# Surface Structure of Au species on TiO<sub>2</sub>(110) by Angle Resolved Total Reflection Fluorescence XAFS (ARTRF-XAFS)

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## **Introduction**

Au-particles below 5 nm in size supported on TiO<sub>2</sub> has unique catalytic properties in CO oxidation[1]. However, there is still no clear picture with respect to the origin of the catalytic activity and the role of metal-support interaction which is considered as a crucial factor. For the further insight of Au-TiO<sub>2</sub> interaction it is important to prepare monoatomic Au species on TiO<sub>2</sub>(110). Tanizawa et al., have shown that organic ligands in organometallic compounds can prevent metal from the aggregation to a large particle on the TiO<sub>2</sub>(110) [2].

In this work, we attempted to prepare monoatomic Au species on  $\text{TiO}_2(110)$  through the chemical vapour deposition with a gold organometallic compound. The surface structure of Au species on  $\text{TiO}_2(110)$  was determined by the ARTRF-XAFS technique[3] that can determine definite three-dimensional surface structure of the overlayer metal species on substrate surfaces at sub-Ångstrom resolution.

## **Experimental**

TiO<sub>2</sub>(110) crystals were cleaned by Ar ion sputtering at room temperature, followed by annealing at 1000 K until a sharp (1 × 1) LEED pattern was obtained. Au was deposited on the clean surface by chemical vapor deposition with AuDMe(acac) (dimethyl diacetoacethyl gold). The Au coverage was 1.4 x 10<sup>14</sup> Au atoms/cm<sup>2</sup> monitored by XPS. ATRF-XAFS was carried out with an in-situ PTRF-XAFS measurement chamber (a base pressure of ca. 8 x 10<sup>-8</sup> Pa) [4]. The Au L<sub>2</sub> edge was used for avoiding small fluorescence signals of W and Ta as a holder material. EXAFS analysis was carried out by REX 2000 (Rigaku Co., Japan) and FEFF8.02 code[5].

### **Results and Discussion**

Fig. 1(a) shows the observed Au  $L_2$ -edge XANES spectra of AuDMe(acac) on TiO<sub>2</sub>(110) with Au foil. First, there was no difference in all ARTRF-XANES oscillations. It indicates the surface structure should be a symmetric structure. Second, the characteristic peaks observed in Au foil were observed in all XANES spectra, but the intensity was weaker than that of Au foil. It

suggests that small Au particles should be formed on the  $TiO_{2}(110)$  surface.

In EXAFS region (Fig.1 (b)), all spectra showed similar features. The  $\chi^2$  test [6] showed no polarization dependency in all orientation. It is in agreement with the XANES result. Curve fitting analysis showed the presence of Au-Au interaction for all orientations at 0.270 nm which is 0.014 nm shorter than that of Au bulk. It indicates the presence of small Au particles on TiO<sub>2</sub>(110) surface.

ARTRF-XAFS results described that the AuDMe(acac) compound decomposed and aggregated to small Au particles on  $TiO_2(110)$  at room temperature. We are now exploring other approaches for obtaining monoatomic Au species.



Fig. 1 The ARTRF-XAFS spectra of AuDMe(acac) on  $TiO_2(110)$ . (a) XANES; (b) EXAFS.

### **References**

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