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CRYSTALLOGRAPHY OF DYNAMICS OF METAL NANOCLUSTERS DURING CHEMICAL REACTION AT THEIR SURFACE

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In heterogenous catalysis surface structure of metal catalyst may change what modifies surface interactions that in turn affect the structure. The process may generate dynamics of surface that can constitute true origin of chemical activity. One can consider concept of 'actve processes' instead of 'active sites'. In our laboratory we have developed in situ powder diffraction technique that is able to register subtle changes of scattered intensities due to modifications of the nanocrystal surface and to interpret these changes via molecular simulations. Our results allowed quantitative distinction between surface relaxations and reconstructions [1]. The surface reconstruction in response to changing atmosphere appears to be quite common for metal nanocrystals. Sometimes it can lead to cyclic or turbulent phenomena if the reconstruction triggers change in the adsorbate coverage that in turn causes re-reconstruction (or cancels it out) [2]. Gold appears as the metal especially prone to reconstruction. Our results point to gold surface reconstruction occurring on adsorption of many reactive gases. Interpreting precisely peak shape and position we could detect reversible size changes along given crystallographic direction pointing to reversible changes of the nanocrystal shape [3]. Gold surface appears to be mobile enough to quickly increase surface of crystal faces interacting more favorably with the adsorbate. Monitoring oxidation of CO we detected also appearance of a new form of nanocrystalline gold with deep reconstruction of crystal faces leading to a 200 and 220 peak split. The transition may deactivate gold as a catalyst. Precise monitoring of the metal peak position and shape during chemical reaction can provide insight into its structure and dynamics. Degree of the Bragg law violations for various peaks can indicate difference in the interaction with adsorbate on various crystall faces.

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