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Surface energy bands of p(1 × 1)Cr(1 0 0) and p(1 × 1)O/Cr(1 0 0)

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Abstract

Angle resolved photoemission spectra have been measured on clean p(1 × 1)/Cr(1 0 0) and p(1 × 1)O/Cr(1 0 0) using a He discharge lamp as an excitation source. The dispersion curves of surface energy bands have been obtained. The results are compared with reported results of the energy band calculation. The measured energy band dispersion curves for the surface states of a clean sample agree well with the calculated bands for the surface state with aligned spins. Some parts of the dispersion curves of the surface bands agree with those of the bulk band. The energy bands observed here appear to be favourable to the surface ferromagnetic state. In case of the sample with adsorbed oxygen, the band dispersion obtained here for the deep band region coincides with the reported data. The bands with binding energies larger than 5 eV are attributed to the O 2p state forming the surface band. The bands within a binding energy of 4 eV from the Fermi level, are ascribed to the bands caused by Cr atoms in the first sub-layer forming the O–Cr bond.

Keywords: Angle resolved photoemission; Energy band dispersion; Antiferromagnetism; Spin density wave; Oxygen adsorption

Physical properties of Cr metal are quite interesting, for it is antiferromagnetic. Since the valence electrons of Cr are itinerant an important question arises: How is the antiferromagnetism generated? Up to the present, general understanding of investigators is that the antiferromagnetism is caused by the formation of spin density waves [1,2]. Spin density waves can exist in Cr owing to the electronic structure near the Fermi level. Hole pockets occur there and this is very important to the solid state properties peculiar to Cr. It should also be remarked that some of the properties are surface sensitive.

Thus, the investigation of the electronic structure of Cr, both bulk and surface, by means of spin polarized photoemission is an attractive subject of solid state physics [3]. In the present report our final goal is the elucidation of the surface magnetism, although this purpose has not yet been achieved.

Experiments were carried out in Photon Factory of KEK. A He discharge lamp was used as the source for exciting photoelectrons. The angular resolution was 0.5° and the total energy resolution was 150 meV. A commercially available single crystal of Cr (1 0 0) was used. Ordinary surface clearing procedures were employed to prepare a clean surface: Ar^+ ion sputtering and heating by electron bombardment. Measurements were performed at a pressure in the range of 10^{-11} Torr. The surface condition was examined by the Auger spectroscopy and LEED pattern analyses. We obtained a sample with adsorbed oxygen by heating the sample at 350 °C in the atmosphere of O_2 gas at a pressure about 1.3×10^{-8} Torr.

Figs. 1 and 2 show photoelectron energy distribution curves (EDC's) of photoelectrons from the clean p(1 × 1) surface of Cr(1 0 0) by excitation at 21.22 eV using He(I) light incident along the (0 1 1) direction. EDC's in Fig. 1 were measured with photoelectron emission angles being varied in the (0 1 0) plane.

Various curves in Fig. 1 correspond to EDC's measured at different emission angle, θ. Ignoring the Umklapp process,

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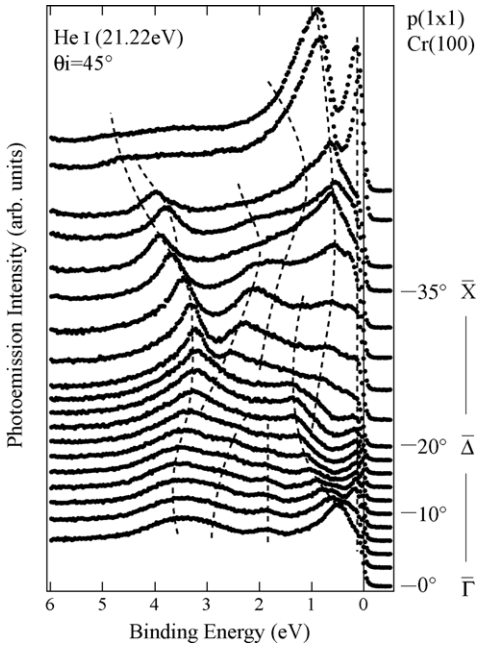

Fig. 1. Angular dependence of EDC's of photoemission from clean p(1 × 1) Cr(1 0 0). The emission angle is varied in the (0 1 0) plane. $k_{||}$ changes along the $\bar{\Delta}$ axis. Excitation light is incident along the (0 1 1) direction on the (0 0 1) surface. Excitation energy is 21.22 eV.

we obtain the component of the electron wave vector, $k_{||}$, parallel to the crystal surface as

$$k_{||} = 0.51(\mathring{A}^{-1})\sqrt{\varepsilon_k(\mathrm{eV})}\sin\theta$$

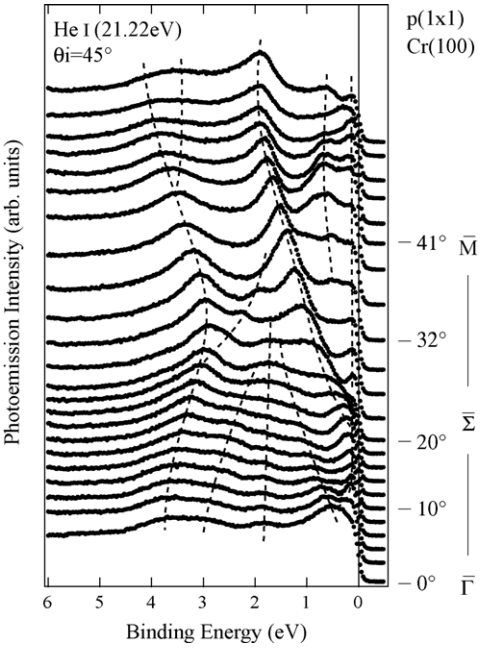

Fig. 2. Angular dependence of photoemission from clean p(1 × 1) Cr(1 0 0). The emission angle is varied in the (1 1 0) plane, $k_{||}$ changes along the $\bar{\Sigma}$ line. Excitation light is incident along the (0 1 1) direction on the (0 0 1) surface. Excitation energy is 21.22 eV.

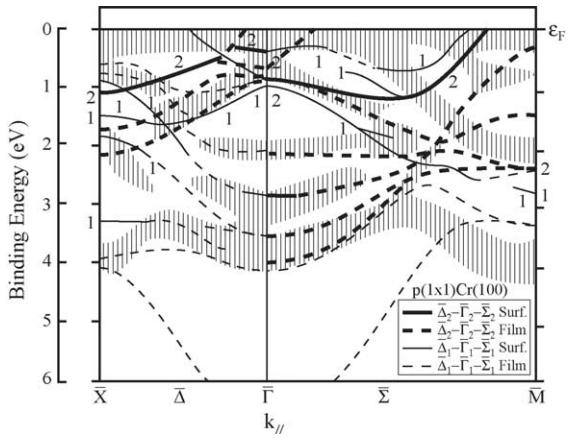

Fig. 3. Comparison of the measured energy bands of Cr(1 0 0) with those calculated by Fu and Freeman [5]. Wide hatched curves are measured $E(k)$ curves. Thick full curves are surface bands calculated along the $\bar{X}_2 - \bar{\Delta}_2 - \bar{\Gamma}_2$ and $\bar{\Gamma}_2 - \bar{\Sigma}_2 - \bar{M}_2$ lines. Thick broken curves are the energy bands calculated along the $\bar{X}_2 - \bar{\Delta}_2 - \bar{\Gamma}_2$ and $\bar{\Gamma}_2 - \bar{\Sigma}_2 - \bar{M}_2$ lines on a thin film consisting of seven layers. Thin full curves represent the surface energy bands calculated along the $\bar{X}_1 - \bar{\Delta}_1 - \bar{\Gamma}_1$ and $\bar{\Gamma}_1 - \bar{\Sigma}_1 - \bar{M}_1$ lines. Thin broken lines represent the energy bands calculated along the $\bar{X}_1 - \bar{\Delta}_1 - \bar{\Gamma}_1$ and $\bar{\Gamma}_1 - \bar{\Sigma}_1 - \bar{M}_1$ lines on a thin film consisting of seven layers. Arabic numbers in the figure distinguish the different symmetric lines or points. All the calculated energy bands are for the majority spin states.

Here ε_k is the photoelectron kinetic energy. The energy dispersion curves of a surface energy band are obtained from pairs of parameters, (ε_B, $k_{||}$). EDC's in Fig. 1 are measured at θ from 0° (normal emission) to 20° at an interval of 2°. For $\theta > 20°$, we measured EDC's at an interval of θ of 3°. With the experimental configuration made here we can trace the energy band dispersion along the $\bar{\Gamma} - \bar{\Delta} - \bar{X}$ direction in the surface Brillouin zone.

Fig. 2 shows EDC's of clean p(1 × 1)Cr(1 0 0) measured in the configuration to trace the energy band dispersion along the $\bar{\Gamma} - \bar{\Sigma} - \bar{M}$ axis. The condition of the measurements is the same as that in the case of Fig. 1 except that emission angles were varied in the $(\bar{1}10)$ plane.

Using the data illustrated in Figs. 1 and 2, the dispersion curves of the surface energy bands are shown by hatched curves in Fig. 3. The widths of hatches illustrate the amounts of the experimental inaccuracy. In the figure, the energy bands calculated by Fu and Freeman are also shown for comparison [5]. Fu and Freeman performed self-consistent all electron local-density-functional calculation of the electronic energy states of Cr(1 0 0) consisting of seven layers using the full-potential linearized augmented plane wave method. They also calculated the $E(k)$ curves for the surface energy bands.

Thick full curves in Fig. 3 are calculated surface bands for the majority spin states along the $\bar{X}_2 - \bar{\Delta}_2 - \bar{\Gamma}_2$ and $\bar{M}_2 - \bar{\Sigma}_2 - \bar{\Gamma}_2$ lines. Thick broken curves represent the energy bands for electrons with majority spin calculated on a seven layer film along the $\bar{X}_2 - \bar{\Delta}_2 - \bar{\Gamma}_2$ and $\bar{M}_2 - \bar{\Sigma}_2 - \bar{\Gamma}_2$ lines. Thin full curves represent the calculated surface energy bands for the majority spin electrons in the $\bar{X}_1 - \bar{\Delta}_1 - \bar{\Gamma}_1$ and $\bar{M}_1 - \bar{\Sigma}_1 - \bar{\Gamma}_1$ lines.

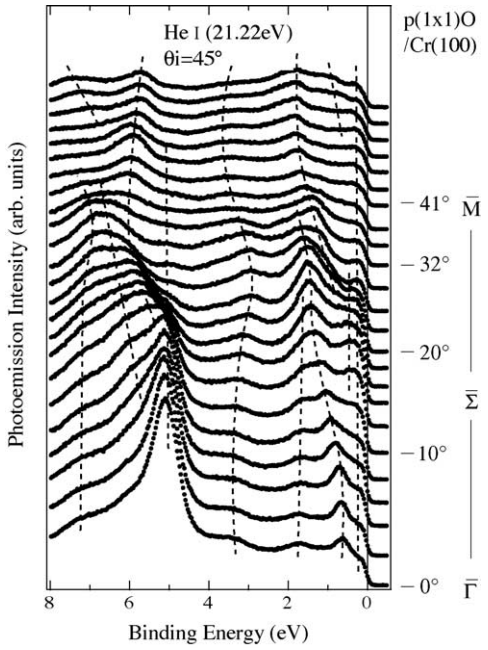

Fig. 4. Angular dependence of EDC's of photoelectrons from p(1 × 1)O/Cr(1 0 0). Excitation light is incident along the (0 1 1) direction on the (0 0 1) surface. Excitation energy is 21.22 eV. Emitted photoelectron beams are in the $(\bar{1}10)$ plane. $k_{||}$ varies along the $\bar{\Sigma}$ axis.

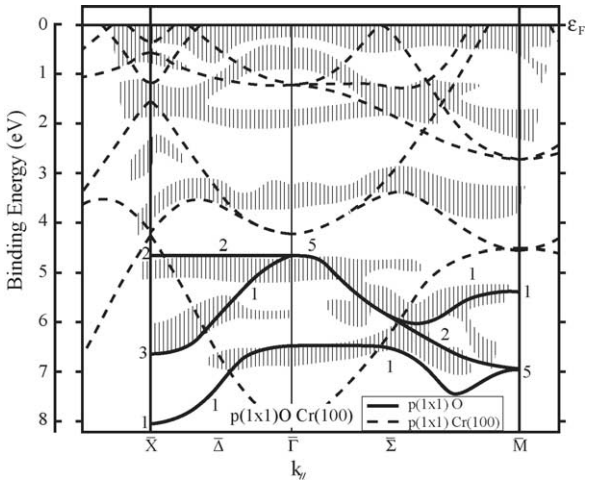

Fig. 5. Comparison of $E(k)$ curves of p(1 × 1)O/Cr(100) measured in the present work with the surface energy bands obtained experimentally by Gewinner et al. [7]. Wide hatched curves are the dispersion curves, $E(k)$, obtained in the present work. Full lines are those measured by Gewinner et al. The dispersion curves in $\bar{X} - \bar{\Delta} - \bar{\Gamma}$ and $\bar{\Gamma} - \bar{\Sigma} - \bar{M}$ directions are shown. For comparison, the $E(k)$ curves for the bulk energy bands calculated by Skriver are also shown with broken lines [6]. Arabic numbers in the figure distinguish the different symmetry lines or points in the Brillouin zone.

Many energy dispersion curves, $E(k)$, of Fu-Freeman's results are omitted here and only representative ones are exhibited in Fig. 3. The comparison of their dispersion curves with the $E(k)$ curves measured here indicates that their surface bands along the $\bar{\Delta}_2$ and $\bar{\Sigma}_2$ lines do not agree with our experimental bands. The surface bands (thick, full), which they show in the symmetry lines, $\bar{X}_2 - \bar{\Delta}_2 - \bar{\Gamma}_2$ and $\bar{\Gamma}_2 - \bar{\Sigma}_2 - \bar{M}_2$, are not found in our data. On the other hand, the seven layer bands shown by thick broken curves have reasonable agreement with our measured bands in the $\bar{\Sigma}_2$ lines. Agreement is not well in the bands along the $\bar{\Delta}_2$ lines. The agreement recognized here is quite contrasted to the Skriver's bulk energy bands that do not agree with the present data in this binding energy region [6].

In the binding energy region lower than 3 eV, agreement is fair in $\bar{\Delta}_1$ and $\bar{\Sigma}_1$ bands both in the surface and thin film bands. In Fu-Freeman's $E(k)$ curves, the surface bands with either $\bar{\Delta}_1$ or $\bar{\Sigma}_1$ symmetry occur in the binding energy region below 2 eV. Agreement with the measured bands is good in the region between 1 and 2 eV. In the region above 2 eV, the $E(k)$ curves calculated on the film agree fair with the bands measured here. The agreement is better with Skriver's bulk energy bands shown later in Fig. 5 in the high binding energy region [6].

Fig. 4 shows the EDC's similar to those shown in Fig. 2 measured on p(1 × 1)O/Cr(1 0 0). The spectra are quite different from those of clean p(1 × 1)Cr(1 0 0), since the first layer of p(1 × 1)O/Cr(1 0 0) is the oxygen layer which influences the electronic structure of the second layer. The second layer is very much influenced by the oxygen on the surface.

The measured EDC's are summarized in the form of the $E(k)$ curves in Fig. 5. In the figure, wide hatched curves represent the energy band dispersion obtained in the present work. For comparison, the $E(k)$ curves for p(1 × 1)1ML O/Cr(1 0 0) obtained experimentally by Gewinner et al. [7] are illustrated with full lines. Broken lines represent the bulk energy bands calculated by Skriver [6]. Arabic numbers in the figure distinguishes the different symmetry lines and points in the Brillouin zone. In Fig. 5, it is recognized that the energy bands for p(1 × 1) 1 ML O/Cr(1 0 0) obtained by Gewinner et al. agree reasonably with the dispersion curves obtained in the present work in the binding energy region above 5 eV. This good agreement is found both on the $\bar{\Delta}$ axis and the $\bar{\Sigma}$ axis. The energy bands calculated for the bulk crystal do not agree with the experimental results.

It is obvious that the bands occurring at binding energies above 5 eV are caused by oxygen. In particular, the band occurring around 5 eV becomes quite intense at oxygen concentration above 3%. The bands with binding energies larger than 5 eV are attributed to the O 2p state forming the surface energy band. The bands within a binding energy of 4 eV from the Fermi level are ascribed to the bands caused by Cr atoms in the first sub-layer forming the O–Cr bond.

Finally, we should point out an important problem. Since the energy of excitation light (He I) is low, the region of the k space, which can be examined is limited. We ignored this and compared the experimental results with theory along directions with good symmetry. The observed transition therefore have $k_{||}$ components to some extent. This may compromise the quality of the comparison.

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