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# Surface Structure of Au Species on a Hydroxylated TiO,(110) Surface

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#### **Introduction**

Gold has been regarded as an inert metal for catalytic applications before Haruta et al. have reported that the Au particles below 10 nm in size supported on  $\text{TiO}_2$  has unique catalytic properties in CO oxidation reaction [1]. However, there is still no clear picture with respect to the origin of the catalytic activity and the role of metal-support interaction. To understand the further insight of Au-TiO<sub>2</sub> interaction, it is important to prepare highly dispersed Au species, in particular, monatomic species on an atomically flat TiO<sub>2</sub> single crystal surface.

In this work, we attempted to prepare monatomic Au species on a hydroxylated  $\text{TiO}_2(110)$  surface using the chemical vapor deposition (CVD) with AuDMe(acac) (dimethyl diacetoacethyl gold) at RT. Yuan et al. previously produced highly active Au cluster using organic Au compounds and hydroxide covered surface.[2] Organic ligands in the organometallic compound may react with hydroxyl group on the  $\text{TiO}_2(110)$  surface to form chemical bonds to fix Au species. The surface structure of the Au species formed on the hydroxylated  $\text{TiO}_2(110)$  by the CVD was determined by the Polarization-dependent Total Reflection XAFS (PTRF-XAFS) technique [3].

#### **Experimental**

TiO<sub>2</sub>(110) surface was cleaned by cycles of Ar ion sputtering at RT and annealing at 1000 K until a sharp (1x1) LEED pattern was observed. A hydroxylated surface was prepared as follows; The cleaned  $TiO_{2}(110)$ surface was sputtered again by Ar ion at 3 keV for 10 min, followed by annealing at 870 K for 10 min. Then the sample was exposed to 10 L water at RT to form hydroxyl groups on the surface. Au was deposited on the hydroxylated surface by CVD with AuDMe(acac). The Au coverage was estimated to be ca. 0.09 ML by XPS. PTRF-XAFS was carried out with in-situ PTRF-XAFS chamber (base pressure: 8 x  $10^{-8}$  Pa) [3]. The Au L<sub>2</sub>-edge was used to avoid small fluorescence signals of W and Ta as a holder material. XAFS analysis was carried out using REX 2000 and FEFF8.0.

### **Results and Discussion**

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

In EXAFS region (Fig. 1(b)), all spectra showed similar features, which is in agreement with the XANES result. The characteristic oscillation due to Au-Au interaction was observed for all spectra, but the periodicity was longer than that of Au foil. It indicates that Au-Au bond was shorter than that of Au foil, suggesting the formation of small Au particles. The XAFS results showed that the AuDMe(acac) was easily decomposed and aggregated to small particles on the hydroxylated  $TiO_2(110)$  at RT. We are now trying other approaches to obtain monatomic Au species.



Fig. 1 The PTRF-XAFS spectra of AuDMe(acac) on the hydroxylated  $TiO_{2}(110)$  surface. (a): XANES;

## **References**

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