

Angle-resolved photoelectron spectroscopy of O/W(001)

Takenori YAMAMOTO*, Naoaki ITOH, Yoshiyuki ISAWA, Masatoshi TANAKA

Faculty of Engineering, Yokohama National University, Hodogaya-ku, Yokohama
240-8501, Japan

Introduction

Gas adsorption on W(001) surface is one of the typical adsorption systems, and oxygen adsorption has been frequently studied since the dawn of surface science. It is well established that 0.5ML adsorption at room temperature induces $p(4 \times 1)$ LEED pattern. For this system, the double-row structure, in which dissociated oxygen atoms are situated the near bridge sites on the line from the bridge site to the fourfold hollow site, was proposed from the measurement of high-resolution electron energy loss spectroscopy [1]. On the other hand, it was suggested from the measurement of low-energy ion scattering spectroscopy [2] that oxygen in the double-row sits on the bridge site rather than the near bridge site. Thus, the structure of the adsorption system has not yet been clearly determined. The aim of this study is to investigate the undetermined structure from a point of view of electronic states, that is, combination of angle resolved photoelectron spectroscopy and band calculation.

Experimental

The experiment was performed at BL-18A of Photon Factory, KEK. The specimen was a (001) surface of a

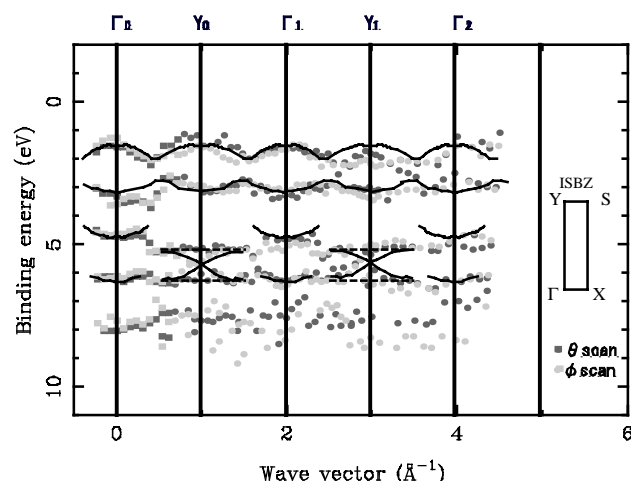


Fig. 1 The band structure of the W(001)- $p(4 \times 1)$ -O surface. The dark- and light-grey solid circles correspond to the peaks in the angle-resolved photoelectron spectra. The solid lines are drawn in order to clearly show periodicity of the structure. The right rectangle is the irreducible surface Brillouin zone of the surface.

tungsten single crystal in a disc shape with a diameter of 9mm and a thickness of 3mm. The surface was cleaned by heating at about 2500K for about 20h and flashing at about 2700K for a few seconds. When the specimen was cooled to about 540K, pure oxygen gases were introduced into the chamber through a variable leak valve at a constant pressure 1×10^{-8} or 1×10^{-7} mbar. $p(4 \times 1)$ LEED pattern was confirmed after 0.5L exposure (0.5ML). Angle-resolved photoelectron spectra were measured at ≈ 85 eV along-Y axis in the surface Brillouin zone.

Result and discussion

The photoelectron spectra have four main structures located at $E_B = 2, 3, 5,$ and 6 eV. The electronic states located at $E_B = 6$ eV correspond to the states originating from oxygen. The binding energy of oxygen-originated states and overall features of the density of states are well reproduced by the cluster-model calculation for the near bridge site [3]. The reproduction is poor both for the bridge site and the four fold hollow site. The photoemission spectra therefore support the adsorption structure with oxygen at the near bridge site. Fig. 1 shows the dispersion of the electronic states for the $p(4 \times 1)$ -O surface obtained from the angle-resolved photoelectron spectra. Periodicity of the fundamental reciprocal lattice vector is found, which means long-range order is formed on the surface. Obtained dispersion of the electronic states is confronted with the band calculation under way. The procedure will provide more precise information about the adsorption structure.

References

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* d99ja008@ynu.ac.jp