SMR/207 - 5

WORKSHOP ON
"SURFACE SCIENCE AND CATALYSIS"
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SHORT INTRODUCTION TO
SURFACE SCIENCE AND HETEROGENEOUS CATALYSIS

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These are preliminary lecture notes, intended only for distribution to participants.

Short Introduction to
Surface Science and Heterogeneous Catalysis

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When an added material enhances (or retards) the rate of a chemical reaction without the simultaneous consumption of this material, the reaction is said to be catalytic. The additive is called the catalyst. When the catalyst is a solid, the reaction is heterogeneous.

The rate change of the catalyzed reaction, in thermodynamic terms, is due to a decreased activation energy for this reaction (Fig. 1). The origin of the lowered activation energy lies in the heterogeneous nature of the catalytic reaction, all reactants are being adsorbed (exothermic reaction) on the surface of the catalyst prior to reacting.

Heterogeneous catalysis thus involves the continuous exchange of material between gaseous and adsorbed phase. The formation of products takes place on the surface of the catalyst in the adsorbed phase. In order to have maximum efficiency, the surface of the catalyst has to be very large. Individual surface processes involve adsorption, desorption, diffusion and surface reaction (Fig. 2).

Fundamental research of catalysis concentrates on the characterization of the catalyst and on a detailed investigation of all elementary surface processes involved. For this reason many analytical techniques are being applied in this area. Obviously surface-sensitive techniques are most important. One distinguishes the "conventional" and the "surface science" approach of research in heterogeneous catalysis (Fig. 3). These approaches differ in the type of catalyst being studied, the pressure regime, and the principle investigative tools applied. Gas phase analysis plays an important role in conventional catalysis research.

The "surface science approach" is essentially governed by the multitude of surface-sensitive techniques that are able to yield detailed information about surface composition and structure, about the electronic structure of

the catalyst and of adsorbed species, etc. In general, these techniques require flat extended surfaces, mostly under vacuum. Thus research conditions in surface science create a methodology gap (catalyst, pressure, techniques) which needs to be bridged if results obtained under idealized conditions are supposed to be relevant for heterogeneous catalysis under realistic conditions (Fig. 4).

The most important catalyst variables are its surface structure and composition. Hence a lot of effort is devoted to studying the structural dependence of reactions and also the materials dependence. Traditionally one speaks of the "structure factor" and of the "electronic factor" in heterogeneous catalysis (Figs. 5 and 6). Both phenomena are studied extensively by the conventional and the surface science approach. The structural dependence in conventional catalysis is usually synonymous with a particle size effect of highly dispersed supported catalysts with a large specific surface area ($> 10 \, m^2/g$ of active catalyst). In surface science the structural dependence is studied fundamentally by using well-oriented single crystals (of metals) whose surfaces may contain specific additives.

References

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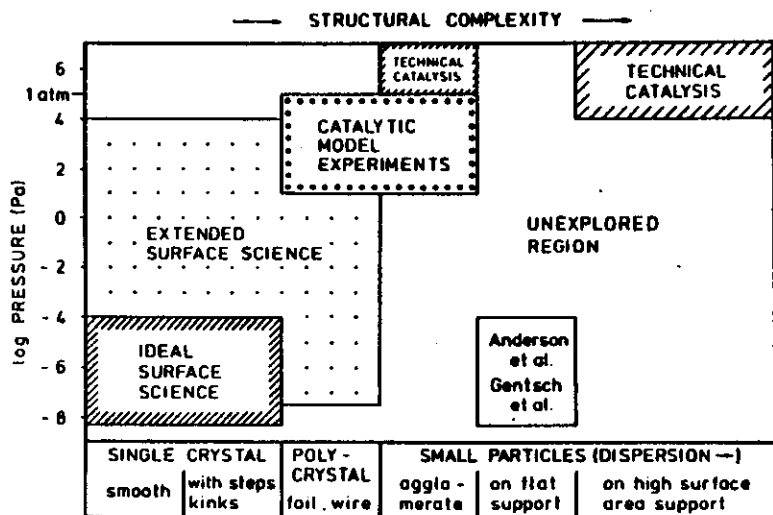(6) G. Ertl, Catal. Rev. Sci. Eng. 21 (1980) 201.

$$CO + \frac{1}{2} O_2 \rightarrow CO_2$$

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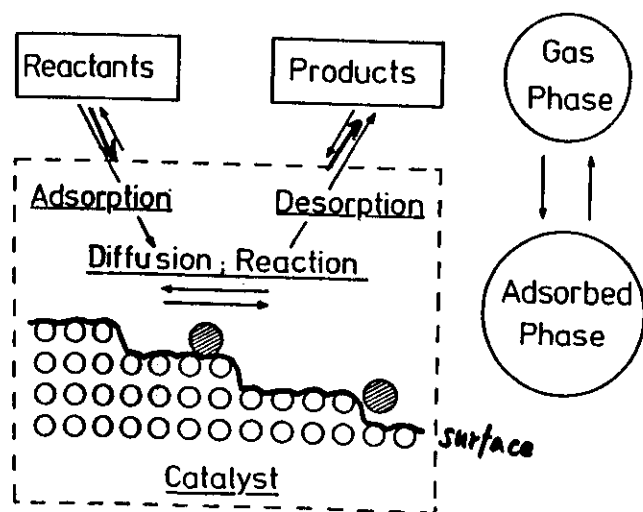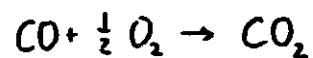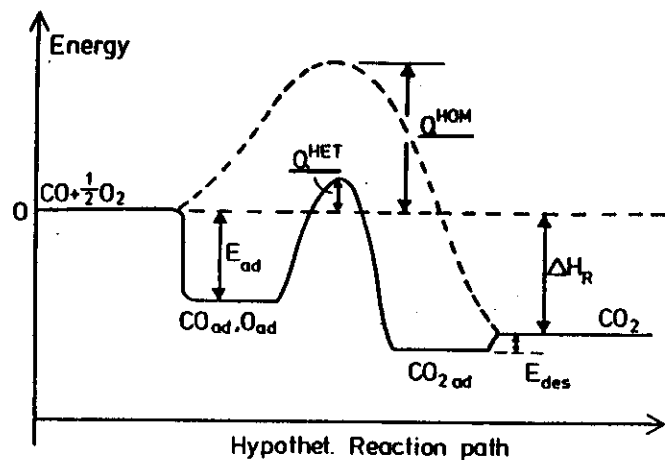
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Research of heterogeneous catalysis

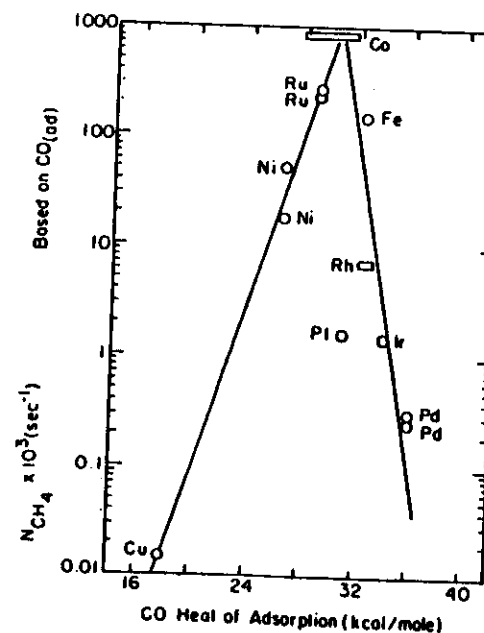|	by conventional approach	by Surface Science approach
catalyst	highly dispersed, supported particles	extended surface, single crystal
pressure	high	low
principle studies	gas phase analysis, some surface analysis, kinetics: $r(P,T)$	surface analysis surface kinetics, surface structure
structure	mostly unknown	known
surface composition	mostly unknown	known
adsorbate coverages	mostly indirect, some analysis (IR)	known in detail
time dependent kinetics	difficult	yes

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Ref. 3

⑤

STRUCTURAL COMPLEXITY ⟶

④

Ref. 4

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