

---

# **Contents**

## **Part I**

### **Diffraction and Imaging of Elastically Scattered Electrons**

#### **1. Basic Kinematic Electron Diffraction**

1.1. Wave Properties of Electrons . . . . .	3
1.2. Plane Wave . . . . .	4
1.3. Single-Atom Scattering . . . . .	5
1.4. Mott Formula . . . . .	6
	8
1.6. Reciprocal Space . . . . .	11
1.7. Bragg's Law . . . . .	12
1.8. Abbe's Imaging Theory . . . . .	16
1.9. Some Mathematical Operations . . . . .	18
1.9.1. Fourier Transformation . . . . .	18
1.9.2. Convolution Calculation . . . . .	18
1.9.3. Dirac Delta Function . . . . .	20

#### **2. Dynamic Elastic Electron Scattering I: Bloch Wave Theory**

2.1. Relativistic Corrections in Single-Electron Scattering Theory . . . . .	23
2.2. Bethe Theory . . . . .	25
2.2.1. Basic Equations . . . . .	25
2.2.2. Characteristics of Bloch Waves . . . . .	28
2.2.3. Orthonormal Relationship of Bloch Waves . . . . .	29
2.2.4. Bethel . . . . .	30
2.3. Two-Beam Theory . . . . .	31
	35
	37

2.6. Critical Voltage Effect . . . . .	40
2.7. Diffraction of Layered Materials . . . . .	42
2.8. HOLZ Reflections . . . . .	44
2.9. Real-Space Bloch Wave Theory of ZOLZ Reflections . . . . .	44
2.9.1. Projected Potential Approximation . . . . .	45
2.9.2. ZOLZ Reflections . . . . .	45
2.9.3. Effects of HOLZ Reflections . . . . .	47
2.10. Diffraction Contrast Images of Imperfect Crystals . . . . .	47
2.10.1. Potential of Imperfect Crystals . . . . .	49
2.10.2. Modified Bloch Wave Theory. . . . .	50
2.10.3. Column Approximation . . . . .	50
2.10.4. Howie-Whelan Equation . . . . .	51
2.10.5. a Coefficient Method . . . . .	54
2.11. Weak-Beam Imaging . . . . .	54
2.12. Absorption Effect in Dynamical Calculations . . . . .	59
2.13. Summary . . . . .	60

### 3. Dynamic Elastic Electron Scattering II: Multislice Theory

3.1. Physical Optics Approach . . . . .	61
3.1.1. Phase Object Approximation . . . . .	62
3.1.2. Huygens' Principle . . . . .	63
3.1.3. Multislice Theory . . . . .	65
3.2. Quantum Mechanical Basis of Multislice Theory . . . . .	65
3.2.1. Inclined Incident Beam Case . . . . .	65
3.2.2. Multislice Solution of the Schrodinger Equation . . . . .	68
3.3. Simulations of HRTEM Images and Electron Microdiffraction Patterns . . . . .	70
3.4. Calculations of HOLZ Reflections . . . . .	74
3.5. Improved Multislice Approaches . . . . .	75
3.5.1. Modified Multislice Theory for ZOLZ Reflections . . . . .	75
3.5.2. Modified Multislice Theory for HOLZ Reflections . . . . .	77
3.6. Effects of a Magnetic Field . . . . .	80
3.7. Summary.. . . . .	81

### 4. Dynamic Elastic Electron Scattering III: Other Approaches

4.1. Scattering Matrix Theory . . . . .	83
4.2. Green's Function Theory . . . . .	85
4.3. Semireciprocal Space Method . . . . .	87
4.4. Scattering Operator in Electron Diffraction . . . . .	88
4.5. Diffraction in Imperfect Crystals . . . . .	90

4.6. Equivalence among Various Theories . . . . .	91
4.7. Comparing of Bloch Wave and Multislice Theories . . . . .	94

## 5. Diffraction and Imaging of Reflected High-Energy Electrons from Bulk Crystal Surfaces

5.1. Geometry of RHEED . . . . .	97
5.2. Bloch Wave Theory . . . . .	100
5.3. Parallel-to-Surface Multislice Theories . . . . .	106
5.3.1. Method I. . . . .	107
5.3.2. Method II . . . . .	112
5.4. Perpendicular-to-Surface Multislice Theory . . . . .	116
5.5. Electron Reflection Process in RHEED . . . . .	118
5.6. Thermal Diffuse Scattering in RHEED . . . . .	123
5.7. Summary . . . . .	126

## Part II

### DIFFRACTION AND IMAGING OF INELASTICALLY SCATTERED ELECTRONS

## 6. Inelastic Excitations and Absorption Effect in Electron Diffraction

6.1. Kikuchi Patterns . . . . .	129
6.1.1. Formation of Kikuchi Lines. . . . .	131
6.1.2. Inelastic Excitations in Crystals . . . . .	132
6.1.3. Bremsstrahlung . . . . .	135
6.1.4. Electron Compton Scattering . . . . .	136
6.2. Yoshioka's Equations for Inelastically Scattered Electrons . . . . .	137
6.2.1. Basic Equations . . . . .	137
6.2.2. Incoherence and Coherence of Inelastically Scattered Electrons . . . . .	139
6.2.3. Conservation of Intensity . . . . .	140
6.2.4. Absorption Phenomenon . . . . .	141
6.3. Effects of Inelastic Excitations on an Elastic Wave . . . . .	141
6.3.1. Mixed Dynamic Form Factor . . . . .	142
6.3.2. Absorption Potential-Reciprocal-Space Description . . . . .	144
6.3.3. Absorption Potential-Real-Space Description . . . . .	145
6.3.4. Interpreting the Imaginary Potential . . . . .	146
6.3.5. Effect of Inelastic Absorption in Quantitative Electron Microscopy . . . . .	148

6.3.6. Virtual Inelastic Scattering . . . . .	149
6.4. Inelastic-Scattering Process I: Phonon Excitation . . . . .	150
6.4.1. Phonons in Crystals . . . . .	150
6.4.2. Perturbation Effect of Atomic Vibrations on Crystal Potential . . . . .	153
6.4.3. Electron-Phonon Interactions . . . . .	155
6.4.4. Phonon Dispersion Surfaces . . . . .	157
6.4.5. Debye-Waller Factor . . . . .	159
6.4.6. Mixed Dynamic Form Factor for Multiphonon Excitations	160
6.4.7. Absorption Potential . . . . .	164
6.5. Inelastic-Scattering Process II: Valence Excitation . . . . .	167
6.5.1. Dielectric Response Theory of Valence Excitations . . . . .	167
6.5.2. Mean Free Path and Absorption Potential . . . . .	169
6.5.3. Interface and Surface Excitations . . . . .	170
6.5.4. The Mixed Dynamic Form Factor and Generalized Dielectric Function . . . . .	175
6.6. Inelastic-Scattering Process III: Atomic Inner Shell Excitation . . . . .	176
6.6.1. Excitation Matrix . . . . .	177
6.6.2. Absorption Potential . . . . .	178
6.7. Diffraction and Channeling Effects in X-Ray and Auger Electron Emissions . . . . .	180
6.7.1. Localization in Atomic Inner Shell Excitation . . . . .	180
6.7.2. Delocalization in Electron Impact Ionization in Crystals . . . . .	181
6.8. Minimum Momentum Transfer in Inelastic Scattering . . . . .	185
6.8.1. Conservation of Energy . . . . .	185
6.8.2. Conservation of Momentum . . . . .	185
6.9. Summary . . . . .	187

## 7. Semiclassical Theory of Thermal Diffuse Scattering

7.1. Frozen Lattice Model . . . . .	189
7.2. Two-Beam TDS Theory . . . . .	192
7.3. Total Absorption Coefficient . . . . .	196
7.4. Many-Beam TDS Theory . . . . .	198
7.5. Multiphonon Excitations . . . . .	200
7.6. Evaluating the Debye-Waller Factor . . . . .	207
7.7. Coherent Length in Thermal Diffuse Scattering . . . . .	208
7.8. Diffuse Scattering of Imperfect Crystals . . . . .	212
7.8.1. Huang Scattering . . . . .	212
7.8.2. Diffuse Scattering Produced by Point Defects . . . . .	213
7.9. Summary . . . . .	216

**8. Dynamic Inelastic Electron Scattering I: Bloch Wave Theory**

8.1. Solution of Yoshioka's Equations . . . . .	217
8.2. Iterative Method . . . . .	220
8.3. Diffraction of Single Inelastically Scattered Electrons . . . . .	221
8.4. Theory of Kikuchi Patterns . . . . .	224
8.5. Diffraction of Double Inelastically Scattered Electrons . . . . .	226
8.6. Coherent Double Inelastic Scattering under Delta Function Localization Approximation . . . . .	231
8.7. Diffraction Contrast Images of Inelastically Scattered Electrons . .	234
8.7.1. Images of Stacking Faults . . . . .	235
8.7.2. Solution of Yoshioka's Equations for Imperfect Crystals . .	236
8.7.3. Diffraction Contrast Imaging of Single Inelastically Scattered Electrons . . . . .	238
8.8. Summary . . . . .	239

**9. Reciprocity in Electron Diffraction and Imaging**

9.1. Reciprocity Theorem for Elastically Scattered Electrons . . . . .	241
9.2. Equivalence of TEM and STEM . . . . .	243
9.3. Reciprocity Theorem for Inelastically Scattered Electrons . . . .	247
9.4. Summary . . . . .	250

**10. Dynamic Inelastic Electron Scattering II: Green's Function Theory**

10.1. Generalized Reciprocity Theorem . . . . .	251
10.2. Fourier Transform of Green's Function . . . . .	253
10.3. First-Order TDS . . . . .	255
10.4. Atomic Inner Shell Single Inelastic Excitation . . . . .	257
10.5. Double Inelastic Electron Scattering . . . . .	258
10.6. Summary  . . . . .	263

**11. Dynamic Inelastic Electron Scattering III: Multislice Theory**

11.1. Multislice Solution of Yoshioka's Equations . . . . .	265
11.2. Conservation of Total Electrons . . . . .	271
11.3. First-Order Results . . . . .	272
11.4. Special Cases of Only One Excited State . . . . .	273
11.4.1. Valence-Loss Scattering . . . . .	274
11.4.2. Thermal Diffuse Scattering . . . . .	275
11.5. Imaging with TDS Electrons in STEM . . . . .	278

11.5.1. Image Formation . . . . .	278
11.5.2. Contribution of Bragg-Reflected Electrons . . . . .	281
11.5.3. Contribution of TDS Electrons . . . . .	281
11.5.4. Effects of Multiphonon and Multiple Phonon Scattering	285
11.5.5. Effects of Coherent TDS . . . . .	286
11.5.6. Detection Geometry and Coherence in HAADF- STEM Imaging . . . . .	293
11.6. Imaging with TDS Electrons in TEM . . . . .	294
11.6.1. Image Formation . . . . .	294
11.6.2. Incoherent Imaging Theory . . . . .	296
11.7. Effect of Phase Correlation Between Atom Vibrations in TDS Electron Imaging . . . . .	298
11.8. Effect of Huang Scattering in Composition-Sensitive Imaging .	299
11.9. Resolution of an Incoherent Image . . . . .	303
11.10. Real-Space Multislice Theory of TDS . . . . .	305
11.10.1. Basic Equations . . . . .	305
11.10.2. Atomic-Number-Sensitive Imaging in STEM—the Exact Theory . . . . .	307
11.10.3. Multislice Calculation of Dynamic Scattering Operator $O_p$ . . . . .	312
11.10.4. Atomic-Number-Sensitive Imaging in TEM—the Exact Theory . . . . .	314
11.10.5. Dislocation Contrast Due to Huang Scattering . . . .	315
11.11. Summary . . . . .	320

## 12. Dynamic Inelastic Electron Scattering IV: Modified Multislice Theory

12.1. General Theory . . . . .	321
12.2. Single Inelastic Scattering . . . . .	323
12.3. Equivalence with Multislice Theory . . . . .	325
12.4. Absorption Function . . . . .	327
12.5. Localized Inelastic Scattering . . . . .	328
12.6. Diffraction of TDS Electrons-Semiclassical Approach . . . .	329
12.6.1. Basic Equations . . . . .	329
12.6.2. Streaks in TDS Electron Diffraction Patterns . . . .	332
12.7. Diffraction of Phonon-Scattered Electrons-Quantum Mechanical Approach . . . . .	336
12.7.1. Fundamental Treatment . . . . .	337
12.7.2. Diffraction Patterns of Phonon-Scattered Electrons . .	339
12.7.3. Directions of TDS Streaks . . . . .	341

12.8. Equivalence of Frozen Lattice Model and Phonon Excitation Theories for TDS . . . . .	349
12.9. Diffraction of Atomic Inner Shell Scattered Electrons . . . . .	351
12.10. Summary . . . . .	354

## 13. Inelastic Scattering in High-Resolution Transmission Electron Imaging

13.1. Contribution of Valence Loss Electrons . . . . .	356
13.1.1. Diffraction of Valence Loss Electrons . . . . .	356
13.1.2. Energy-Filtered HRTEM Images of Valence Loss Electrons . . . . .	358
13.1.3. Approaching the Completely Delocalized Scattering Model . . . . .	359
13.1.4. Perturbation Theory for Calculating $\Psi$ . . . . .	361
13.1.5. Effect of Surface Plasmon Excitation . . . . .	362
13.1.6. Energy-Filtered Inelastic Images of Interfaces . . . . .	364
13.2. Contribution of Phonon-Scattered Electrons . . . . .	367
13.3. TDS in High-Resolution Off-Axis Electron Holography . . . . .	370
13.3.1. Electron Holography with Time-Dependent Perturbation . . . . .	370
13.3.2. Multislice Calculation of $\langle\Phi\rangle$ . . . . .	373
13.3.3. Inelastic Scattering in Electron Holography . . . . .	375
13.4. Summary . . . . .	375

## 14. Multiple Inelastic Electron Scattering

14.1. Transport Equation Theory . . . . .	377
14.1.1. Energy Distribution of Plural Inelastically Scattered Electrons . . . . .	378
14.1.2. Angular Distribution of Plural Inelastically Scattered Electrons . . . . .	380
14.2. Improved Theories . . . . .	383
14.3. Density Matrix Theory of Electron Diffraction . . . . .	385
14.3.1. Kinetic Equation of Multiple Inelastic Electron Scattering . . . . .	386
14.3.2. Absorption Effect in Calculating Green's Function . . . . .	388
14.3.3. Delocalized Multiple Inelastic Scattering . . . . .	391
14.4. A Modified Multislice Theory . . . . .	393
14.4.1. Double Inelastic Scattering . . . . .	393
14.4.2. $\wp$ Function . . . . .	397
14.4.3. Multiple Scattering Theory . . . . .	397
14.4.4. Multiple Phonon Scattering in HAADF-STEM Imaging	399
14.5. Summary . . . . .	401

## 15. Inelastic Excitation of Crystals in Thermal Equilibrium with the Environment

15.1. Basic Equations . . . . .	403
15.2. Electron Images and Diffraction Patterns . . . . .	406
15.3. Solution to a Fluctuating Component . . . . .	406
15.4. Contributions of Fluctuating Components to Electron Diffraction Pattern and Image . . . . .	408
15.5. Nonfluctuating Inelastic Components . . . . .	410
15.6. Absorption Effect for Elastic Waves . . . . .	412
15.7. Applications in Phonon Scattering . . . . .	412

APPENDICES

A. Physical Constants, Electron Wavelengths, and Wave Numbers . . . . .	419
B. Properties of Fourier Transforms . . . . .	421
B.1. Identities . . . . .	422
C. Some Properties of Dirac Delta Functions . . . . .	423
C.1. Defining Relationships and Normalization Conditions . . . . .	423
C.2. Useful Representations of the Delta Function . . . . .	423
D. Integral Form of the Schrödinger Equation . . . . .	427
E. Some Useful Mathematical Relations . . . . .	431
<b>References , , , , , . . . . .</b>	<b>433</b>
<b>I n d e x . . . . .</b>	<b>4 4 3</b>