

Contents

LEED Intensities – Experimental Progress and New Possibilities of Surface Structure Determination

By K. Heinz and K. Müller. With 29 Figures

1. Introduction	1
2. Structural Determination by Comparison of Experimental and Calculated Intensities	3
2.1 Comparison of Theoretical and Experimental Spectra	4
2.2 Comparison of Experimental Spectra from Different Measurements	7
2.3 Sources of Experimental Error	9
2.4 Classical Methods for Intensity Measurements	13
3. New Experimental Methods for Intensity Data Collection	18
3.1 Photographic Methods	18
3.2 TV Computer Methods	20
3.2.1 Data Acquisition Rate Lower than TV Rate	21
3.2.2 Data Acquisition Rate Equal to TV Rate	27
4. Examples for Reliable Intensity Data Obtained by the New Methods	33
4.1 Influence of Sample Misalignment	33
4.2 Influence of Background Subtraction	36
4.3 Influence of Residual Gas Adsorption	38
4.4 Influence of Adsorbate Decomposition and Desorption	38
5. New Possibilities Using Modern Intensity Measurement Methods	39
5.1 Integral Intensities of Rapidly Varying Surface Systems	39
5.2 Spot Profiles of Rapidly Varying Surface Systems	42
5.3 Extension of Intensity Measurements to Varying Temperature	43
5.4 Extension of Intensity Measurements to the Medium-Energy Range	45
6. Summary and Outlook	48
References	49

Structural Studies of Surfaces with Atomic and Molecular Beam Diffraction

By T. Engel and K.-H. Rieder. With 91 Figures

1. Introduction	55
2. The Particle-Surface Interaction Potential	57
2.1 Physical Basis	57
2.2 Short Survey of Theoretical Efforts	58
2.3 Determination of the Surface Potential from Bound-State Energy Data	65
3. Quantum Theory of Particle Diffraction	71
3.1 The Corrugated Hard-Wall Model	71
3.2 Diffraction Condition and Ewald Construction	72
3.3 Calculation of Diffraction Intensities—General Method	75
3.4 Calculation of Intensities—Rayleigh Hypothesis	78
3.4.1 The GR Method	79
3.4.2 The Eikonal Approximation	79
3.5 Calculation of Intensities—Iterative Series	83
3.6 A Few Illustrative Examples	86
3.7 The Inversion Problem	90
3.8 Effects Due to the Softness of the Repulsive Potential	92
4. Inelastic Scattering of Atoms from Surfaces	93
4.1 The Dependence of the Scattering on the Time Scale of the Interaction	93
4.2 The Debye-Waller Factor in the Time-Dependent Interaction Regime	95
4.3 The Size Effect in the Debye-Waller Factor for Atom Scattering	97
4.4 Experimental Investigations of the Debye-Waller Factor for Atom-Surface Scattering	98
5. Influence of the Attractive Part of the Potential on Diffraction Intensities	103
5.1 Modifications for the Calculation of Diffraction Intensities	103
5.2 Bound Surface States and Resonant Transitions	105
5.3 Theory of Atom Scattering from a Corrugated Hard Wall with an Attractive Well	111
5.4 Inelastic Effects in Resonant Scattering	114
6. Experimental Aspects of Gas-Surface Scattering	118
6.1 Requirements on an Apparatus to Perform Gas-Surface Scattering Experiments	118

6.2 Beam Sources	119
6.2.1 Effusive Beam Sources	119
6.2.2 Nozzle-Beam Sources	119
6.3 Beam Energy Variation for Effusive and Nozzle-Beam Sources	123
6.4 The Design of Nozzle-Beam Systems	124
6.5 Molecular-Beam Detectors	126
6.6 Detector Rotation	128
6.7 Sample Manipulators	129
6.8 Beam-Modulation Devices	131
6.9 Experimental Systems for Diffractive Scattering from Surfaces	133
6.10 The Influence of the Transfer Width of the Apparatus and of Surface Perfection on Measured Intensities	137
7. Structural Investigations on Surfaces of Ionic Crystals	140
7.1 Diffraction Studies on LiF(100)	140
7.2 Diffraction Studies on NiO(100)	146
7.3 Diffraction from Other Ionic Materials	147
8. Structural Investigations on Semiconductor Surfaces	148
8.1 Helium-Diffraction Studies on Si(111) and Si(100)	148
8.2 Helium Diffraction from GaAs(110)	152
8.3 Diffraction from Graphite	154
8.4 Diffraction from Layer Compounds	155
8.5 Helium-Diffraction Studies from Other Surfaces	156
9. Structural Investigations on Metal Surfaces	157
9.1 Introduction	157
9.2 Helium and Hydrogen Diffraction from Close-Packed Metal Surfaces	157
9.3 Helium Diffraction from fcc(110) and bcc(112) Planes	158
9.4 Helium Diffraction from Stepped Metal Surfaces	160
10. Structural Studies on Adsorbate-Covered Surfaces	162
10.1 Introduction	162
10.2 Hydrogen Adsorption on Ni(110)	163
10.3 Oxygen Adsorption on Ni(110)	171
10.4 Oxygen Adsorption on Cu(110)	173
References	174