

Contents

Preface XIII

1	Introduction	1
1.1	Examples for the Application of X-Ray–Matter Interaction	3
1.1.1	Medical Imaging with X Rays	4
1.1.2	X-Ray Scattering and Spectroscopy	5
1.1.3	Short-Pulse X-Ray Probing of Matter	7
1.2	Electromagnetic Spectrum	7
1.3	X-Ray Light Sources	9
1.3.1	X-Ray Tubes	9
1.3.2	Laser-Produced X-Ray Sources	10
1.3.3	X-Ray Lasers	11
1.3.4	Z-Pinch	12
1.3.5	Novel X-Ray Source Capabilities	13
1.4	Fundamental Models to Describe X-Ray–Matter Interaction	14
1.4.1	Maxwell Equations	14
1.4.2	Relation of Maxwell Equations to Quantum Electrodynamics and the Semiclassical Treatment	17
1.5	Introduction to X-Ray–Matter Interaction Processes	19
1.5.1	Atomic and Electronic X-Ray–Matter Interaction Processes	19
1.5.2	Energy and Time Scales	21
1.5.3	Length Scales	22
1.5.4	Size Effects	24
1.6	Databases Relevant to Photon–Matter Interaction	24
	References	25
2	Atomic Physics	29
2.1	Atomic States	29
2.1.1	Center-of-Mass Motion	30
2.1.2	Constants of Motion	31
2.1.3	Atoms with a Single Electron	32
2.1.3.1	One-Body Schrödinger Equation	32
2.1.3.2	The Radial Schrödinger Equation	32

Contents

2.1.3.3	The Schrödinger Equation as the Nonrelativistic Limit of the Dirac Equation	33
2.1.4	Atoms with Multiple Electrons	36
2.1.5	The Periodic System of the Elements	37
2.1.6	Screened Hydrogenic Model	39
2.1.6.1	Semiclassical Approximation (WKB Method)	40
2.1.6.2	Semiclassical Approximation for Single Electrons in a Centrally Symmetric Field	41
2.1.6.3	The Screened Hydrogenic Ionization Model	43
2.2	Atomic Processes	44
2.2.1	Interaction of Atoms with Photons	45
2.2.1.1	Quantization of Free Electromagnetic Fields	46
2.2.1.2	Dipole Approximation in the X-Ray Regime	48
2.2.1.3	Principle of Detailed Balance	48
2.2.2	Radiative Excitation and Spontaneous Decay	49
2.2.3	Photoionization and Radiative Recombination	51
2.2.4	Electron Impact Ionization and Three-Body Recombination	52
2.2.5	Electron Impact Excitation and Deexcitation	53
2.2.6	Autoionization and Dielectronic Recombination	54
2.2.7	Shake Processes	55
2.3	Effect of Plasma Environment	56
2.3.1	Modification of Atomic Structure	57
2.3.1.1	Physical Models	57
2.3.1.2	Chemical Models	57
2.3.1.3	Energy Level Shifts	58
2.3.2	Modification of Atomic Processes	59
	References	59
3	Scattering of X-Ray Radiation	61
3.1	Scattering by Free Charges	61
3.1.1	Classical Description (Thomson Formula)	61
3.1.2	Relativistic Quantum-Mechanical Description (Klein–Nishina Formula)	63
3.2	Scattering by Atoms and Ions	64
3.2.1	Quantum-Mechanical Treatment of Scattering	64
3.2.1.1	Scattering by Atoms	65
3.2.1.2	Tabulated Atomic Structure Factors	68
3.3	Scattering by Gases, Liquids, and Amorphous Solids	69
3.4	Scattering by Plasmas	73
3.5	Scattering by Crystals	76
3.5.1	Kinematic Diffraction by Crystals	77
3.5.1.1	Diffraction by a Lattice of Finite Volume	77
3.5.1.2	Structure Factors for Monoatomic Crystals	79
3.5.1.3	Finite Temperature	81
3.5.1.4	Experimental Configurations	82

3.5.2	Dynamical Diffraction by Crystals	83
3.5.2.1	Diffraction from a Single Layer of Atoms	84
3.5.2.2	Kinematical Diffraction from Several Layers of Atoms	85
3.5.2.3	Index of Refraction	87
3.5.2.4	Reflection from a Perfect Crystal	88
	References	90
4	Electromagnetic Wave Propagation	93
4.1	Electromagnetic Waves in Matter	93
4.1.1	Scalar Wave Propagation	95
4.1.2	Laser Modes	96
4.2	Reflection and Refraction at Interfaces	97
4.2.1	Electromagnetic Field in the Reflecting Medium	100
4.2.2	Polarization by Reflection	100
4.2.3	Critical Angle	102
4.2.4	Evanescent Waves for Grazing-Incidence Reflection	103
4.3	Reflection by Thin Films, Bilayers, and Multilayers	105
4.3.1	Optical Properties of a Multilayer Stack	105
4.3.2	Field Intensity in the Multilayer Stack	107
4.3.3	Multilayers in the X-Ray Regime	107
4.3.4	Reflection by Thin Films and Bilayers	110
4.4	Dispersive Interaction of Wavepackets with Materials	111
4.4.1	Interaction with Optical Elements	113
4.5	Kramers–Kronig Relation	114
	References	115
5	Electron Dynamics	117
5.1	Transition of Solids into Plasmas	118
5.2	Directional Emission of Photoelectrons	119
5.3	Electron Scattering	122
5.3.1	Elastic Electron Scattering	124
5.3.1.1	Elastic Scattering of Fast Electrons	125
5.3.1.2	Elastic Scattering of Slow Electrons	126
5.3.1.3	Elastic Scattering in Solids	126
5.3.2	Inelastic Electron Scattering	128
5.3.2.1	Inelastic Scattering of Fast Electrons	128
5.3.2.2	Inelastic Scattering of Slow Electrons	128
5.4	Energy Loss Mechanisms	130
5.4.1	Energy Loss through Plasmon Excitation	130
5.4.2	Energy Loss through Phonon Excitation	131
5.5	Electron Dynamics in Plasmas	132
5.6	Statistical Description of Electron Dynamics	132
5.7	Bremsstrahlung Emission and Inverse Bremsstrahlung Absorption	133
5.7.1	Electron–Ion Bremsstrahlung	133
5.7.2	Electron–Electron Bremsstrahlung	134
5.7.3	Inverse Bremsstrahlung Absorption	134

5.8	Charge Trapping in Small Objects	135
5.8.1	Charge Trapping in Solid, Spherical Objects	135
5.8.2	Charge Trapping in Semi-infinite Objects and Thin Films	136
	References	138
6	Short X-Ray Pulses	141
6.1	Characteristics of Short X-Ray Pulses	142
6.1.1	Coherence and Photon Statistics	142
6.1.2	Chirped X-Ray Pulses	143
6.1.3	Bandwidth-Limited X-Ray Pulses	144
6.1.4	Propagation in Free Space	146
6.2	Generating Short X-Ray Pulses	147
6.2.1	Short-Pulse X-Ray Sources	147
6.2.1.1	High-Harmonic Generation	148
6.2.1.2	Thomson Scattering	148
6.2.1.3	Ultrafast X-Ray Tubes	148
6.2.1.4	Laser Plasma Sources	149
6.2.1.5	Synchrotrons	149
6.2.1.6	Energy Recovery Linacs	151
6.2.1.7	X-Ray Free-Electron Lasers	151
6.2.2	Reducing Pulse Lengths through Time-Slicing	153
6.2.3	Reducing Pulse Length through Pulse Compression	154
6.2.4	Generating Ultrashort X-Ray Pulses	155
6.3	Characterizing Short X-Ray Pulses	155
6.3.1	X-Ray Streak Cameras	156
6.3.2	Correlation Methods	156
6.3.3	Examples	157
6.4	Characteristic Time Scales in Matter	158
6.5	Short-Pulse X-Ray-Matter Interaction Processes	159
6.5.1	Atomic Processes	160
6.5.2	Fast Structural Changes	160
6.6	Single-Pulse X-Ray Optics	162
	References	164
7	High-Intensity Effects in the X-Ray Regime	169
7.1	Intensity and Electric Field of Intense X-Ray Sources	170
7.2	High-X-Ray-Intensity Effects in Atoms	171
7.2.1	Multiphoton Absorption	172
7.2.1.1	Multiphoton Absorption Cross Section	172
7.2.1.2	Two-Photon Absorption by Hydrogen	172
7.2.2	Tunneling Ionization	174
7.2.3	Onset of Strong Photon-Field Effects	175
7.2.4	Multiple Ionization and Hollow Atoms	176
7.2.5	Stabilization of Atoms	176
7.3	Nonlinear Optics	178
7.3.1	Nonlinear Optics in the Visible Regime	178

7.3.2	Nonlinear Optics in the X-Ray Regime	179
7.3.2.1	Nonlinear Optics with Quasi-Free Electrons	179
7.3.2.2	Magnitude of Nonlinear Effects in the X-Ray Regime	182
7.4	High-Intensity Effects in Plasmas	182
7.4.1	Plasma Wakefield Accelerators	183
7.4.2	Plasma Instabilities at High Intensities	183
7.5	High-Field Physics	184
7.5.1	High-Intensity QED Effects: Pair Production	185
7.5.2	Experimental Verification of Quantum Field Theory	186
	References	187
8	Dynamics of X-Ray-Irradiated Materials	191
8.1	X-Ray–Matter Interaction Time Scales	191
8.2	The Influence of X-Ray Heating on Absorption	192
8.2.1	Temperature-Dependence of X-Ray Absorption	192
8.2.2	Time Dependence of X-Ray–Matter Interaction	195
8.2.3	Pulse Length Dependence of X-Ray Absorption	196
8.3	Thermodynamics of Phase Transformation	199
8.3.1	Solid–Liquid Transitions	200
8.3.2	Liquid–Gas Transition	202
8.3.3	Solid–Gas Transition	202
8.3.4	Example Phase Diagram	203
8.4	Ablation	203
8.5	Intensity Dependence of X-Ray–Matter Interaction	205
8.5.1	Interaction of Short X-Ray Pulses with Crystals	207
8.6	X-Ray-Induced Mechanical Damage	207
8.7	X-Ray Damage in Inertial Confinement Fusion	208
8.8	X-Ray Damage in Semiconductors	209
8.8.1	X-Ray Damage in Semiconductor Processing	209
8.8.2	X-Ray-Damage-Resistant Semiconductors	209
8.9	Damage to Biomolecules in X-Ray Imaging	210
	References	212
9	Simulation of X-Ray–Matter Interaction	215
9.1	Models for Different Time- and Length Scales	215
9.2	Atomistic Models	216
9.2.1	Molecular Dynamics and Particle-in-Cell Models	217
9.2.1.1	Molecular Dynamics Models	217
9.2.1.2	Particle-in-Cell Method	218
9.2.1.3	Hybrid Methods	218
9.2.1.4	Quantum Molecular Dynamics Models	219
9.2.2	Monte Carlo Models	219
9.2.2.1	Monte Carlo Methods to Sample Phase Space	220
9.2.2.2	Monte Carlo Methods to Sample Particle Trajectories	220
9.3	Statistical Kinetics Models	224
9.3.1	Kinetics Equations	224

Contents

9.3.1.1	Klimontovich Distribution	224
9.3.1.2	Liouville Distribution	225
9.3.1.3	BBGKY Hierarchy	225
9.3.1.4	Boltzmann and Vlasov Equation	226
9.3.1.5	Fokker–Planck Equation	227
9.3.2	Atomic Kinetics	228
9.3.3	Using Statistical Kinetics Models to Describe X-Ray–Matter Interaction	228
9.4	Hydrodynamic Models	229
9.4.1	Fluid Models	229
9.4.2	Using Hydrodynamic Models to Describe X-Ray–Matter Interaction	233
	References	235
10	Examples of X-Ray–Matter Interaction	239
10.1	Interaction of Intense X-Ray Radiation with Atoms and Molecules	239
10.2	Interaction of Intense X-Ray Pulses with Atomic Clusters	240
10.2.1	Interaction of Clusters with High-Intensity 12.7-eV Radiation	241
10.2.2	Interaction of Clusters with High-Intensity 40- to 100-eV Radiation	242
10.2.3	Interaction of Clusters with High-Intensity Hard X-Ray Radiation	243
10.3	Biological Imaging	245
10.3.1	Image Formation	245
10.3.2	Protein X-Ray Crystallography	246
10.3.3	Coherent Diffractive Imaging	247
10.3.3.1	Dynamic Damage Limits	249
10.3.3.2	Coherent Diffractive Imaging at X-Ray Free-Electron Lasers	250
10.3.4	Outlook	250
10.4	X-Ray Scattering Diagnostics of Dense Plasmas	251
10.4.1	Experimental Setups	252
10.4.2	Collective and Noncollective Scattering	254
10.4.3	Theoretical Description of Inelastic X-Ray Scattering	255
	References	256
	Index	263