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Angle Resolved Photoemission Spectroscopy Study of O/α-Mo₂C(0001)

Masao KATO¹, Ken-ichi OZAWA¹, Tomohiko SATO¹, Kazuyuki EDAMOTO² ¹Tokyo Institute of Technology, Ookayama, Meguro-ku, Tokyo 152-8550, Japan ²Rikkyo Univ., Nishiikebukuro, Toshima-ku, Tokyo 171-8501, Japan

Introduction

Recently Mo₂C has attracted much attention because of its characteristic catalytic activities; Mo₂C has been proved to have catalytic activities similar to those of noble metal catalysis. Moreover, it has been reported that the Mo₂C's catalytic activities are often improved when subjected to slight oxidation. In this work, in order to examine the cause of the improvement of catalytic activity by oxidation, we investigated the electronic structure of , especially around the Fermi level E_F oxygen-covered α -Mo₂C(0001) by ARPES.

Experimental

ARPES measurements were performed at BL-3B using a hemispherical electron-energy analyzer of 180° hemispherical sector type. The surface was cleaned by cycles of Ar⁺-ion bombardment and annealing (~1600°).

Results & Discussion

Fig.1 shows the normal-emission spectra of α -Mo₂C(0001) exposed to various amount of O₂. The O₂ exposure induces bands at 4-7 eV, which are interpreted as O2p, C2p, Mo5sp hybrid bands[1]. In addition to these bands, a peak is grown just below E_F with increasing O₂ exposure. The oxygen induced state around E_F is characteristic of the O/Mo₂C(0001) system.

We map the valence band dispersion of the $20L-O_2$ -exposed surface. The result is shown as a gray scale in Fig.2. The O-induced state around E_F shows a clear dispersion which has energy minimum at the Γ point, and seems to cross E_F at some points.

LEED study has revealed that the O_2 exposure of $Mo_2C(0001)$ sharpens the (1×1) pattern. Since the O-induced state shows a clear dispersion, the adsorbed O atoms are thought to form a (1×1) lattice. It is also found that a metallic band is built in the vicinity of E_F after O_2 exposure, which may have substantial contribution to the activation of Mo_2C surface.

Reference

[1] K.Edamoto et al., Surf. Sci. 561, 101(2004)



Fig.1 PE spectrum was dependence on oxygen coverage.



Fig.2 oxygen 20L exposed surface valence band map around $\Gamma.$