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

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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 Eₚ, 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°C).

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 Eₚ with increasing O₂ exposure. The oxygen induced state around Eₚ is characteristic of the O/Mo₂C(0001) system.

We map the valence band dispersion of the 20L-O₂-exposed surface. The result is shown as a gray scale in Fig.2. The O-induced state around Eₚ shows a clear dispersion which has energy minimum at the Γ point, and seems to cross Eₚ at some points.

LEED study has revealed that the O₂ exposure of Mo₂C(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 Eₚ after O₂ exposure, which may have substantial contribution to the activation of Mo₂C surface.

Reference