

List of Tables

- 1.1 Physical and chemical properties of atomic, gaseous, liquid and solid hydrogen 10
- 3.1 Summary of experimental NMR parameters that can be related to hydrogen isotope diffusion properties 102
- 3.2 Summary of hydrogen diffusion parameters for TiFeH_x and related systems 116
- 3.3 Summary of hydrogen diffusion parameters for Mg_2NiH_x 117
- 3.4 Summary of LaNi_5H_x diffusion parameters 118
- 3.5 Effects of alloy substitution on diffusion behaviour in $\text{LaNi}_{5-x}\text{M}_x\text{H}_z$ systems 119
- 3.6 Diffusion parameters for hydrides of Laves alloys 119
- 3.7 Summary of hydrogen diffusion parameters for A_2BH_x 120
- 3.8 Comparison of activation energies U (meV) obtained from different proton NMR parameters 120
- 4.1 Comparison of LaNi_5 – H kinetics data 173
- 4.2 Kinetic model for iron-titanium hydrogenation/dehydrogenation 187
- 5.1 Intermetallic – impurity interactions 206
- 5.2 Damage model parameters for various intermetallic – impurity interactions 207
- 5.3 Comparison of H_2 storage parameters 211
- 5.4 a–c Summary of large stationary hydride vessels 214–215
- 5.5 Energy density of automotive power sources 217
- 5.6 a–c Summary of vehicular hydride systems 218–219
- 5.7 Volume of heat-storage systems for 100 kWh (approximate heat consumption per winter day of a German one-family house) 229
- 5.8 Summary of hydride heat pump and refrigerator demonstrations 235
- 5.9 Specification of the Ni-metal hydride rechargeable battery of AA size, AB_5 type alloy, and C size, Ti-Ni-Zr-V-Cr alloy 244
- 6.1 Some properties of nuclear probes which are often used in perturbed angular correlation experiments 264
- 6.2 Summary of published PAC experiments on metal-hydrogen systems 281
- 7.1 Some resonant scatterers with significant temperature effect 296
- 7.2 Experimental values of the temperature effect R (77 K, 300 K, 135°), for ^{62}Ni and ^{48}Ti in several compounds and deduced values of θ_D 299

- 7.3 Measured scattered intensity ratios R , with an accuracy of about 2 %, normalized to pure nickel (after background and self-absorption corrections), and deduced effective temperature $T_{\text{eff, Ni}}$ at $T = 298 \text{ K}$ 301

Subject Index

- A_2B , A_2B hydride 202, 239
- A_2B_{17} diffusion Table 3.7; 239
- AB , AB hydride 202, 207, 212, 216
 - impurity effect 206
- AB_5 , AB_5 hydride 73, 207, 212, 226, 227, 235, 242
- AB_2 , AB_2 hydride 202, 211, 220, 239, 243
 - diffusion Table 3.7
 - kinetics 189
 - surface 80
- Absorption pressure 201
- Acoustic emission 171
 - vibration 97, 112
- Actinide 16
- Activation 1, 15, 23, 40, 50, 177, 183, 202, 227, 243
 - barrier 18, 22, 29, 41, 65, 70
 - energy 1, 17, 32, 120, 167, 279
 - getter 71, 227
- Activity 37
- Actuator 206, 237
- Adatom 22, 31
- Additive 81
- Adsorbate 23, 28
- Aftereffect, elastic 101
- Al 220
 - composites 204, 205
- Alkali metal 37
- Ammonia
 - purge gas 222
 - synthesis 239, 240
- Amorphization 4
- Amorphous alloy hydride 42, 83, 137, 152, 243, 281
 - diffusion, dynamics 137
 - relaxation 99
- Anatase 38
- Anderson impurity model 31
- Anderson-Newns 31
- Angular distribution 33
- Anharmonic, anharmonicity 33, 115, 147
- Annealing 201, 209
- Annihilation 33
- Antibonding level 29
- Applications 2; Chap. 5
- Arrhenius factor 33, 167, 186, 276
- Atom probe 24
- Atomic H 21, 84, 210, 239
- Auger electron spectroscopy AES 24, 46, 51, 191
- Augmented plane waves APW 39
- Automobile, Automotive Table 5.5; 3, 217
- Ball-milling 180
- Band
 - mode 112
 - structure 28
- Battery Table 5.5; 240, 243
- Beryllium-filter 115
- Bimetallic catalyst 16
- Binder 243
- Bloch theory 28
- Blocking 39
- Bloembergen model BPP 105
- Bloembergen, Purcell, Pound analysis BPP 124
- Bond length 29
- Bonding 21
 - level 29
 - strength 294
- Born/Haber cycle 32
- Born-Mayer potential 151
- Breakthrough
 - front 222
 - phenomena 223
- Bus 217
- Capacity 209
 - electrochemical 240
 - gas 221
 - loss 221
 - rule of reversed capacity 300
- $CaNi_5$, $CaNi_5$ hydride 209, 225, 229, 240, 245
- Carbon 40

- Catalysis, catalysts 15, 16, 23, 40, 43, 181, 210, 239
 ammonia 239
 bimetallic 16
 dissociation 65, 225
 electrochemical 240
 ignition 246
 methanation 239
 Catalytic activity 36
 Cd electrode 242
 Charge transfer 34
 Chemical
 bond 18
 diffusion coefficient 138
 diffusion constant 123
 potential 22
 Chemisorption 15, 21, 24, 154, 168
 activated 18
 dissociative 17
 energy 31
 heat of 17
 model 24
 on metal oxide 35
 Chudley Elliott model CE 108
 Clean surface 50
 Cluster, clustering 18, 28, 179
 calculation 36
 Coating 36, 37
 Coefficient of performance 233
 Coercivity 28
 Coherent 276
 potential approximation CPA 28
 Cohesive energy 29
 Cold fusion 9, 34
 Composite 220
 Compressor 202, 206, 213, 227, 228, 237, 245
 Conducting polymers 243
 Conduction band 35
 Container, containment Tables 5.4, 5.6; 203, 211, 215
 bulging 203
 composite 220
 rupture 203
 Contamination 40
 Conversion-electron Mössbauer spectroscopy
 CEMS 54
 Cooling 220
 Coordination number 24
 Core level shift 27, 32, 51
 Corrugation function 52, 59
 Cosine distribution 56
 Costs 202, 228, 236
 Count rate 260
 Coverage 35
 Cu, Cu-H 65
 Cycle, cyclic 9, 202, 203
 life 206, 242
 stability 208
 D-D fusion rate 46
 d-transition metal 1, 16
 Damage
 function 208
 model, exponential 207
 model parameter Table 5.2
 Debye temperature 294, 298
 Debye-Waller factor 113, 115, 259
 Decohesion 3
 Decrepitation 8, 203, 242, 244
 Defect 18, 22, 36, 169
 Density
 functional method 24
 of state 25, 39
 Dephasing of the precession 266
 Depth profiling 50, 54, 80
 Deuterium D, D₂ 15, 39, 46, 223, 224, 278
 Diffraction 21
 Diffusion Chap. 3; 1, 18, 36, 98, 107, 116, 259;
 Sect. 6.5; 224, 275, 278
 coefficient 10, 111, 172, 277
 of H isotopes 278
 Direct recoil 3, 52, 285
 spectroscopy 49
 Disordered 20, 28
 alloy surface 28
 Disproportionation 9, 208, 234, 237
 Dissociation, dissociative 17, 22, 41, 70, 81, 84, 225
 adsorption 17
 chemisorption 22, 29
 pressure 224
 Doppler 295
 Dynamics 2
 bulk Chap. 3
 surface 33
 Economic 215, 220
 Effective medium 25, 31
 Elastic incoherent structure factor EISF 136
 Electric
 energy storage 245
 field gradient EFG 259, 262, 267
 or magnetic field 34
 peak shaving 212
 quadrupole moments 259
 storage 245
 Electrical resistivity 171
 Electrochemical 137

- catalysts 240, 244
- cell 3
- Electrode 17, 243
 - reaction 240
- Electrolyte metal interface 34
- Electrolyzer 244
- Electromigration 2, 5
- Electron
 - energy loss spectroscopy EELS 35, 50, 53
 - hole pair excitation 33, 34, 47
- Electronegative 37
- Electronic
 - properties 24
 - structure 28, 62
- Electropositive 37
- Embedded atom 25, 31
 - method 63
 - theory 21
- Embrittlement 2, 11, 15, 36, 40, 210, 244
- Energy density Tables 5.5, 5.9; 242
- Enthalpy 23, 230
 - change ΔH 198
- Entropy change ΔS 198
- Environment 2
- Epitaxial 37
- Equation of state 11
- European community 212
- Excitation 33
- Expansion 203, 213
- Exponential damage model 207

- F centre 37
- FeTi, FeTi hydride 197, 201, 205, 208, 212, 216, 220, 229, 240
 - applications Chap. 5; 217
 - diffusion Table 3.2
 - gaseous impurity 206
 - historical 197
 - kinetics Table 4.2; 183
 - plateau slope 201
 - surface 76
- Fermi level 39
- Field-gradient spin-echo FGSE 104
- Fire detector 3, 238
- First wall interaction 17
- Force constant 33
- Forklift trucks 217
- Frozen phonon 145
- Fuel 216
 - cell 243, 245
 - storage 216
- Fusion 9, 17

- γ - γ cascade 259
- γ -ray 259
- Gas
 - impedance 203, 204
 - permeability 204
- Getter 15, 23, 40, 82, 226
 - alloys 45
- Gorsky effect 2, 99, 112, 139, 141
- Grain boundary 81
- Grinding 181

- H₂-D₂ exchange reaction 49, 54, 76
- Hall effect, proton 2
- He diffraction 21, 59
- Heat
 - ballast 175
 - capacity 166
 - engine 202, 206, 228, 237
 - exchange Tables 5.4, 5.6; 211, 220
 - of chemisorption 17, 21
 - of dissociation 17
 - of physisorption 17, 21
 - of reaction 203, 228
 - of segregation 23
 - of surface segregation 28
 - pump 199, 202, 203, 206, 228, 234, 236, 237
 - storage 205, 228
 - transfer 166, 174, 184, 204, 213, 222, 228
 - upgrading 233
- Heavy metal 40
- Helium 4, 173
 - atom diffraction 52
- Heterogeneous 22, 165
- Hf, Hf alloy, hydride PAC Table 6.2
- High pressure cell 8
- High purity H₂ 212, 220
- Homogeneity 23
- Hybridization 30
- HYCSOS system 234
- Hydride
 - actuator 238
 - heat pump 231
- Hydrogen H, H₂
 - as a probe 22
 - economy 211
 - electrode battery 244
 - environmental effect 201
 - equation of state 11
 - evolution cathode 244
 - excitation 6
 - fuel 216
 - metallic 4
 - occupancy 156
 - oxygen surface interaction 292
 - potential 6, 33, 145

- Hydrogen H, H₂
 - recovery 222
 - separation 222
 - site determination 148
 - amorphous metals 152
 - intermetallic compounds 148
 - metal oxides 153
 - surface 153
 - solid 4
 - storage 211
 - vibration 143
- Hydrogenation 239
- Hyperfine interaction 263
- Hysteresis 200, 230, 234, 237
 - dynamic 201
 - static 201
 - temperature 201
- Impurity 18
 - effect 206
 - hydride surface interaction 206
- Incoherent 104, 276
 - inelastic neutron scattering IINS 53
 - scattering 110, 136
- Induction period 179
- Inelastic scattering 35, 106
 - electron 53
 - neutron Chap. 4
 - neutron at surface 53
- Inert gas blanketing 221
- Infrared absorption 35
- Inhibition, inhibitor 39
- Innocuous 206
- Intermetallic
 - compounds, PAC 271
 - impurity interaction Table 5.1; 206, 207
- Internal friction 139
- Intrinsic 166
- Inverse
 - isotope effect 224
 - photoemission 32, 51
- Isomer shift 259
- Isotope H, D, T, μ^+ 1, 15, 223, 278
 - effect 46, 224
 - exchange 49
 - inverse 224
 - normal 224
 - scrambling 173
 - separation 46
- Jellium 24, 31, 34
- Johnson-Mehl equation 177
- Jump
 - frequency, rate 1, 276
 - matrix 109, 110
- Kinetics Chap. 4; 2, 17, 35, 64, 81, 165, 206, 215
- Kink 22
- KOH electrolyte 242
- LaNi, LaNi₅ hydride 201, 208, 212, 222, 229, 238, 240, 242
 - diffusion Table 3.4
 - electrode 242
 - gas separation 222
 - gaseous impurity 206
 - historical 197
 - kinetics Table 4.1
 - neutron scattering 122, 131
 - NMR 131
 - plateau slope 201
 - poison 206
 - surface 72
- LaNi_{5-x}M_x, LaNi_{5-x}M_x hydride 209, 222, 226, 239, 242
- Larmor frequency 263
- Lattice gas model 56
- Laves phase, Laves phase hydride 130, 189
 - (C15) structure 271
 - diffusion Table 3.6
- Lennard-Jones potential 18
- Life prediction 208
- Liquid alloy 4
- Liquid LH₂ 211, 220, 238
 - boil-off 238, 239
 - vehicle 220
- Local
 - electric field gradient EFG 259
 - magnetic field 259, 263
 - mode 97
 - probe 22, 259
- Localized mode 112
- Loss, capacity 221
- Low energy electron diffraction LEED 50, 51
- Magnetic
 - dipole moments 259
 - moment 37
 - recording 43
 - structure 28
 - surface 28
 - susceptibility 73, 78, 147
- Many-body effect 24
- Martensitic transition 271
- Mass transfer 166, 206, 230
- Mean field theory 21
- Mean residence time 277
- Mechanically driven heat pump 230

- Metal
 - foam 204
 - oxyde 35, 153
 - surface 153
- Metal-oxide-semiconductor device with Pd-gate
 - Pd-MOS 54, 67
- Metallic H, metallization 4, 8
- Metallic glasses 99, 137
- Methanation 239, 240
- Mg, MgH₂ 81, 178, 291
- Mg alloy, Mg alloy hydride 81, 178, 215
- Mg₂Cu 216
- Mg₂Ni, Mg₂Ni hydride 81, 182, 201, 209, 211, 216, 220, 240
 - diffusion Table 3.3
 - kinetics 178, 215
 - plateau slope 201
 - surface 81
- Microencapsulation 205, 242
- Microstructure 184, 243
- Migration 31, 33
- Mine vehicles 220
- Mischmetal Mm 184, 200, 239
- Missing-row model 60
- MmNi₅, MmNi₅ hydride 200, 239
- Molecular beam 21
- Mössbauer effect 99
- Motional narrowing 279
- Motor vehicle 216
- Multi
 - component alloy 42
 - component electrodes 242
 - layer 84
 - phonon processes 34
 - stage 228
- Muon 1
 - spin resonance 111
 - spin rotation 125
- Network material 204
- Neutron diffraction, scattering Chap. 3; 2, 21, 104, 192
 - at surface 35
 - inelastic 106
 - quasielastic 104
- Neutron vibrational spectroscopy 112
- Ni-Zr, Ni-Zr hydride 197, 227, 281
- Ni, Ni-H 55
- Ni-hydrogen battery, Ni-Cd batteries 240, 242
- Noble metal surface 29
- Nuclear
 - conversion 276
 - probe 54
 - reaction 98
- Nuclear magnetic resonance NMR 2, 97, 101
 - amorphous, glassy, metal 141
- Nuclear resonant scattering of γ -rays Chap. 7; 3, 294
- Nucleation and growth 2, 17, 77, 167, 177, 181, 186
- Nuclei, radioactive 259
- Optical
 - mode 97
 - vibration 112
- Ordered 28
 - phase 57
 - surface 20
- Order-disorder 4
 - transformation 63
- Ortho para conversion 34, 46
- Overcharging 243
- Overlayer 37, 38, 84
- Overpotential 40
- Oxidation 38, 42, 45, 50
- Oxide
 - layer 38, 179
 - surface 36
- Oxygen 37, 38, 39, 221, 243; Table 5.1
 - diffusion 46
- Packing 203
- Pairing-row model 60
- Paramagnetic relaxation 103, 131
- Particle size 203
- Passivation 41
- Pauli
 - paramagnetic 78
 - repulsion 29
- Pd, Pd-H 60, 147, 224, 267; Table 6.2; 309
- Permanent magnet 8, 15, 17, 43, 244
- Permeation 1, 37, 40
- Perturbed angular correlation PAC Chap. 6; Table 6.2; 2, 259
- Phase
 - diagrams 267
 - transition 177
- Phonon 33
- Photoelectron diffraction XPD 51
- Photoelectron spectroscopy UPS, XPS 24, 46, 50, 51
- Photoemission 32, 50
- Physisorption 15, 21, 29
 - heat of 17
- Plasma-wall interaction 15
- Plasmon 24, 66
- Plateau
 - pressure 198, 209, 224

- Plateau
 - slope 200, 230, 234
- Point charge model 267, 268
- Poison, poisoning 1, 23, 32, 37, 40, 177, 192, 204, 206, 228
- Polarization 29, 51
- Pollution 3, 242
- Polymer 243
- Potential energy 29
 - curve 18
 - surface 70
 - well 33
- Porous metallic-matrix hydrides PMH 204
- Power
 - generation 234
 - sources Table 5.5
- Precipitation 276
- Precoverage 33, 37
- Preparation techniques 9, 201
- Pressed metal hydrides PMH 192
- Pressure
 - composition isotherm 22
 - composition loop 200
 - temperature relations Chap. 5; 198
- Probe 22
- Promote, promoter 32, 37
- Prototype 212, 234
- Purification, purifier 9, 205, 208, 220, 222
- Pyrophoric, pyrophoricity 83, 209

- Quadrupole interaction 260
 - splitting 262
- Quantum
 - diffusion 275
 - phenomena 46
- Quasielastic neutron scattering QNS Chap. 3; 97, 106
 - incoherent 104

- Radioactive nuclei 259
- Raman spectroscopy 35, 49
- Raney nickel 154
- Rapid cooling 275
- Rare earth hydride 16, 40, 43, 66, 292
- Rare gas 40
- Rate
 - constant 35, 166
 - determining step 165
- Reactant 207, 228
- Reaction 206, 226
 - rate 176, 204
- Reactivation 41
- Reactor 170
 - autoclave 170
 - double wall 171
 - thin disc 170
- Recombination 225
- Recombinative desorption 17
- Reconstructed 20
- Recovery 207
- Refrigeration, refrigerator 228, 234, 236
- Relaxation 33, 278
 - anelastic 99
 - mechanical 99
 - Snoek 99
 - spin lattice 103
 - strength 101
- Remote power generation 245
- Retardant, retardation 206, 207
- Reversible capacity 200, 202
- Rotation 18
- Rotational excitation 65
- Rule of reversed capacity 302
- Rutile 36, 38

- Safety 10, 203, 209, 211, 220
- Scanning tunneling microscope STM 52, 59
- Secondary ion mass spectroscopy SIMS 53
- Selective oxidation 71, 73, 80
- Self
 - correlation function 107, 128
 - diffusion 111
 - discharge 242
- Semiconductor-metal transition 32
- Sensors
 - hydrogen 8
 - Pd-MOS 8
 - temperature 237
- Separation, separators 205, 208, 220, 223, 226
 - factor 224, 226
- SEXAFS 52
- Sieverts apparatus 169
- Simple metal surface 21, 29, 55, 69
 - oxide 36
- Slab 25, 26
 - calculation 36
- Slurry 203
- Small polaron hopping theory 277
- Snoek
 - effect 100, 138, 141
 - relaxation 99
- Solar energy 229, 234, 237, 245
 - heat 232, 236
 - powered 237
 - storage 230
- Solid
 - gas reaction 165, 167
 - hydrogen 4

- solution phase 172
- Solidification 201
- Spillover 46, 81
- Spin
 - density 26
 - echo 104
 - lattice relaxation 103
 - polarization 26, 27, 51, 78
- Sputtering 50
- Stainless steel 11
- Stationary storage 212
- Statistical distribution 268
- Sternheimer factor 267
- Sticking 18, 33, 46, 84
 - coefficient 47, 54, 57, 65
 - probability 17, 33
- Stirling engine 237
- Stochastic model 278
- Storage 199, 205, 211, 215, 220, 234
 - capacity 241
 - electric energy 245
 - electrochemical 240
 - electrode 242
 - fuel 216
 - gaseous 211
 - heat 228; Table 5.7
 - liquid 211
 - stationary 212; Table 5.4
- Strain
 - field 4
 - modulation 84
- Strength relaxation 101
- Strong metal support interaction SMSI 37, 43
- Substitutional impurities 274
- Subsurface 22, 31, 34, 37
 - hydrogen 18, 21
 - site 2, 34, 62
- Sulphur 39, 40
- Superconductivity 8, 37, 147
- Superlattice 5, 37, 84, 180
- Superparamagnetic 73
- Supersaturation 177
- Superstructure 26
- Surface 7, 15, 16, 24, 226, 228
 - activation 41, 243
 - area 203
 - cleanliness 50
 - composition 289
 - contamination 40
 - crystallographic notation 19
 - defect 36
 - density of states 26
 - diffusion 42
 - dipole layer 25
 - dynamics 33
 - effect 15, 17, 192
 - electronic structure 28, 32, 37, 39, 290
 - exchange 225
 - extended X-ray adsorption fine structure SEXAFS 52
 - hydride 21, 35, 57, 64, 66, 84, 168
 - magnetism 23, 26, 32, 67
 - migration 33, 168
 - noble metal 1, 19
 - ordered, disordered 20
 - phase 20
 - poisoning 40
 - rare earth metal 16, 32, 66
 - reactivity 175
 - reconstruction 20, 27, 57, 59
 - relaxation 20
 - segregation 16, 20, 23, 42, 71, 80, 293
 - heat 28
 - hydrogen induced 23
 - model 16, 43, 44
 - oxygen induced 23
 - semiconductor-metal transition 67
 - simple metal 1, 29
 - site 307
 - state 25, 35
 - step 22
 - structure 19, 21, 51, 76, 290
 - temperature 34
 - transition metal 1, 29
 - valence 24, 27
 - vibration 20, 33, 53
- Synchrotron radiation 50, 52
- Ta, Ta alloy, hydride PAC Table 6.2; 261, 269, 271
- Temperature
 - programmed desorption 46
 - sensor 206, 237
 - upgrading 231
- Terrace 22
- Thermal, thermally
 - conductivity 165, 204, 213, 220, 230, 237
 - desorption spectroscopy TDS 53, 191, 285, 304
 - driven 231, 233, 234
 - hydride refrigerator 234
 - system 230
- Thermodynamic
 - equilibrium 22, 33
 - factor 101
- Thermogravimetry 169, 171, 175
- Thermometers 238
- Thermotransport 2

- Ti alloy, Ti alloy hydride
 - diffusion Table 3.7
 - Jahn-Teller effect 300
 - kinetics 189
- TiFe, TiFe hydride 197, 201, 205, 208, 212, 216, 220, 229, 240
 - applications Chap. 5; 217
 - diffusion Table 3.2
 - gaseous impurity 206
 - historical 197
 - kinetics Table 4.2; 183
 - plateau slope 201
 - poison 206
 - surface 76
- Tight binding 31
 - method LCAO 25
 - model 63
- Time
 - of direct recoils TOF-DR 52, 287
 - of flight analysis 3
- TOF-DR 70
- Total energy calculation 25, 31
- Trace correlation factor 104
- Tractors 217
- Transportation 213, 215
- Transition metal 43, 55
 - oxide 35
 - surface 29
- Trap, trapping 46, 116, 128; Chap. 6.4; 208, 259, 272
 - model 125
- Tritium T, T₂ 4, 7, 46, 82, 98, 223, 227, 278
 - imaging 51
- Tunnelling 2, 34, 48, 276
 - state 272
- Two-state model 126
- Unidirectional solidification 9
- Vacuum microbalance 171
- Valance change 68
- Van 217
- Van der Waals 20, 21
 - attraction 29
- Van't Hoff 198, 227, 230, 234
- Vehicles, vehicular Table 5.6; 218
 - hydrogen storage 217
 - indoor industrial 217, 220
 - liquid hydrogen LH₂ 20
 - mine 220
 - road 216, 220
- Velocity distribution 33
- Vibration, vibrational 18, 33
 - acoustic, optical 112
 - excitation 65
 - mode 20, 33, 34
 - spectroscopy neutron 112
 - spectroscopy surface 53
 - state 33
- Volume
 - change 203, 209, 244
 - expansion 242
- Volumetry 169
- Water pumping 237
- Wind energy 245
- Work function 25, 32, 40, 50, 51
- X-ray diffraction 171
- Z+1 approximation 28
- Zr, Zr alloy, hydride Table 6.2; 197, 227, 240, 271, 303, 309
 - diffusion 141, 280
 - getter 226
 - NMR 141
 - PAC 271, 280