

Contents

Physics of solid surfaces

Subvolume a: Structure

1 General introduction (G. CHIAROTTI)	1
1.1 Motivations for a Landolt-Börnstein volume on surface physics	1
1.2 Outline of the volume	2
1.3 How to consult the volume	12
1.4 List of frequently used symbols and abbreviations	13
1.5 Conversion tables	20
1.6 Crystal structures and bulk lattice parameters of materials quoted in the volume	21
1.7 References for 1	27
2 The structure of surfaces	29
2.1 The structure of ideal surfaces (J.F. NICHOLAS)	29
2.1.1 Introduction	29
2.1.1.1 Definitions	29
2.1.1.2 Description of a half-crystal defined by an (hkl) plane	30
2.1.1.3 Symmetry	31
2.1.1.3.1 Symmetry of a half-crystal	31
2.1.1.3.2 Symmetry of a surface layer	31
2.1.1.4 Coordination of surface atoms	34
2.1.1.4.1 Theory	34
2.1.1.4.2 Results for nearest neighbour bonds in face- and body-centred cubic crystals	35
2.1.1.5 Models of surfaces	37
2.1.1.5.1 The terrace-ledge-kink (TLK) model	37
2.1.1.5.2 Ball models of surfaces	40
2.1.1.6 Some useful crystallographic formulae	40
2.1.2 Surface diagrams	42
2.1.2.1 Positions of surface atoms in particular surfaces	42
2.1.2.1.1 Face-centred and body-centred cubic crystals	42
2.1.2.1.2 NaCl and diamond type structures	55
2.1.2.1.3 Hexagonal close-packed structures	102
2.1.2.2 Conversion formulae and extension to other atoms	123
2.1.3 References for 2.1	124
2.2 Surface reconstruction and relaxation (A. FASOLINO, A. SELLONI, A. SHKREBTII)	125
2.2.1 Introduction	125
2.2.1.1 Outline	125
2.2.1.2 Relaxation and reconstruction	126
2.2.1.3 Surface periodicity: notations for surface structures	128
2.2.1.4 Techniques	129
2.2.1.5 Surface preparation	130
2.2.1.6 Models of reconstruction	130

2.2.2 Data	131
2.2.2.1 Metals	131
2.2.2.2 Semiconductors and insulators	171
2.2.3 References for 2.2	208
2.3 Structural defects at surfaces (H. HENZLER, W. RANKE)	225
2.3.1 Introduction	225
2.3.1.1 Preliminary remarks	225
2.3.1.2 Methods of investigation	228
2.3.1.2.1 Microscopy	229
2.3.1.2.2 Diffraction	230
2.3.1.2.3 Ion scattering	231
2.3.1.2.4 Other methods	231
2.3.2 Data	232
2.3.2.1 Experimentally observed stability of surfaces, stepped surfaces	232
2.3.2.1.1 Metals and metal alloys	233
2.3.2.1.2 Group IV semiconductors	278
2.3.2.1.3 III-V semiconductors	312
2.3.2.1.4 Chalcogenides	321
2.3.2.1.5 Halides	324
2.3.2.2 Phase transitions	330
2.3.2.2.1 Roughening transition of stepped metal surfaces	330
2.3.2.2.2 Phase transitions on low index metal surfaces	336
2.3.3 References for 2.3	352