主　論　文　要　旨

論文題名　**The Mechanism of Emerging Catalytic Activity of Gold Nano-clusters in CO Oxidation Reaction**

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主論文要旨

It is well known that Au is the noblest of all the metals. However, Haruta found a strong catalytic activity of Au nano-clusters dispersed on rutile TiO_2 particles even at low temperatures for the size below ~5nm. Up to now, many efforts have been made experimentally and also theoretically to elucidate the mechanism of emerging catalytic activity of Au nano-clusters in CO oxidation reaction. In spite of many efforts, however, the mechanism leading to a strong catalytic activity of Au nano-clusters is still a debatable issue.

In this study, we demonstrate a pronounced enhancement of the CO oxidation reaction by Au nano-clusters deposited on rutile TiO_2(110) surfaces. We first analyzed the grown mode of Au nano-clusters on TiO_2(110) by high-resolution medium energy ion scattering (MEIS). Then, we revealed that CO oxidation kinetics is dependent on the surface structure of TiO_2(110) by MEIS and photoemission spectroscopy(PES). Finally, we found a pronounced enhancement of the CO oxidation reaction by Au nano-clusters deposited on the rutile TiO_2(110) surface.

For the CO oxidation on TiO_2(110) surfaces, a residual surface electronic charge plays a very important role. The residual charge appears as defect states in the band gap. There reported so far two probable sources of the gap state, (i) the Ti atoms (Ti^{3+}) beneath a bridging O vacancy and (ii) Ti interstitials segregated near the surface by sputter/annealing in vacuum. We demonstrate quantitatively that the Ti interstitials are dominant for TiO_2(110) subjected to many sputter/annealing cycles low sheet resistance below ~200 Ω/□, while the bridging O vacancies becomes primary source for the samples with relatively high sheet resistance exceeding ~200 Ω/□.