CRYSTALLITE MORPHOLOGY IN GOLD CATALYSTS OBTAINED VIA RIETVELD REFINEMENT

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Rutile was prepared at 90 °C, and heated at temperatures between 300 and 700 °C to get it with different crystallite sizes. On these rutile samples, 5 wt % gold was deposited to produce nanocrystallite gold particles with dimensions between 1 and 3 nm, which functioned as catalysts for CO oxidation. The crystalline phases of the catalyst, rutile and cubic gold, were characterized with X-ray powder diffraction and transmission electron microscopy. The crystallite structures were refined by using the Rietveld method where the crystallite morphology was modeled with a basis of spherical harmonics. Rutile particles were polycrystalline fibers made of crystallites oriented parallel to their *c* axis, which defined the growing direction of the fibers. This texture gave rise to large microstrains that decreased with temperature and functioned as pinning centers for the gold particles. Although the gold concentration was low and the gold crystallite size was small, crystallite size and morphology was obtained from the refinement of the gold crystalline structure. The gold crystallite morphology was based on a cuboctahedron, with a preferential crystallite growing on their eight faces parallel to the family of equivalent {111} planes. This produced cubic crystallites with a conic hole on each of their six faces. As the gold crystallite grew the enlargement of the crystallite along the family of {111} planes was larger, which decreased the number of catalytic active sites, and with that its catalytic activity for CO oxidation.