

## 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  $[1\bar{1}0]$  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  $(\text{NO})_x$  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  $[1\bar{1}0]$  and  $[001]$ . The wave number of the photoelectron used here was  $10.7 \text{ \AA}^{-1}$ , 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  $[1\bar{1}0]$  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  $[1\bar{1}0]$  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  $[1\bar{1}0]$  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  $(\text{NO})_x$  polymeric chain on the close-packed Pt rows. NO molecules adsorbed on the close-packed rows occupy the atop site, tilting only by  $14 \pm 2^\circ$  from the surface normal towards  $40 \pm 20^\circ$  from the  $[1\bar{1}0]$  azimuth.

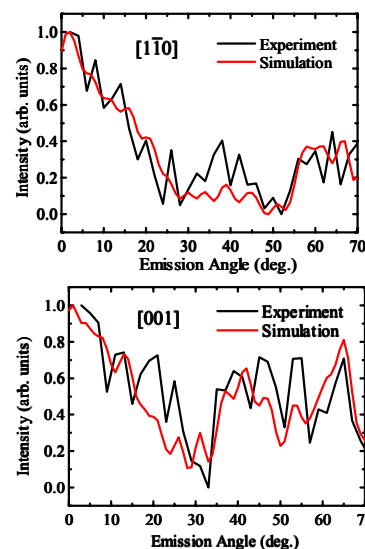


Fig. 1. Comparison of experimental (black) and best-fit simulated (red) scanned-angle XPD curves for the 1.5NO/(2x1)-Pt(110) surface.

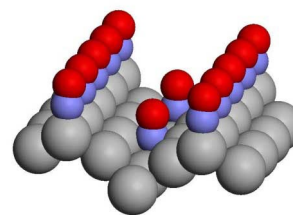


Fig. 2 Schematic view of the best-fit adsorption geometry for the 1.5NO/(2x1)-Pt(110) surface.

### References

- [1] W. A. Brown et al., *J. Phys. Chem. B* 102, 5303 (1998).
- [2] Q. Ge et al., *J. Chem. Phys.* 110, 12082 (1999).
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