Contents

Preface IX
List of Contributors XIII

1 Chirality at Metal Surfaces 1
Chris J. Baddeley and Neville V. Richardson
1.1 Introduction 1
1.1.1 Definition of Chirality 1
1.1.2 Nomenclature of Chirality: The (R),(S) Convention 2
1.2 Surface Chirality Following Molecular Adsorption 4
1.2.1 Achiral Molecules on Achiral Surfaces 4
1.2.2 Lattice Matching 8
1.2.3 Chiral Molecules on Achiral Surfaces 12
1.2.4 Chiral Molecules on Chiral Surfaces 15
1.2.5 Chiral Etching 16
1.3 Chiral Amplification and Recognition 19
1.3.1 Chiral Amplification in Two Dimensions 19
1.3.2 Chiral Switching 20
1.3.3 Chiral Recognition 21
1.3.4 Prochiral Molecules Interacting with Chiral Surfaces 24
1.4 Conclusions 25
References 26

2 The Template Route to Nanostructured Model Catalysts 29
Conrad Becker and Klaus Wandelt
2.1 Introduction 29
2.2 Surfaces as Two-Dimensional Templates 31
2.3 STM Imaging of Oxide Films 34
2.4 STM Imaging of Metal Particles on Oxide Films 39
2.5 Template-Controlled Growth of Model Catalysts 44
2.5.1 Oxides as Templates 44
In Situ STM Studies of Model Catalysts  
Fan Yang and D. Wayne Goodman

In Situ Studies of Model Catalysts

3.1 Introduction  
3.2 Instrumentation  
3.3 Visualizing the Pathway of Catalytic Reactions  
3.3.1 Imaging of Adsorbates and Reaction Intermediates  
3.3.2 Imaging Chemisorption on Metals  
3.3.3 Determining the Sites for Chemisorption on Oxide Surfaces  
3.3.4 Visualizing Reaction Intermediates and the Mechanism of Hydrogen Oxidation  
3.3.5 Measuring the Reaction Kinetics of CO Oxidation  
3.4 Metal Surfaces at High Pressures  
3.5 In Situ Studies of Supported Model Catalysts  
3.5.1 Monitoring the Growth Kinetics of Supported Metal Catalysts  
3.5.2 Studies of the SMSI Effect  
3.5.3 Sintering Kinetics of Supported Au Clusters  
3.6 Outlook  

References

Theory of Scanning Tunneling Microscopy and Applications in Catalysis  
Gilberto Teobaldi, Haiping Lin, and Werner Hofer

4.1 Catalysis and Scanning Tunneling Microscopy  
4.2 Image Formation in an STM  
4.3 Simulating Tunneling Currents  
4.4 Simulating Chemical Reactivity  
4.5 Catalytic Water Production  
4.5.1 TiO₂: A Catalytic Model System  
4.6 Outlook  

References

Characterization and Modification of Electrode Surfaces by In Situ STM  
Dieter M. Kolb and Felice C. Simeone

5.1 Introduction  
5.2 In Situ STM: Principle, Technical Realization and Limitations  
5.2.1 Principle Considerations for In Situ Operation  
5.2.2 Technical Realization  
5.2.2.1 Tip Preparation and Isolation  
5.2.2.2 Electrochemical Cell  
5.2.2.3 Vibration Damping  

References
5.2.3 Limitations 127
5.3 Imaging Single-Crystal Surfaces of Catalytically Relevant Systems 128
5.3.1 Preparation and Imaging of Metal Single-Crystal Surfaces 128
5.3.2 Bimetallic Surfaces 130
5.4 Strategies for Nanostructuring Surfaces 132
5.4.1 Oxidation–Reduction Cycles for Roughening and Faceting Surfaces 132
5.4.2 Surface Modification by an STM: An Overview 134
5.4.3 Metal Nanocluster Deposition via Jump-to-Contact 139

References 144

6 STM Imaging of Oxide Nanolayer Model Systems 147
   Falko P. Netzer and Svetlozar Surnev
6.1 Introduction 147
6.2 Experimental Aspects and Technical Developments 149
6.3 Case Studies: Selected Oxide–Metal Systems 152
6.3.1 Alumina Nanolayers on NiAl Alloys 152
6.3.2 Titanium Oxide Nanolayers 155
6.3.3 Vanadium Oxide Nanolayers 159
6.3.4 Iron Oxides on Pt(1 1 1) 169
6.3.5 Nickel Oxide Nanolayers 173
6.3.6 Ceria Nanolayers on Metal Surfaces 177
6.4 Synopsis and Outlook 182
   References 183

7 Surface Mobility of Atoms and Molecules Studied with High-Pressure Scanning Tunneling Microscopy 189
   Gabor A. Somorjai, Feng Tao, and Derek Butcher
7.1 Introduction 189
7.2 Characterization of Surface Mobility of Molecules and Atoms 189
7.3 High-Pressure STM Technique and Instrumentation 191
7.4 Mobility and Flexibility of Catalyst Surfaces at High-Pressure High-Temperature Reaction Conditions 197
7.5 Adsorbate Mobility During Catalytic Reactions 206
7.5.1 Ethylene Hydrogenation on Pt(1 1 1) 207
7.5.2 Hydrogenation of C6 Cyclic Hydrocarbons on Pt(1 1 1) 209
7.5.3 CO/NO Coadsorption on Rh(1 1 1) 213
7.6 Summary 216
   References 216
# 8 Point Defects on Rutile TiO$_2$(1 1 0): Reactivity, Dynamics, and Tunability

*Chi L. Pang and Geoff Thornton*

## 8.1 Introduction

## 8.2 Methods

## 8.3 Water Dissociation at Oxygen Vacancies and the Identification of Point Defects

## 8.4 O$_2$ Dissociation at Oxygen Vacancies

## 8.5 Alcohol Dissociation at Oxygen Vacancies

## 8.6 Diffusion of Oxygen Vacancies and Surface Hydroxyl

## 8.7 Tuning the Densities of Oxygen Vacancies and Surface Hydroxyl on TiO$_2$(1 1 0)

## 8.8 Outlook

## References

## Index