

Preface	vi
-------------------	----

<i>Chapter 1</i> (J.W. Davenport and P.J. Estrup).	
--	--

Hydrogen on metals	1
1. Introduction.	1
2. Structure	2
2.1 Atomic geometry	2
2.2 Binding energy	7
2.3 Vibrational modes	9
2.4 Nature of the bond	11
2.4.1 Theoretical investigations	11
2.4.2 Experimental investigations	19
2.5 Hydrogen–hydrogen interactions	22
3. Dynamics	25
3.1 Overview	25
3.2 Sticking probability	28
3.3 Diffusion	30
3.4 Thermal desorption	30
3.5 Sorption	32
Acknowledgements	33
References	33

<i>Chapter 2</i> (R. Raval, M.A. Harrison and D.A. King)	
--	--

Nitrogen adsorption on metals	39
1. Introduction.	39
1.1 The review in outline	39
1.2 The nitrogen molecule	40
1.3 Organometallic dinitrogen complexes	42
1.4 Inorganic metal nitrides	43
2. Nitrogen on palladium	45
2.1 Adsorption of dinitrogen	45
2.2 Adsorption of N ₂ activated in the gas phase	45
3. Nitrogen on copper	47
3.1 Adsorption of dinitrogen	47
3.2 Adsorption of N ₂ activated in the gas phase	47
4. Nitrogen on ruthenium	50
5. Nitrogen on nickel	51
5.1 Introduction	51
5.2 Nitrogen adsorption on Ni{100}.	54
5.2.1 Structural studies	54
5.2.2 Thermodynamic measurements	54
5.2.3 Electronic properties	56
5.3 Nitrogen adsorption on Ni{111}.	61
5.3.1 Physisorbed state	61
5.3.2 Chemisorbed states	62
5.4 Nitrogen adsorption on Ni{110}.	63
5.4.1 Electronic properties	63

5.4.2 Kinetic and thermodynamic data	67
5.4.3 Structural studies	68
5.5 Activated molecular and atomic nitrogen adsorption on nickel	72
6. Nitrogen on iron	75
6.1 Introduction	75
6.2 Nitrogen on polycrystalline iron	75
6.3 Nitrogen on Fe{111}	76
6.3.1 β -Nitrogen	76
6.3.2 α -, γ - and δ -nitrogen on Fe{111}	78
6.3.3 Kinetics and thermodynamics of N ₂ on Fe{111}	81
6.4 Nitrogen on Fe{100}	88
6.5 Nitrogen on Fe{110}	90
6.6 Nitrogen on Fe{1210}	92
6.7 Bulk diffusion of nitrogen in iron	92
7. Nitrogen adsorption on tungsten	93
7.1 Introduction	93
7.1.1 The β state	94
7.1.2 The α state	95
7.1.3 The γ state	95
7.2 Nitrogen adsorbed on W{110}	96
7.2.1 γ -Nitrogen	96
7.2.2 β -Nitrogen	98
7.3 Nitrogen adsorbed on W{111}	102
7.4 Adsorption of N ₂ on W{100}	103
7.4.1 The γ state	103
7.4.2 The β state	104
7.5 Nitrogen adsorption on high index planes of tungsten	118
8. Summary	123
References	124

Chapter 3 (C.R. Brundle and J.Q. Broughton)

The initial interaction of oxygen with well-defined transition metal surfaces	131
1. Introduction	131
1.1 General	131
1.2 The nature of the clean surface	134
1.3 Molecular oxygen adsorption	135
1.4 Conversion to "oxide"	136
1.5 Unwanted co-adsorption reactions	137
2. Chromium, molybdenum and tungsten	137
2.1 General	137
2.2 Chromium	140
2.2.1 Cr{110}	140
2.2.2 Cr{100}	141
2.2.3 Cr{111}	146
2.2.4 Summary of Cr results	146
2.3 Molybdenum	150
2.3.1 Mo{110}	151
2.3.2 Mo{100}	152
2.3.3 Mo{111}	157
2.3.4 Summary of Mo results	158
2.4 Tungsten. General	159
2.5 W{110}	160

2.5.1	Some aspects of very low temperature adsorption	161
2.5.2	0–0.5 Monolayer O range. S, θ measurements	163
2.5.3	0–0.5 Monolayer O range. Location of O normal to surface	168
2.5.4	0–0.5 Monolayer O range. Geometric structure.	170
2.5.5	0–0.5 Monolayer range. Phase diagram	174
2.5.6	0–0.5 Monolayer range. Electronic structure effects	178
2.5.7	Greater than 0.5 monolayer O range. General	181
2.5.8	Greater than 0.5 monolayer O range. S, θ measurements	182
2.5.9	Greater than 0.5 monolayer O range. Location of O normal to the surface.	183
2.5.10	Greater than 0.5 monolayer O range. Geometric structure	185
2.5.11	Greater than 0.5 monolayer O range. Phase diagram	187
2.5.12	Greater than 0.5 monolayer O range. Electronic structure effects.	187
2.5.13	Diffusion of O on W{110}	188
2.5.14	Stepped W{110} surfaces	190
2.6	W{100}	198
2.6.1	S, θ measurements	199
2.6.2	Location of O normal to the surface	202
2.6.3	Geometric structure.	208
2.6.4	Electronic structure effects	219
2.6.5.	Diffusion of O on W{100} surfaces	223
2.7	W{111}	225
2.7.1	S, θ measurements	225
2.7.2	Location of O normal to the W{111} surface.	228
2.7.3	Electronic structure effects	230
2.7.4	Adsorption geometries for W{111}/O	232
2.7.5	Summary.	233
2.8	ESD and PSD on W/O surfaces	234
2.8.1	W{110}.	238
2.8.2	W{100}.	241
2.8.3	W{111}.	250
2.8.4	Conclusions	252
2.9	Thermal desorption from W/O surfaces	254
2.9.1	W{110}.	256
2.9.2	W{100}.	257
2.9.3	W{111}.	257
2.10	Secondary ion mass spectroscopy (SIMS) from W/O surfaces	258
2.11	Summary of tungsten data	264
2.11.1	300 K and below	264
2.11.2	High temperature	265
2.11.3	Steps and defects	267
2.12	General comparison of trends for Cr, Mo, W	267
3.	Nickel	268
3.1	Ni{100}.	270
3.1.1	General reaction scheme. 300 K and above.	270
3.1.2	General reaction scheme. Low temperature	275
3.1.3	Problems of co-adsorption and reaction	276
3.1.4	Geometric structure of p(2 × 2) O and c(2 × 2) O	278
3.1.5	Thin oxide epitaxy and geometry	289
3.1.6	Electronic structure aspects	292
3.1.7	Kinetics and mechanisms. General	305
3.1.8	Kinetics and mechanism of chemisorption.	306
3.1.9	Kinetics and mechanism of oxide nucleation and island growth	314
3.2	Ni{110}.	321

3.2.1	General reaction scheme. 300 K and above.	321
3.2.2	General reaction scheme. Low temperature	323
3.2.3	Geometric structure of chemisorbed species. General.	323
3.2.4	Geometry of the p(2 × 1) structure. $\theta \approx 0.25\text{--}0.3\text{ mL}$	327
3.2.5	Geometry of the p(3 × 1) initial structure. $\theta \approx 0.15\text{ mL}$	333
3.2.6	Geometry of the p(3 × 1) final structure. $\theta \approx 0.3\text{--}0.6\text{ mL}$	333
3.2.7	Summary of chemisorbed structures	335
3.2.8	Geometric structure of the oxide species	336
3.2.9	Electronic structure aspects	338
3.2.10	Kinetics and mechanisms. General	341
3.2.11	Kinetics and mechanism of chemisorption.	341
3.2.12	Kinetics and mechanism of oxide nucleation and island growth	347
3.3	Ni{111}.	351
3.3.1	General reaction scheme. 300 K and above.	351
3.3.2	General reaction scheme. Low temperature	352
3.3.3	Phase diagram	353
3.3.4	Geometric structure of chemisorbed species	356
3.3.5	Geometric structure of the oxide species	360
3.3.6	Electronic structure aspects	362
3.3.7	Kinetics and mechanisms. General	364
3.3.8	Kinetics and mechanism of chemisorption.	365
3.3.9	Kinetics and mechanism of oxide nucleation and island growth	368
3.4	Intercomparison of Ni{100}, {110}, and {111} surfaces.	370
3.4.1	General reaction scheme.	370
3.4.2	Geometric structure of chemisorbed and oxide species	371
3.4.3	Electronic structure of chemisorbed and oxide states.	372
3.4.4	Kinetics and mechanism of chemisorption and initial oxidation	373
3.5	Secondary ion mass spectroscopy (SIMS) of Ni/O surfaces.	375
4.	Conclusions	379
	References.	381

Chapter 4 (J.C. Campuzano)

	The adsorption of carbon monoxide by the transition metals	389
1.	Introduction.	389
2.	The carbon monoxide molecule	390
3.	The bonding of CO in metal carbonyls	392
4.	The bonding of CO to bulk metal surfaces	393
5.	Plan of this review.	395
6.	Titanium	396
7.	Vanadium.	397
8.	Chromium.	397
9.	Manganese	399
10.	Iron	400
11.	Cobalt	402
11.1	Co(0001)	403
11.2	Co(1012)	405
12.	Nickel	406
12.1	Ni(100)	406
12.2	Ni(110)	409
12.3	Ni(111)	411
13.	Copper	415
13.1	Cu(110)	418
13.2	Cu(111).	419

14. Zirconium	421
15. Niobium	422
16. Molybdenum	422
16.1 Mo(100)	422
16.2 Mo(110)	424
17. Ruthenium	425
17.1 Ru(0001)	425
17.2 Other Ru faces	431
18. Rhodium	431
18.1 Rh(111)	432
18.2 Rh(110)	434
19. Palladium	435
19.1 Pd(100)	435
19.2 Pd(110)	438
19.3 Pd(111)	439
19.4 Pd(210)	440
19.5 Other surfaces	441
20. Silver	442
21. Tantalum	443
22. Tungsten	444
22.1 W(110)	445
22.2 W(100)	446
22.3 W(111)	449
23. Rhenium	449
24. Iridium	451
25. Platinum	453
25.1 Pt(111)	453
25.2 Pt(110)	456
25.3 Pt(100)	458
Acknowledgements	459
References	460
Index	471