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## *Book Review*

# HANDBOOK OF HETEROGENEOUS CATALYSIS

Second, Completely Revised and Enlarged Edition

Volume 3

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The third volume of the **Handbook of Heterogeneous Catalysis** is organized in three sections: *Model systems*, *Elementary Steps and Mechanisms* and *Macrokinetics and Transport Processes*.

Since solid catalysts are typically complex materials, researchers have often used structurally simple models in their attempts to identify the catalytic sites and understand the reaction mechanisms.

Consequently, the first chapter (***Model Systems***) covers the structures that can be used as models for industrial catalysts. Among these, Single Crystals are usually used as models for metal catalysts because they are highly uniform, crystalline, and pure materials. Some examples given in this book are indicative for the concepts that were developed using the single crystal models: (i) the nature of the active site can be easily revealed by comparing the turnover rates on industrial, supported catalysts and single crystal catalysts for the catalytic reaction of ammonia synthesis; (ii) the classification of a reaction as structure-sensitive or structure-insensitive may be made directly by measuring the rates on the different planes of a single crystal.

The second group of model systems deals with the Supported Metal Cluster Catalysts. Metals are among the most important industrial catalysts, and in practice they are usually dispersed on supports, so that a large fraction of the metal atoms are exposed at surfaces and accessible to reactants. The aims of this chapter are to summarize methods of synthesis and characterization of supported metal clusters made from molecular precursors, and to illustrate their catalytic properties. Metallic Glasses, also referred to as "glassy metals" have gained considerable interest in catalysis research due to their unique structural and chemical properties. In this chapter, a brief account of the state-of-the-art is provided, and some important facets of the knowledge gained are discussed. Based on the results reported so far, two principal opportunities for the use of glassy metals in catalysis have emerged, namely *as-quenched* state (based on the surface structure which, ideally, should be structurally and chemically isotropic and exhibiting no-long range ordering of the constituents, as well as on the ability to tailor the electronic properties) or as *catalyst precursors* (which opened new routes for the preparation of supported metal catalysts with unusual chemical and structural properties). Bimetallic Model Catalysts offer advantages due to "synergy": the two active metals somehow cooperate to enhance activity and/or selectivity in ways which are not seen in catalysts based only on the individual metals. In this chapter, the properties of bimetallic surfaces that contain transition and *s, p* metals are examined. Because this subject was previously reviewed in the First Edition of this Handbook, the attention is focused only on the recent studies with well-defined model catalysts, placing importance on investigations that illustrate new concepts or provide results that lead to a general and coherent picture of the behavior of bimetallic surfaces. The chapter Ultrathin Oxide Films is focused on the recent developments in the investigations of thin oxide films supported on metal single crystals. The material taken into consideration is organized as follows: first, a prototype system (MgO(100) surface) is addressed, before discussing surfaces of other oxide materials. Also, the interaction of oxide surfaces with metal and metal oxide

deposits, and how these composite systems interact with gas-phase reactants are included in this chapter. The Reactions of Model Metal Oxide Surfaces are of exceptional significance in areas such as catalysis. So far, in spite of their wide-range applications, metal oxides have been less addressed than the metals in the studies on the industrial process. The presence of two different atoms (metal and oxygen) increases the number and complexity of the surface structures, and many are less stable than their metal counterparts at elevated temperatures. The chapter Microcrystalline Oxides: Bridging the Gap between Single Crystals and Dispersed Oxides intends to show that the gap between "believed perfect" single-crystal surfaces and high-surface-area samples can be progressively reduced. The approach of this contribution (limited to MgO) should not be considered as too restricted because a lesson derived from one single example has sufficient generality to be extended to other systems. The last chapter is devoted to the Oxide Solid Solutions which covers the preparation, characterization and the catalytic applications of these materials. The catalytic applications are limited to the most relevant reactions and catalysts.

The next chapter, on ***Elementary steps and mechanisms***, gives comprehensive details about the "intimacy" between catalyst and the molecules being converted. All these things are properly presented a long of five sub-chapters. First information is given on Chemisorption where principles of chemisorption, thermodynamics and energetics, surface diffusion and structure sensitivity are very well documented. The discussion is going further with Microkinetics. This sub-chapter deals with the concept of turnover frequency (TOF) and provides examples of how this concept allows us to think about heterogeneous catalysis. How to collect the kinetic reactions data and build mechanistically-based "microkinetic" models are discussed, as well. Further, the use of the transition state theory to estimate the entropies of the adsorbed species in the models is shown. Finally, the concept of kinetically significant steps, as determined by Campbell's degree of rate control, is discussed. The third sub-chapter is devoted to the Factors Influencing Catalytic Action. Few examples and case studies are chosen in order to better understand the mechanism of the action of catalysts and, perhaps more importantly, how promoters and poisons influence this chemistry. Hydrocarbon Reaction Mechanisms provides a brief, introductory summary of mechanistic information about hydrocarbon reactions, restricted for brevity to those catalyzed by solid acids or by metals. Related information is presented in the parts of this Handbook dealing with acidity and basicity, computer simulation of sorption, diffusion and shape selectivity, petroleum refining reactions and petrochemical conversions. In addition, various chapters are concerned with catalysis by acids and metals. The fifth chapter, on Computer Simulations, proposes to show how molecular simulation is a useful tool in catalysis. In this respect, three possible applications are presented here such as (i) modeling of structures and reactivity of solids catalysts, (ii) computer simulation of sorption and transport in zeolites and (iii) computer simulations of shape selectivity effects. It is shown that recent developments in novel simulation techniques and force field have allowed for computing the properties of catalysts to a sufficient degree of accuracy so that, they may be considered as a good alternative for real experiment data.

The chapter ending this volume of the Handbook, consisting in six sub-chapters, treats the ***Macrokinetics and Transport Processes***. The sub-chapter Rates Procurement and Kinetic Modeling describes the methods to obtain relevant data for kinetic modeling and comparison of catalysts activities for the ultimate purpose of engineering applications. Discussions on the diffusion phenomenon including (i) definitions, (ii) measurement of transport diffusion, (iii) measurement of self-diffusion, diffusion in multicomponent systems, and (iv) the correlation among different diffusivities are accurately exploited in the sub-chapter Determination of Diffusion Coefficients in Porous Media. The objective of the sub-chapter Simultaneous Heat and Mass Transfer and Chemical Reaction is to make the chemists and chemical engineers familiar with the basic concepts for a quick and effective study of the phenomena of simultaneous heat and mass transfer combined with simultaneous chemical reactions in porous media. The first part of sub-chapter Magnetic Resonance Imaging (MRI) summarizes the basic principles of this procedure and transport measurement techniques and highlights the recent developments in the field. In the second part, several examples are presented with the aim of giving the reader an overview of the state-of-the-art capabilities of MRI applied to catalysts and catalytic reactions. The sub-chapter $^{11}C$, $^{13}N$ and $^{15}O$ Positron ($\beta^+$) Emitters in Catalysis Research briefly describes the radiation properties of $\beta$-emitters, the production and synthesis of $\beta$-labeled compounds and the *in situ* detection of $\beta$-labels. Several applications of $^{11}C$, $^{13}N$ and $^{15}O$ in heterogeneous catalysis are also summarized. The last topic of the chapter is Computational Fluid Dynamics Simulation of Catalytic Reactions. This sub-chapter introduces the applications of CFD simulations to obtain a better understanding of the interactions between mass and heat transport and chemical reactions in catalytic reactors. Concepts for modeling and numerical simulation of catalytic reactors are presented, which describe the coupling of the physical and chemical processes in detail. The ultimate objective of these approaches is to understand and, finally, to optimize the behavior of the catalytic reactors.

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