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Surface Structure of Ni on TiO_2(110) surface

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Introduction

Metal-oxide interaction is one of the most important issues in many fields such as catalysts, sensors, and electronic devices. Recent development in SPM (Scanning probe microscopy) and surface X-ray can provide the registry, morphology and texture of the deposited metal. But the problem about the type of chemical bond between the metal and metal oxide is still under debate. Polarization-dependent surface EXAFS is a suitable technique and we have determined the structures of the Cu and the Mo oxide on TiO_2 (110) by this technique.[1,2] In this paper we will report the structure of Ni on TiO_2(110) surface. The oxide supported Ni is a typical metal catalyst used for hydrogenation reactions. TiO_2-supported Ni catalysts often show interesting phenomena called "strong-metal support interaction" (SMSI).[3]

Experimental

A TiO_2(110) surface was cleaned by Ar^+-sputtering and 873 K-annealing cycles which gave a clean (1x1) LEED pattern. The Ni was evaporated from a tungsten filament which was wrapped with a Ni wire. The amount of Ni was monitored by XPS. Polarization dependent XAFS was measured at BL9A beam line in a total reflection fluorescence mode. The sample was kept under 10^{-8} Pa. The fluorescence X-ray was detected by a Canberra 19-element SSD.

Results and Discussion

Figure 1 shows the polarization dependent XAFS oscillations for 0.05 ML. Envelope of the XAFS oscillations indicated the presence of Ni-O bonding and the larger amplitude in [110] direction might be corresponding to the larger contribution of Ni-O in this direction. Table 1 shows the best fitting results. The Ni-O bond length was found at 1.92 Å The agreement was tremendously improved when the additional Ni-Ni bond was postulated. This means that the Ni-Ni was present even in as low coverage as 0.02 ML. This result is contrasted to the Ni on α-Al_2O_3 (0001) surface where only monoatomically dispersed Ni was found at the coverage of 0.05 ML. This difference may arise from the fact that Ni atoms on the three fold oxygen sites of the TiO_2 (110) surface should find the repulsive interaction of Ti cations because they would be located less than 2.5 Å away from the adsorbed Ni. Consequently Ni atoms should be expelled from the three-fold position and the Ni clusters were formed at a very low coverage.

References

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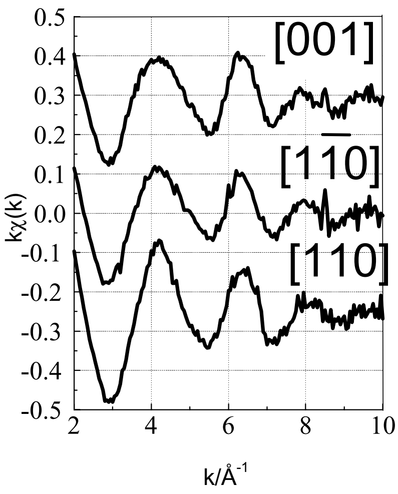

Fig. 1 polarization dependent XAFS of 0.05 ML Ni/TiO_2(110)

Table 1 Best fitting results of XAFS analysis for Ni/TiO2(110).

		Coordination Number	r /Å
[001]	Ni-O	1.2	1.92
	Ni-Ni	0.9	2.43
[$1\bar{1}0$]	Ni-O	1.3	1.92
	Ni-Ni	0.7	2.43
[110]	Ni-O	1.8	1.91
	Ni-Ni	0.8	2.43

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