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Tracking the facet-resolved strain state of a PtRh nanoparticle under catalytic reaction conditions

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Oxide-supported nanoparticles are important heterogeneous catalysts. The nanoparticles shapes and type of facets are decisive for the catalyst activity and lifetime. During a catalytic reaction, the nanoparticle may be subject to shape changes, and segregation in alloys may adjust the termination of the surface to a changing gas environment.

Here we report on the evolution of the 3D strain state in a single alloy PtRh nanoparticle operando followed by coherent X-ray diffraction imaging (CXDI). At a temperature of T=700 K the nanoparticle environment was switched between the gas compositions (I) inert Ar, (II) CO+Ar, (III) CO+O_2+Ar and (IV) CO+Ar resembling different adsorption and catalytic reaction scenarios on the nanoparticle surface.

$SrTiO_3$ supported nanoparticles were grown by co-deposition of Pt and Rh and annealed in UHV to induce the equilibrium shape. A single nanoparticle was pre-selected in an SEM and subsequently, hierarchical Pt fiducial markers were deposited in the vicinity of the selected nanoparticle and used to re-locate the same particle in the X-ray beam.

The nanoparticle exhibited solely low index <100> and <111> type facet surfaces, intriguingly showing distinct, facet-family specific strain states. Under the catalytic reaction condition (III) we observed significant strain relaxations for all facets accompanied with a preferential segregation of Rh to the nanoparticle surface, in line with density functional theory calculations (DFT). The Rh enrichment on the facets turned out to be non-reversible under the subsequent CO reduction condition (IV) as compared to the identical previous gas condition (II).

Tracking the dynamics of facet-specific structural reorganizations of the nanoparticle is one key for the future design of heterogeneous catalysts with optimized efficiency and selectivity.

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