a sample bias voltage of −0.4 V.

Figures 4(a) and 4(b) indicate STM and dI/dV images of the $c(2\times2)$ Cr(001) thin film surfaces with the Fe/W tip, respectively. To investigate correlation between the difference of the peak intensity and surface structures, the two images were simultaneously obtained on the same scan area. The STM image was taken at a sample bias voltage of −0.2 V, where there is no feature in both dI/dV spectra shown in Fig. 3. The dI/dV image was taken at a sample bias voltage of +0.1 V, where the surface state of the $c(2\times2)$ Cr(001) thin film surfaces exists. Therefore, the STM and the dI/dV images would be independently obtained.

The STM image shown in Fig. 4(a) indicates that the $c(2\times2)$ Cr(001) thin film surfaces have a step-terrace based structure. The terraces labeled with **A** and **B** are neighbor terraces separated by a step. Figure 4(c) shows a cross-sectional line profile taken along a dashed white line as marked in Fig. 4(a). The line profile crosses over three terraces, **A**,**B**, and another **A**. The step height separating the terraces **A** and **B** is about 0.14 nm, which is in good agreement with monatomic step height, 0.144 nm. In the dI/dV image shown in Fig. 4(b), dark and bright areas are distinguished, which correspond to areas exhibiting small and large intensities of the surface state peak in the dI/dV spectra, respectively. As compared with the STM image, the terraces labeled with **A** in the dI/dV image are clearly imaged darker than those with **B**. Moreover, the step areas indicated by the white arrows in Fig. 4(b) are imaged further darker than the label **A** terraces. This is attributed to the absence of the surface state as shown in Fig. 5. Figure 4 reveals that the surface state peak intensity on the $c(2\times2)$ Cr(001) thin film surfaces is alternately changed in every terrace separated by

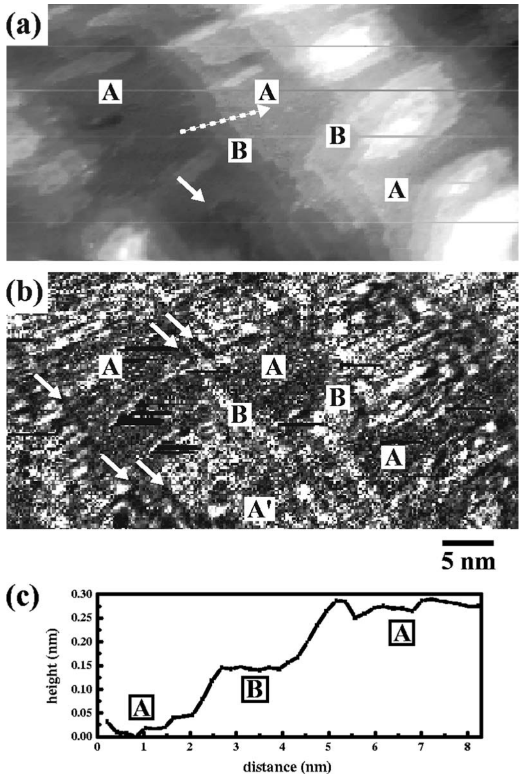

FIG. 4. STM and dI/dV images of the $c(2\times2)$ Cr(001) thin film surfaces with the Fe/W tip. (a) STM image obtained in constant current mode. Labels **A** and **B** indicate adjacent terraces separated by a monatomic high step. A white arrow shows a screw dislocation. $V_s=-0.2$ V, $I_T=0.5$ nA, 25×50 nm^2. (b) dI/dV image simultaneously taken with (a) at a sample bias voltage of +0.1 V. The white arrows indicate monatomic high step lines. (c) Cross-sectional line profile taken along the dashed white line indicated in (a).

the monatomic high step, as is the case with the (1×1) Cr(001) surfaces.[7] This result leads to the conclusion that the shifted surface state on the $c(2\times2)$ Cr(001) thin film surfaces still has spin-polarized nature. However, at the lower middle in Fig. 4(b), it is seen that one terrace exhibits two contrasts, which correspond to areas around labels **A** and **A**′. Kleiber *et al.* and Kawagoe *et al.* reported that domain walls were formed by spin frustration around a screw dislocation.[7,13] A screw dislocation exists as marked by a white arrow in Fig. 4(a). Therefore, the contrast change between labels **A** and **A**′ would originate from the same reason.

IV. CONCLUSION

SP-STM/STS measurements were performed on the $c(2\times2)$ Cr(001) thin film surfaces. The surface state energy observed on the surfaces shifted upward to about +0.1 eV as compared with that on the (1×1) Cr(001) surfaces. The dI/dV image obtained at the shifted surface state energy revealed that the intensity of the surface state peak exhibited alternate change whenever a monatomic high step is crossed. This result clearly shows that the shifted surface state on the $c(2\times2)$ Cr(001) thin film surfaces is still spin polarized.

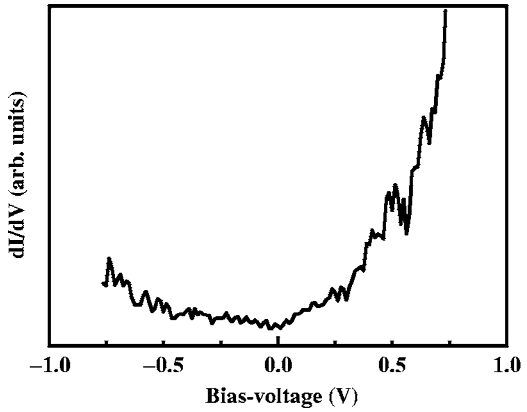

FIG. 5. Averaged dI/dV spectrum taken on the steps with the Fe/W tip. There is no peak corresponding to the surface state.

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