



Foundations of Surface Science

Stephen J. Jenkins

Professor of Physical and Computational Surface Chemistry

Yusuf Hamied Department of Chemistry, University of Cambridge

OXFORD
UNIVERSITY PRESS

Contents

Preface	v
1 Thermodynamics	1
1.1 Introduction	1
1.2 Dividing plane and surface excess	1
1.3 Specific surface energy and surface free energy	4
1.4 Surface tension and surface stress	5
1.5 Surface curvature and its consequences	11
1.6 Surfactants and the Gibbs isotherm	14
1.7 Gas/solid isotherms and relative coverage	17
1.8 Heats of adsorption and lateral interactions	22
1.9 Exercises	25
1.10 Summary	25
Further reading	26
2 Symmetry and Structure	27
2.1 Introduction	27
2.2 Bulk lattices and crystals	27
2.3 Miller indices and ideal surfaces	30
2.4 Relaxation and reconstruction	37
2.5 Notation for superstructure	40
2.6 Reciprocal space	42
2.7 Exercises	45
2.8 Summary	46
Further reading	47
3 Electronic Structure	48
3.1 Introduction	48
3.2 Surface dipole and work function	48
3.3 Surface-localised electronic states	56
3.4 Adsorbate-surface bonding	64
3.5 Exercises	68
3.6 Summary	69
Further reading	70

4 Kinetics and Dynamics	71
4.1 Introduction	71
4.2 Adsorption	71
4.3 Desorption	78
4.4 Vibration	82
4.5 Reaction	87
4.6 Exercises	91
4.7 Summary	91
Further reading	92
5 Techniques	94
5.1 Introduction	94
5.2 Electron diffraction techniques	95
5.3 Scanning probe techniques	97
5.4 Photoemission techniques	102
5.5 Auger Electron Spectroscopy (AES)	105
5.6 Near-Edge X-ray Absorption Fine Structure (NEXAFS)	107
5.7 Molecular beam techniques	108
5.8 Vibrational spectroscopies	112
5.9 Density Functional Theory (DFT)	115
5.10 Exercises	120
5.11 Summary	121
Further reading	121
Glossary	123
Index	128