Contents

List of symbols		xix
Preface		xxv
	Chapter 1. General features and fundamental concepts	1
1.1	Introduction	1
1.2	Range distributions	4
1.3	Lattice disorder	5
1.4	Atomic and planar densities	6
1.5	Energy and particles	8
1.6	The Bohr velocity and radius	11
	Suggested reading	12
	Problems	12
	Chapter 2. Interatomic potentials	14
2.1	Introduction	14
2.2	Interatomic forces	14
2.3	Short- and long-range interatomic forces	15
2.4	Model interatomic potentials	16
2.4.1	Hard-sphere potential	16
2.4.2	Square-well potential	17
2.4.3	Inverse power potential	17
2.4.4	Lennard–Jones potential	17
2.5	Interatomic forces in solids	17
2.6	Physical properties of a solid	19
2.6.1	Binding energy	19
2.6.2	Elastic modulus	20
2.6.3	Thermal properties	21
2.7	Energetic collisions of atoms and ions	23
2.8	Thomas–Fermi statistical model	25
2.9	Solutions of the TF equation	27

2.10	The TF screening function (approximations)	27
2.11	Interatomic potentials	32
2.12	Universal interatomic potential	33
	References	37
	Suggested reading	37
	Problems	37
	Chapter 3. Dynamics of binary elastic collisions	39
3.1	Introduction	39
3.2	Classical scattering theory	40
3.3	Kinematics of elastic collisions	41
3.4	Classical two-particle scattering	44
3.5	Motion under a central force	49
3.5.1	Conservation of angular momentum	50
3.5.2	Energy conservation in a central force	52
3.5.3	Angular orbital momentum and the impact parameter	52
3.6	The classical scattering integral	55
3.7	Distance of closest approach	59
	References	60
	Suggested reading	60
	Problems	61
	Chapter 4. Cross-section	62
4.1	Introduction	62
4.2	Angular differential scattering cross-section	63
4.3	Energy-transfer differential scattering cross-section	71
4.4	Power law potentials and the impulse approximation	74
4.5	Power law energy-transfer cross-section	78
4.6	Reduced cross-section	80
4.7	Hard-sphere potential	83
	References	85
	Suggested reading	86
	Problems	86
	Chapter 5. Ion stopping	88
5.1	Introduction	88
5.2	The energy-loss process	89
5.3	Nuclear stopping	90
5.4	Nuclear stopping: reduced notation	92
5.5	ZBL nuclear stopping cross-section	95
5.6	ZBL universal scattering formula	98
5.7	Electronic stopping	99
5.7.1	Effective charge of moving ions	100

5.7.2	High-energy electronic energy loss	101
5.7.3	Low-energy electronic energy loss	105
5.7.3.1	Fermi–Teller model	105
5.7.3.2	The Firsov and Lindhard–Scharff models	106
5.7.3.3	Z_1 oscillations in electronic stopping	111
	References	113
	Suggested reading	113
	Problems	114
	Chapter 6. Ion range and range distribution	115
6.1	Range concepts	115
6.2	Range distributions	117
6.3	Calculations	120
6.3.1	Range	121
6.3.2	Range approximations	124
6.3.3	Projected range	128
6.3.4	Range straggling	130
6.3.5	Polyatomic targets	131
6.4	Channeling	133
6.4.1	General principles	134
6.4.2	The maximum range, R_{max}	138
	References	139
	Suggested reading	139
	Problems	139
	Chapter 7. Radiation damage and spikes	141
7.1	Introduction	141
7.2	Radiation damage and displacement energy	141
7.3	Displacements produced by a primary knock-on	147
7.4	PKA damage energy	152
7.4.1	The Norgett, Robinson, and Torrens (NRT) model of damage energy	154
7.5	Ion irradiation damage	155
7.5.1	Displacements produced by an energetic ion	155
7.5.2	Ion damage energy	160
7.5.3	Spatial distribution of deposited energy	162
7.6	Damage production rate	165
7.7	Primary recoil spectrum	167
7.8	Fractional damage function	168
7.9	Displacement damage in polyatomic materials	168
7.9.1	Damage energy	169
7.9.2	Displacement damage	171

7.10	Replacement collision sequences	173
7.11	Spikes	176
7.11.1	Mean free path and the displacement spike	176
7.11.2	Thermal spike	180
7.11.3	Deposited energy density, θ_D	181
7.11.4	The cascade volume and the deposited energy density	182
7.11.5	Deposited damage energy and materials properties	185
	References	187
	Suggested reading	188
	Problems	189
	Chapter 8. Ion–solid simulations and diffusion	191
8.1	Introduction	191
8.2	Monte Carlo simulations	191
8.2.1	An example of a Monte Carlo program, PIPER	192
8.2.2	Nuclear scattering	192
8.2.3	Electronic energy loss	193
8.2.4	Calculation procedure	194
8.2.5	An example from TRIM	197
8.3	Molecular dynamic simulations	200
8.4	Irradiation enhanced diffusion	204
8.4.1	Diffusion	204
8.4.2	Radiation enhanced diffusion (RED)	205
8.5	Diffusion in thermal spikes	209
	References	216
	Suggested reading	217
	Chapter 9. Sputtering	218
9.1	Introduction	218
9.2	Sputtering of single element targets	219
9.2.1	Nuclear stopping cross-section	221
9.2.2	Deposited energy	222
9.2.3	Sputtering yield	223
9.3	Semi-empirical formula for sputtering of single elemental targets	223
9.4	Sputtering yield of monoatomic solids at glancing angles	225
9.5	Ion implantation and the steady-state concentration	228
9.6	Sputtering of alloys and compounds	229
9.6.1	Preferential sputtering	230
9.6.2	Composition changes	232
9.6.3	Composition depth profiles	233
9.7	High-dose ion implantation	235

9.8	Concentrations of implanted species	238
9.8.1	Si implanted with 45 keV Pt ions	239
9.8.2	Pt implanted with 45 keV Si ions	240
9.8.3	PtSi implanted with Si	241
9.9	Factors that influence concentrations in high dose ion implantation	243
9.10	Sputtering from spikes	244
9.11	Computer simulation	247
	References	250
	Suggested reading	251
	Problems	252
	Chapter 10. Order–disorder and ion implantation metallurgy	254
10.1	Irradiation induced chemical order–disorder	254
10.1.1	The long-range order parameter, S_{LR}	254
10.1.2	Irradiation induced disordering: point defects	255
10.1.3	Irradiation induced disordering: dense cascades	257
10.1.4	Irradiation enhanced thermal reordering	261
10.2	Ion implantation metallurgy: introduction	262
10.3	Ion implantation metallurgy and phase formation	265
10.3.1	Simple equilibrium binary phase diagrams: solid solutions	265
10.3.2	Rapid thermal quenched metal systems: metastable alloys	269
10.3.3	Lattice location of implanted impurity atoms	272
10.3.3.1	Replacement collisions: kinematic picture	273
10.3.3.2	Hume-Rothery rules	276
10.3.3.3	Miedema rules	279
10.3.3.4	Impurity atom–lattice defect interactions	281
10.4	Ion implantation: high-dose regime	286
10.4.1	Geometry effects	288
10.4.2	Surface chemistry effects	288
	References	290
	Suggested reading	292
	Problems	293
	Chapter 11. Ion beam mixing	295
11.1	Introduction	295
11.2	Ballistic mixing	299
11.2.1	Recoil mixing	300
11.2.2	Cascade mixing	302

11.3	Thermodynamic effects in ion mixing	305
11.3.1	Heat of mixing	307
11.3.2	Influence of cohesive energy	313
11.3.3	Model of mixing	315
11.3.4	Cascade parameters	318
11.4	Thermally assisted ion mixing	319
11.4.1	Liquid state diffusion	321
11.5	Transition temperature	322
11.6	Phase formation	323
11.6.1	Kinetics	324
11.6.2	Nucleation	324
11.6.3	Thermodynamics	326
	References	328
	Suggested reading	330
	Problems	330
	Chapter 12. Phase transformations	332
12.1	Introduction	332
12.2	Energetics of phase transformations and ion irradiation	334
12.2.1	Metastable phases	335
12.2.2	Energy differences between amorphous and crystalline states	336
12.2.3	Enthalpy of the order–disorder transformation	338
12.3	Irradiation induced defects and damage accumulation	342
12.3.1	Vacancy–interstitial defects	343
12.3.2	Anti-site defects	343
12.3.3	Dislocations	344
12.3.4	Strain energy and elastic instability	346
12.4	Phase transformations by cascades and thermal spikes	348
12.4.1	Cascade recovery: driving force	349
12.4.2	Cascade recovery: nucleation constraints	350
12.4.3	Cascade recovery: kinetic constraints	351
12.5	Kinetics and the formation of metastable phases	351
12.6	Amorphous phase	354
12.6.1	Complex unit cell	354
12.6.2	Width of the phase field	355
12.7	Overview	359
	References	359
	Suggested reading	361
	Problems	361

	Chapter 13. Ion beam assisted deposition	363
13.1	Introduction	363
13.2	Microstructure development during the growth of metallic films	365
13.2.1	Zone I, $T_s < 0.15T_m$	365
13.2.2	Zone T, $0.15T_m < T_s < 0.3T_m$	366
13.2.3	Zone II, $0.3T_m < T_s < 0.5T_m$	366
13.2.4	Zone III, $T_s > 0.5T_m$	366
13.3	Non-reactive IBAD processing: effect of ions on film growth	366
13.3.1	Microstructure development during IBAD	370
13.3.2	Densification	374
13.3.2.1	Densification: Monte Carlo calculations	374
13.3.2.2	Densification: molecular dynamic calculations	379
13.3.3	Intrinsic stress	380
13.3.4	Grain size	384
13.3.5	Texture	387
13.3.6	Epitaxy	390
13.3.7	Adhesion	396
13.4	Reactive IBAD processing: compound synthesis	399
13.4.1	Reactive IBAD: processing model	399
13.4.2	Reactive IBAD: The Hubler–van Vechten model	400
	References	403
	Problems	406
	Chapter 14. Applications of ion beam processing techniques	408
14.1	Introduction	408
14.2	Ion implantation – advantages and limitations of the technique	408
14.3	Tribology	410
14.3.1	Nitrogen implantation	412
14.3.2	Dual ion implantation and ion beam mixing	412
14.3.3	Industrial tribological applications	413
14.4	Fatigue	415
14.5	High-temperature oxidation	418
14.6	Aqueous corrosion	420
14.7	Catalysis: solid/gas, solid/liquid interface reactions	425
14.8	Ceramics	427
14.9	Polymers	427

14.10	Applications and research areas of IBAD processing	428
14.10.1	Metastable compound formation	429
14.10.2	Optical and electronic coatings	433
14.10.2.1	Dielectric coatings	434
14.10.2.2	Rugate filter production	436
14.10.2.3	Transparent conducting films	437
14.10.2.4	Reflective coatings	438
14.10.2.5	Thermochromic VO_2 coatings	439
14.10.2.6	Magnetic thin films	439
14.10.2.7	Diffusion barriers	440
14.10.3	Tribological coatings	440
14.10.3.1	Hard coatings	440
14.10.3.2	Solid lubricant coatings	442
14.10.4	Aqueous corrosion resistant coatings	444
14.11	Ionized cluster beam (ICB) deposition	446
	References	450
	Suggested reading	453
	Chapter 15. Ion beam system features	455
15.1	Introduction	455
15.2	Directed beam ion implantation	456
15.2.1	Ion implantation ion sources	456
15.2.1.1	Freeman ion source	457
15.2.1.2	High-temperature ion source (CHORDIS)	459
15.2.1.3	MEVVA ion source	459
15.2.2	Ion beam mass analysis	461
15.2.3	Ion beam transport, beam scanning, target manipulation	462
15.2.4	Dose determination	463
15.2.5	Substrate temperature considerations	463
15.3	Plasma source ion implantation*	467
15.4	Ion beam assisted deposition (IBAD) system ion sources	474
15.4.1	Broad-beam gridded ion sources	474
15.4.2	End–Hall source	478
15.4.3	Electron cyclotron resonance (ECR) source	479
15.5	Physical vapor deposition systems and monitors	480
	References	481
	Suggested reading	482

* This section is written by Donald J. Rej.

Appendix A Crystallography 483
A.1 Crystallography and notation 483
A.2 Directions and planes 485
A.3 Spacing between planes of the same Miller indices 486
A.4 Interatomic spacing 488
A.5 Plane spacings 488
Appendix B Table of the elements 491
Appendix C Density of states 498
C.1 Wavelike properties of electrons 498
C.2 Standing waves and an electron in a box 499
C.3 Density of states 500
Suggested reading 502
Appendix D Derivation of the Thomas–Fermi differential equation 503
Appendix E Center-of-mass and laboratory scattering angles 505
Suggested reading 508
Appendix F Miedema's semi-empirical model for the enthalpy of formation in the liquid and solid states 509
F.1 Introduction 509
F.2 Concentration-dependent enthalpy of formation 511
F.2.1 Alloys of two transition metals 512
F.2.2 Alloys of two non-transition metals 513
F.2.3 Alloys of two polyvalent non-transition metals and gaseous elements 513
F.2.4 Alloys of transition metals with non-transition metals 514
F.3 Solutions of infinite dilution 514
F.4 Amorphous solid solutions 515
References 518
Suggested reading 518
Appendix G Implantation metallurgy – study of equilibrium alloys 519
G.1 Study of metallurgical phenomena 519
G.2 Diffusion and the composition profile 519
G.3 Experimental determination of diffusion coefficients 520
G.4 Solid solubilities 525
References 528
Appendix H Physical constants, conversions and useful combinations 529
Index 531