W. Kress F.W. de Wette (Eds.)

Surface Phonons

With Contributions by
G. Benedek J.E. Black V. Celli
W. Kress A.A. Maradudin L. Miglio
D.L. Mills G.I. Stegeman J.P. Toennies
S. Y. Tong F.W. de Wette

With 160 Figures

Springer-Verlag

Berlin Heidelberg New York London Paris Tokyo Hong Kong Barcelona Budapest

Contents

| 1. | | Oduction V. Kress and F.W. de Wette | 1 | | |
|----|---|---|----------|--|--|
| 2. | Surf | ace Acoustic Waves | | | |
| | By A.A. Maradudin and G.I. Stegeman (With 10 Figures) | | | | |
| | 2.1 | Surface Acoustic Waves on Various Media | . 6 | | |
| | | 2.1.1 Elastic Media | 6 | | |
| | | 2.1.2 Piezoelectric Media | 16 | | |
| | 2.2 | Generation and Detection of Surface Acoustic Waves | 24 | | |
| | | 2.2.1 Electrical Generation and Detection | | | |
| | | in Piezoelectric Media | 25 | | |
| | | 2.2.2 Generation on Non-piezoelectric Media | 27 | | |
| | | 2.2.3 Acousto-optic Detection | | | |
| | | of Generated Surface Acoustic Waves | 28 | | |
| | | 2.2.4 Brillouin Scattering from Surface Waves | 28 | | |
| | 2.3 | Some Applications of Surface Acoustic Waves | 30 | | |
| | | 2.3.1 Applications to Electronic Signal Processing | 30 | | |
| | | 2.3.2 Measurements of Intrinsic Material Properties | 32 | | |
| | Refe | rences | 34 | | |
| | | | | | |
| 3. | | Green's Function Method | | | |
| • | | ne Surface Lattice Dynamics of Ionic Crystals | | | |
| | • | G. Benedek and L. Miglio (With 10 Figures) | 37 | | |
| | 3.1 | Outline of the Time-Independent Green's Function Method | 37 | | |
| | 3.2 | The Green's Function Method in Surface Dynamics | 42 46 | | |
| | 3.3 | The Intrinsic Perturbation for a Semi-Infinite Lattice | | | |
| | 3.4 The Electronic Contribution to Surface Dynamics | | | | |
| | | in the Framework of Shell Models | 50 | | |
| | 3.5 | Surface Phonon Polaritons | 53 | | |
| | 3.6 | Surface Vibrations in Alkali Halides | 55 | | |
| | 3.7 | Further Developments: | | | |
| | | The Study of Surface Phonon Anomalies | 62 | | |
| | Refe | rences | 65 | | |
| | | | | | |

VII

| 1 . | rface Phonons by the Slab Method | (7 | | |
|------------|----------------------------------|---------|--|----------|
| | - | | Vette (With 20 Figures) | 67 |
| | 4.1 | Formal | | 69 |
| | | 4.1.1 | Slab Dynamics | 69 |
| | | 4.1.2 | Use of Symmetry | 73 |
| | | 4.1.3 | Slab Vibrational Modes | 7.4 |
| | | 414 | and Their Dispersion Curves | 74 |
| | | 4.1.4 | Macroscopic and Microscopic Surface Modes | 78 70 |
| | | 4.1.5 | Attenuation Curves | 78 |
| | | 4.1.6 | Systematic Features of Surface Modes | 80 |
| | 4.2 | | utational Considerations | 81 |
| | | 4.2.1 | Diagonalization Techniques | 81 |
| | | 4.2.2 | Surface Brillouin Zone Sampling | 82 |
| | 4.3 | | ction Models | 85 |
| | | 4.3.1 | Simple Pair Potentials (Molecular Crystals) | 85 |
| | | 4.3.2 | Shell Models (Ionic Crystals) | 86 |
| | | 4.3.3 | Force Constant Models (Semiconductors, Metals) | 88 |
| | 4.4 | Results | | 89 |
| | | 4.4.1 | Relaxation and Dynamics | |
| | | | of the (001) Surfaces of Alkali Halides | 89 |
| | | 4.4.2 | Results for fcc and bcc Metals | · 92 |
| | | 4.4.3 | Layered Structure – Graphite | 95 |
| | 4.5 | Derive | ed Physical Quantities | 97 |
| | | 4.5.1 | Mean-Square Amplitudes of Vibration | |
| | | | and Vibrational Correlation Functions | 97 |
| | | 4.5.2 | Surface Debye Temperature | 103 |
| | | 4.5.3 | Surface Thermodynamic Quantities | 104 |
| | 4.6 | Conclu | uding Remarks | 107 |
| | Refe | rences | | 108 |
| | | | | |
| | | | | |
| 5. | _ | | al Determination of Surface Phonons | |
| | - | | Atom and Electron Energy Loss Spectroscopy | |
| | By J | | nnies (With 30 Figures) | 111 |
| | 5.1 | | etical Background | 112 |
| | 5.2 | Kinem | natics | 116 |
| | 5.3 | Heliun | m Scattering | 123 |
| | | 5.3.1 | General Considerations | 123 |
| | | 5.3.2 | Helium Nozzle Beam Source | 126 |
| | | 5.3.3 | Target Chamber | 131 |
| | | 5.3.4 | Detector | 132 |
| | | 5.3.5 | Typical Measurements and Resolution | 133 |
| | 5.4 | Electro | on Scattering | 140 |
| | | 5.4.1 | Apparatus | 140 |
| | | 5.4.2 | Typical Measurements | 142 |
| | | | | |

| | 5.5 | Intensi | ties | 142 | | | |
|----|--|--------------------------|--|-----|--|--|--|
| | | 5.5.1 | Helium Atom Scattering | 144 | | | |
| | | 5.5.2 | Electron Scattering | 150 | | | |
| | | 5.5.3 | Comparison of Experimental Intensities | 153 | | | |
| | 5.6 | Discus | ssion of Experimental Results and Summary | 154 | | | |
| | | rences | , | 162 | | | |
| | | | | | | | |
| 6. | Theory of Helium Scattering from Surface Phonons | | | | | | |
| | By V | '. Celli (| (With 5 Figures) | 167 | | | |
| | 6.1 | Kinem | natics | 167 | | | |
| | | 6.1.1 Kinematic Focusing | | | | | |
| | 6.2 | Dynan | nical Theory: General Considerations | 171 | | | |
| | | 6.2.1 | Box Normalization and Scattering Geometry | 171 | | | |
| | | 6.2.2 | Cross Sections and Reflection Coefficients | 172 | | | |
| | | 6.2.3 | State-to-State Cross Sections | | | | |
| | | | vs Differential Cross Sections | 173 | | | |
| | 6.3 | One-P | honon Exchange Processes | 173 | | | |
| | | 6.3.1 | The Distorted Wave Born Approximation | 174 | | | |
| | | 6.3.2 | The Phonon Matrix Elements | 176 | | | |
| | | 6.3.3 | The Atom-Surface Matrix Elements | 177 | | | |
| | | 6.3.4 | The Differential Reflection Coefficient | 178 | | | |
| | | 6.3.5 | Relation to Phonon Density of States | | | | |
| | | 0.5.5 | and Correlation Functions | 179 | | | |
| | 6.4 | The In | nelastic Atom-Surface Interaction | 180 | | | |
| | 0.4 | 6.4.1 | The Static Repulsive Potential | 181 | | | |
| | | 6.4.2 | The Static Attractive Potential | 183 | | | |
| | | 6.4.3 | The Total Static Potential | 185 | | | |
| | | 6.4.4 | The Dynamic Repulsion and the Cutoff Factor | 186 | | | |
| | | 6.4.5 | Dynamical Effects of the Attractive Potential | 187 | | | |
| | Dofo | rences | • | 189 | | | |
| | Kele | rences | | 105 | | | |
| 7. | | | of Surface Phonons | | | | |
| | - | | Energy Loss Spectroscopy: | | | | |
| | Theoretical and Experimental Considerations | | | | | | |
| | By L | | lls, S.Y. Tong and J.E. Black (With 2 Figures) | 193 | | | |
| | 7.1 | 7.1 A Brief Review | | | | | |
| | 7.2 The Surface Phonon Excitation Mechanism | | | | | | |
| | in the Impact Regime | | | | | | |
| | 7.3 The Green's Function Approach | | | | | | |
| | to Spectral Density Calculations | | | | | | |
| | 7.4 Calculations of the Cross Section | | | | | | |
| | | | rface Phonon Excitation | 204 | | | |
| | 7.5 Concluding Remarks | | | | | | |
| | | 7.5 Concluding Remarks | | | | | |
| | | | | | | | |

| 8. | Vibr | Vibrational Properties of Clean Surfaces: | | | | | |
|----|---|---|--------------------------------------|-----|--|--|--|
| | Survey of Recent Theoretical and Experimental Results | | | | | | |
| | By W. Kress (With 82 Figures) | | | | | | |
| | 8.1 | Ionic C | Crystals | 211 | | | |
| | | 8.1.1 | Alkali Halides (Rock Salt Structure) | 211 | | | |
| | | 8.1.2 | Metal Oxides | 233 | | | |
| | | 8.1.3 | Refractory Compounds | 236 | | | |
| | | 8.1.4 | Perovskite Structure Compounds | 248 | | | |
| | 8.2 | Metals | | 254 | | | |
| | 'Au | 8.2.1 | Body Centered Cubic Metals | 255 | | | |
| | | 8.2.2 | Face Centered Cubic Metals | 257 | | | |
| | 8.3 Miscellaneous | | | 277 | | | |
| | | 8.3.1 | Diamond Structure Crystals | 277 | | | |
| | | 8.3.2 | Zinc-Blende Structure Crystals | 280 | | | |
| | | 8.3.3 | Layered Structure Crystals | 281 | | | |
| | Refe | rences | | 287 | | | |
| C. | . I 4 | Too all aus | | 293 | | | |
| วเ | in iect | muex . | · | 29, | | | |