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Polarization dependent total reflection fluorescence XAFS(PTRF-XAFS) studies on Ni atoms dispersed on Al_2O_3(0001) surface

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Introduction

Metal deposited on oxides are technologically important. The interaction between metal and oxide is also interesting in a fundamental field. However, it is quite difficult to determine the interface structure between them. EXAFS is one of the promising techniques but the conventional EXAFS provides an average structure over all directions. When the metal is deposited on a single crystal oxide and polarization dependent measurement is carried out, one can get the information about the structure parallel or perpendicular to the oxide surface separately. The method is called as polarization-dependent total reflection fluorescence XAFS(PTRF-XAFS). We have applied this technique to the structure analysis of Ni on Al_2O_3(0001) surface.

Experimental

The details of the the XAFS measurement chamber was described elsewhere[1]. We prepared Ni on Al_2O_3 (0001) using vacuum evaporation. The coverage was estimated by the inflection point of XPS intensities of Ni and O peaks. We measured PTRF-XAFS of Ni/Al_2O_3 sample varying the coverage from 0.02 ML to 2 ML. The XAFS measurement was carried out at BL9A using a Si(111) double crystal monochromator. We accumulated the fluorescence data using a 19-element SSD.

Results and discussion

Fig.1 shows the XAFS oscillations with two directions, parallel to the surface (s-pol) and perpendicular to the surface (p-pol) for 0.04 ML Ni/Al_2O_3 (0001). The XAFS oscillation changed at about 0.1 ML where Ni-Ni started to be observed, indicating the Ni agglomerated to particles at more than 0.1 ML. Here we report the details in the analysis of Ni local structure less than 0.1 ML where Ni was present in an atomically dispersed form.

We carried out FEFF calculations based on a several model structures. As a result, the EXAFS oscillation is found to be due to the scattering from the oxygen and the polarization dependence of coordination number indicated the Ni is located on the three fold site. There is 3 types of three fold sites on the surface of Al_2O_3 (0001) called as A,B and C sites as shown in Fig. 2. Site A is the one theoretically predicted[2]. However, Al should be present below the Ni with Ni-Al distance at about 0.191 nm in the site A. In our EXAFS could not be reproduced when such a short Ni-Al distance was present. Site C is usually occupied by the surface Al. If Ni is adsorbed on this site C, Al is replaced with the Ni. Site B is the one where the next Al should be placed.

We can reproduce the EXAFS oscillation by assuming the Ni location at the Site B but not at the site C. Site C does not have no surface Al contribution to the EXAFS oscillation and hence s pol could not be well simulated.

In summary, the Ni is placed on the B site of Al_2O_3(0001) where the next Al is expected to sit and the conclusion is contradicted with the previous calculation.

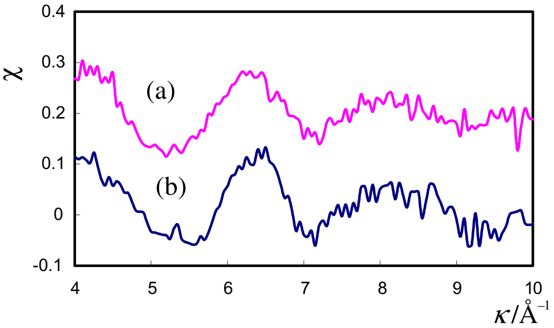

Fig.1 XAFS oscillation of Ni/Al_2O_3 (a): spol, (b): ppol

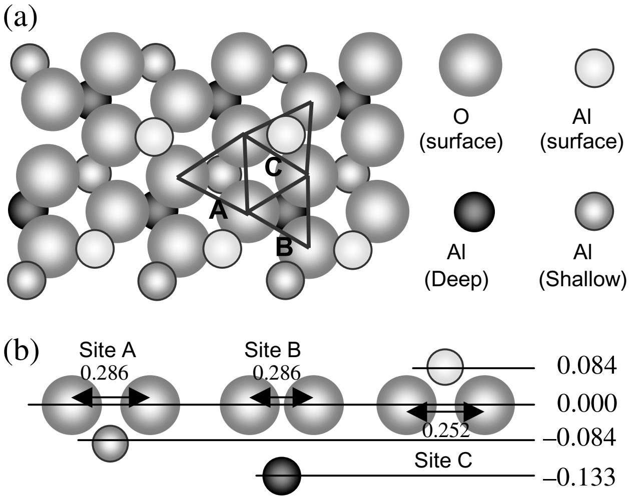

Fig.2 Al_2O_3 (0001) surface structure. (a) top view, (b) side view.

References

[1] W. J. Chun, et.al. J.Synchrotron Rad., **8**, 168 (2001).
[2] Q. Ma,et.al. J.Phys.Chem., **105**, 2212 (2001).

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