Heterogeneous Catalysis: An Analytical Challenge

Robert Schlögl

Fritz-Haber-Institut der Max-Planck-Gesellschaft
Faradayweg 4-6, D-14195 Berlin

The development of heterogeneous catalysts which form the technological basis of about 15% of the world GNP is after a century of research still a problem of trial and error. Despite the enormous factual database and the efforts of surface science, chemical engineering and synthetic chemistry we are still lacking a good theoretical and experimental basis to link the information to a picture accurate enough to predict function from structure and vice versa.

One general problem is the poor knowledge about the structures of operating catalysts. Without this information we are unable to device models and to perform targeted surface science experiments serving as a basis for kinetic models describing the behaviour of the catalysts under technical reaction conditions. The lack of ordering at surfaces of reacting systems and the dynamic solid state behaviour of catalytic systems preclude a standard solid state structural analysis.

We need to performs the investigations under reaction conditions and to explore the solid state dynamics under varying reaction conditions. Under such conditions most analytical methods are only difficult to apply. The contribution reviews several suitable methods including EXAFS, XAS, XRD RAMAN and UV-VIS-NIR spectroscopy in their potential for solving structural problems of metallic and oxidic massive catalyst systems.

It will be demonstrated that a simultaneous knowledge of the gas-phase reaction products and of the spectroscopic parameters is useful to unravel those structural details which govern the catalytic function. So called ex-situ methods like HRTEM or photoemission can be used to back the in-situ observations and to guide the structural analysis by showing possible geometric and electronic structural features. The generally dynamical behaviour of catalysts which represent solids far apart from a thermodynamically controlled situation is the origin of the discrepancies between expected and observed structures and not a "special catalytic chemistry". The lack of information about kinetically labile inorganic solids precludes the appropriate choice of model systems and hinders fundamental and theoretical studies. In this way the analytical description of reactive solids becomes of paramount importance to gain progress towards a rational development of catalysts.