Adsorption of NO on Pt(110): X-ray photoelectron diffraction study

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Introduction
The adsorption of NO on Pt surfaces has attracted considerable attention due to its importance in catalytic processes. The clean surface of Pt(110) undergoes a (2x1) missing row reconstruction, in which every second [1T0] row of surface Pt atoms is removed. NO adsorption on this surface has been experimentally and theoretically studied. Only one peak is observed in infrared reflection-absorption spectroscopy (IRAS). This peak was assigned to NO molecules on the atop sites [1]. For the atop adsorption of NO, formation of a polymeric (NO)x chain structure was proposed by the previous density functional theory calculations [2]. In the present work, the structure of NO on Pt(110) has been investigated using a scanned-angle N1s x-ray photoelectron diffraction (XPD).

Experimental
The experiments were conducted at the bending-magnet station Beamline 7A. The sample was prepared by exposing a clean Pt(110) surface to gaseous NO at a sample temperature of 180 K to the saturation. The saturated surface showed (2x1) LEED pattern. Scanned-angle XPD curves were measured as a function of polar emission angle along the two major azimuths [1T0] and [001]. The wave number of the photoelectron used here was 10.7 Å⁻¹, where photoelectron diffraction is dominated by the forward scattering by the oxygen atoms. The molecular axis orientation was determined by R-factor analyses. The simulations were performed using the multiple-scattering calculation of diffraction (MSCD) package developed by Chen and van Hove [3].

Results and discussion
Fig. 1 shows the XPD data for the [1T0] azimuth (up) and [001] azimuth (bottom), respectively. The black lines show the results of experiments and the red lines show the results of multiple-scattering simulations for the optimized geometry. Each N 1s intensity was normalized by the corresponding O 1s intensity to avoid any angular dependence not directly related to the molecular axis orientation. The structural model was optimized under assumption of NO molecule adsorbed not only on the close-packed [1T0] rows but also on the long-bridge sites between the rows, because the saturation coverage estimated by XPS is approximately 1.5 times with respect to the close-packed [1T0] row. In the previous IRAS study [1] no peak associated with NO at the long-bridge site was detected, probably due to the effective screening of the dynamic dipole situated at the lower level. Fig. 2 shows a schematic illustration of the best-fit model. The present result gives no evidence for the formation of (NO), polymeric chain on the close-packed Pt rows. NO molecules adsorbed on the close-packed rows occupy the atop site, tilting only by 14 ± 2° from the surface normal towards 40 ± 20° from the [1T0] azimuth.

References

Fig. 1. Comparison of experimental (black) and best-fit simulated (red) scanned-angle XPD curves for the 1.5NO/(2x1)-Pt(110) surface.

Fig. 2. Schematic view of the best-fit adsorption geometry for the 1.5NO/(2x1)-Pt(110) surface.

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