

# Material Concepts in Surface Reactivity and Catalysis

*Henry Wise  
Jacques Oudar*

# Contents

Preface ix

Introduction

## 1. Structural Aspects

- A. Symmetry Properties 1
- B. Crystal Planes 3
- C. Packing Fractions 7
- D. Surface Overlayers 13
- E. Catalyst Supports 16
- F. Bulk and Surface Imperfections 18
- References 23

## 2. Crystallite Morphology

- A. Surface Energy and Crystal Shape 25
- B. Metal–Support Interactions 28
- C. Surface Energy and Crystal Orientation 32
- D. Surface Energy of Multicomponent Systems 33
- References 42

## 3. Interface Equilibria

- A. Adsorption Isotherms and Isosteres 44
- B. Model Isotherms 57
- References 63

## 4. Adsorption and Desorption Kinetics

- A. Lennard–Jones Potential Curves 64
- B. Adsorption Kinetics 66
- C. Desorption Kinetics 71
- References 78

5. Binding States and Adsorbate Structures	
A. Low-Energy Electron Diffraction (LEED)	80
B. Photoemission Spectroscopy	86
C. Adsorbate-Induced Surface Reconstruction	100
References	104
6. Interface Reactions between Metals and Support Materials	
A. Metal–Support Reactions	106
B. Intermetallic Compounds	109
References	116
7. Electronic Properties of Nonmetal Catalysts	
A. Defect Structure	117
B. Point Defects	119
C. Defect Thermodynamics	121
D. Surface States	124
E. Catalytic Applications	127
References	134
8. Disorder in Multicomponent Metal Oxides	
A. Metal Oxides	135
B. Spinels	135
C. Perovskites	137
D. Scheelites	141
E. Defect Metal Oxides with Crystallographic Shear Structures	145
References	147
9. Metal Oxide Catalysis	
A. Spinels	149
B. Perovskites	153
C. Scheelites	157
References	160
10. Surface Properties of Grain Boundaries	
A. Grain Boundary Structure	162
B. Grain Boundary Energetics	171
C. Component Segregation at Grain Boundaries	176
D. Model Isotherms	178

E. Selective Segregation in Multicomponent Systems	184
F. Influence of Grain Boundary Structure on Segregation	190
References	195
<b>11. Oxide Layer Formation on Metal Surfaces</b>	
A. General Considerations	199
B. Nucleation and Growth of Oxide Layer	201
C. Diffusion-Controlled Metal Oxidation	205
D. Metal Oxidation Controlled by Interfacial Reaction	216
E. Formation of Volatile Species	219
F. Formation of Epitaxial Oxide Layers	222
G. Stress Effects	224
H. Oxidation of Alloys	231
References	237
<b>12. Metal–Electrolyte Interfaces</b>	
A. General Considerations	239
B. Equilibrium at Metal–Electrolyte Interfaces	240
C. Adsorption at Metal–Electrolyte Interfaces	242
D. Kinetics of Metal Deposition	249
References	254
<b>Index</b>	<b>257</b>