Photoelectron spectroscopic study of CO adsorption on Pd(100) single crystal surface under ambient-pressure conditions

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INTRODUCTION

The adsorption structure of carbon monoxide (CO) on late-transition metal surfaces under atmospheric conditions is an issue of technological and scientific interest. In this study, we conducted a work on CO adsorption on a Pd(100) single crystal, because the Pd has been used as a catalyst of CO oxidation (i.e. three-way catalyst). Under UHV conditions, the adsorption structure has been widely investigated.¹² Ambient-Pressure X-ray Photoelectron Spectroscopy (AP-XPS) enables to measure the XP spectrum even under 1 Torr pressure condition using a differential pumping system.

EXPERIMENTAL SECTION

A Pd(100) single crystal was cleaned using well-established procedures in a preparation chamber, the base pressure was < 2×10⁻¹⁰ Torr. Then it was transferred to a high-pressure experimental chamber. The CO gas (99.99% purity) was introduced to the chamber up to 0.5 Torr at room temperature. The photon energy of 435 eV was used for Pd3d⁵/₂ and C1s XPS.

RESULTS and DISCUSSION

Fig. 1 shows a series of Pd3d⁵/₂ XP spectrum of CO adsorption up to 0.5 Torr. At 1×10⁻⁷ Torr, the bulk and an additional peak component at higher binding energy CO(I) are observed. This is associated with the (2√2×√2)R45⁰ structure. With increasing CO gas pressure, a new component CO(II) appears at about 336 eV, and the (3√2×√2)R45⁰, (II)/(I)=0.5 and (4√2×√2)R45⁰, (II)/(I)=1 is formed. These structures have been found at low temperatures under UHV conditions.

However, a new structure, (II)/(I)>1, is reversibly observed at 0.5 Torr. This is interpreted as a (1×1) structure predicted by theoretical calculations.³

References