

Contents

Part 1: Theory of Ellipsometry	1
1 Polarized Light and Ellipsometry.....	3
1.1 A Quick Guide to Ellipsometry	4
1.1.1 Light Waves and Photons	4
1.1.2 Polarization of Light	6
1.1.3 Ellipsometric Configurations	9
1.1.4 Null Ellipsometry	12
1.1.5 Photometric Ellipsometry and Polarimetry	13
1.2 Maxwell and Wave Equations	19
1.2.1 Linear Local Response	20
1.2.2 Linear Non–Local Response	22
1.2.3 Dipole Moment, Susceptibility and Inductions.....	23
1.2.4 Relationships Between Optical Constants.....	24
1.2.5 Wave Equation for Monochromatic Fields	26
1.2.6 Plane Waves in Isotropic Medium.....	29
1.3 Representations of Polarization.....	31
1.3.1 Representation by Ellipsometric Angles	32
1.3.2 Special Cases: Linear and Circular Polarization.....	35
1.3.3 Orthogonal Polarization States	37
1.3.4 Representation by Complex Numbers.....	37
1.3.5 Light Intensity, Detection of Polarization State	40
1.4 Propagation of Polarized Light	45
1.4.1 Jones Vectors	45
1.4.2 Jones Matrices	48
1.4.3 Quantum Mechanical Description, Partial Polarization....	53
1.4.4 Stokes Vectors.....	56
1.4.5 Mueller Matrices	59
1.5 Reflection and Transmission of Polarized Light at Planar Interfaces	67
1.5.1 Matching Plane Waves at a Planar Interface.....	67
1.5.2 Fresnel Coefficients.....	72
1.5.3 Special Values of the Angle of Incidence.....	74
1.5.4 Ratio of Amplitude Reflectivities.....	76
1.5.5 Propagation Matrices, Stratified Structures.....	80
1.5.6 Substrate–Film–Ambient System	85
1.6 References	90

2 Optical Physics of Materials.....	93
2.1 Introduction	93
2.2 Propagation of Light in Solids	102
2.2.1 Optically Isotropic Solids and the Complex Dielectric Function	102
2.2.2 Optically Anisotropic Solids and the Dielectric Tensor..	110
2.2.3 Dispersion Relationships	124
2.3 Classical Theories of the Optical Properties of Solids.....	125
2.3.1 Semiconductors and Insulators: the Lorentz Oscillator Model	125
2.3.2 Metals: The Drude Free Electron Model	129
2.3.3 Plasmons	132
2.3.4 Optical Sum Rules.....	136
2.4 Quantum Mechanical Theories of the Optical Properties of Solids.....	137
2.4.1 Quantum Theory of Absorption and Dispersion	138
2.4.2 Direct Interband Transitions in Solids.....	146
2.4.3 Band Structure and Critical Points in Solids.....	150
2.4.4 Indirect Interband Transitions in Solids	153
2.4.5 Intraband Transitions in Metals.....	157
2.5 Modeling the Optical Properties of Solids.....	159
2.5.1 Classical Lorentz Oscillator Models	159
2.5.2 Classical Drude Models.....	172
2.5.3 Generalized Quantum Mechanical Models	178
2.5.4 Specialized Quantum Mechanical Models	207
2.6 Overview and Concluding Remarks	227
Acknowledgments	230
2.7 References and Bibliography	230
2.7.1 Numbered References	230
2.7.2 Bibliography	233
3 Data Analysis for Spectroscopic Ellipsometry	237
3.1 Introduction	237
3.2 Ellipsometry Parameters.....	239
3.2.1 Calculated Parameters: Jones Matrices	240
3.2.2 Measured Parameters: Mueller Matrices.....	241
3.2.3 Mueller-Jones Matrices	242
3.3 Calculation of Complex Reflection Coefficients	246
3.3.1 Isotropic, Homogeneous Systems	246
3.3.2 Anisotropic Systems	248
3.3.3 Inhomogeneous Layers.....	251
3.4 Models for Dielectric Functions.....	252

3.4.1 Tabulated Data Sets	253
3.4.2 Lorentz Oscillator Model	254
3.4.3 Optical Functions of Amorphous Materials	255
3.4.4 Models for Crystalline Materials.....	258
3.4.5 Effective Medium Theories	260
3.5 Fitting Models to Data.....	262
3.5.1 Figures of Merit.....	263
3.5.2 Errors in Spectroscopic Ellipsometry	265
3.5.3 Convergence Routines	268
3.5.4 An Example: (a-Si _x N _y :H)	271
3.6 Determination of Optical Functions from Spectroscopic Ellipsometry Data	276
3.6.1 Optical Functions from Parameterization.....	278
3.6.2 Newton-Raphson Algorithm.....	280
3.6.3 Optical Functions of Bulk Isotropic Semiconductors and Insulators.....	282
3.6.4 Optical Functions of Anisotropic Materials	285
3.6.5 Optical Functions of Thin Films	286
3.7 Depolarization	289
Acknowledgements	293
3.8 Further Reading and References	293
Optics and Ellipsometry	293
Data Reduction	294
Numbered References	294
Part 2: Instrumentation	297
4 Optical Components and the Simple PCSA (Polarizer, Compensator, Sample, Analyzer) Ellipsometer	299
4.1 General.....	299
4.2 The Components.....	301
4.2.1 Methods of Obtaining Polarized Light.....	301
4.2.2 Double Refraction	302
4.2.3 Calcite Crystals.....	303
4.2.4 Polarizers and Analyzers	305
4.2.5 Wollaston Prisms	307
4.2.6 Compensators, Quarter-Wave Plates, and Retarders	308
4.2.7 Photoelastic Modulators	316
4.2.8 Monochromators.....	317
4.2.9 Goniometers.....	321
4.3 Ellipsometer Component Configurations	322
4.3.1 Early Null Ellipsometer Configurations.....	322
4.3.2 Photometric Ellipsometer Configurations	323

4.3.3 Spectroscopic Ellipsometers.....	324
4.3.4 Other Configurations	326
4.4 References	327
5 Rotating Polarizer and Analyzer Ellipsometry	329
5.1 Introduction	329
5.2 Comparison of Ellipsometers	333
5.3 Instrumentation Issues	343
5.3.1 Optical Configuration.....	343
5.3.2 Optical Components and Spectral Range.....	345
5.3.3 Alignment	351
5.3.4 Electronic Design and Components	356
5.4 Data Reduction for the Rotating Polarizer and Analyzer Ellipsometers	364
5.4.1 Ideal PXSA _r Configuration	364
5.4.2 Errors in the PXSA _r Configuration	371
5.4.3 P _r XSA Configuration	378
5.5 Precision Considerations	386
5.6 Calibration Procedures	392
5.6.1 Ideal Rotating Polarizer and Analyzer Ellipsometers	394
5.6.2 Detecting and Correcting Errors in Calibration	407
5.6.3 Detecting and Correcting Compensator Errors	423
5.7 Summary: Recent and Future Directions	425
5.8 References	429
6 Polarization Modulation Ellipsometry	433
6.1 Introduction	433
6.2 The Photoelastic Modulator (PEM)	436
6.2.1 General Description and Historical Perspective	436
6.2.2 Mathematical Description of a PEM.....	440
6.2.3 Stokes Vector Descriptions of the PSG and PSA.....	442
6.3 Experimental Configurations of Polarization Modulation Ellipsometers	446
6.3.1 Polarization Modulation Ellipsometry (PME) with Analog Data Acquisition	446
6.3.2 Phase Modulated Ellipsometry (PME) with Digital Data Acquisition	447
6.3.3 Two-Channel Spectroscopic Polarization Modulation Ellipsometer (2-C SPME)	449
6.3.4 Two-Modulator Generalized Ellipsometer (2-MGE)	450
6.4 Light Intensity Through a Polarization Modulation Ellipsometer.....	452
6.4.1 Mueller Matrices for Various Samples.....	452

6.4.2 Intensity for a Standard PME	455
6.4.3 Intensity for the 2-Modulator Generalized Ellipsometer (2-MGE).....	457
6.5 Waveform Analysis.....	461
6.5.1 Basis Function	463
6.5.2 Phase-Sensitive Detection	465
6.5.3 Digital Waveform Analysis	466
6.5.4 Two-Modulator Systems.....	467
6.6 Calibration Procedures	469
6.6.1 One-Modulator PMEs	470
6.6.2 Two-Modulator PMEs.....	472
6.7 Errors	474
6.7.1 General Discussion	474
6.7.2 Systematic Errors of PMEs	475
6.8 Further Reading and References	479
6.8.1 Further Reading	479
6.8.2 Numbered References	479
7 Multichannel Ellipsometry	481
7.1 Introduction	481
7.2 Overview of Instrumentation.....	483
7.2.1 Self-Compensating Designs	483
7.2.2 Rotating-Element Designs.....	487
7.2.3 Phase-Modulation Designs	491
7.2.4 Design Comparisons.....	493
7.2.5 Errors Unique to Multichannel Detection Systems.....	497
7.3 Rotating-Element Designs.....	502
7.3.1 Rotating Polarizer	502
7.3.2 Single Rotating Compensator.....	523
7.3.3 Dual Rotating Compensator	546
7.4 Concluding Remarks	562
Acknowledgements	564
7.5 References	564
Part 3: Critical Reviews of Some Applications	567
8 SiO₂ Films.....	569
8.1 Introduction	569
8.1.1 Preeminence of SiO ₂ in Microelectronics: the Ellipsometry Connection	569
8.1.2 Electronic Passivation	570
8.1.3 Properties of SiO ₂ Films	571
8.2 Historical Perspective – Prior to 1970	578

8.3	Modern Studies – Since 1970	585
8.3.1	Thick SiO ₂ Films	585
8.3.2	Thin SiO ₂ Films	599
8.3.3	Recent Results on Ultra Thin SiO ₂ Films and the Si-SiO ₂ Interface	619
8.4	Conclusions	632
	Acknowledgements	633
8.5	References	633
9	Theory and Application of Generalized Ellipsometry	637
9.1	Introduction	637
9.2	The Generalized Ellipsometry Concept	638
9.2.1	Comments on Notations in GE	638
9.2.2	The Optical Jones Matrix	640
9.2.3	The Generalized Ellipsometry Parameters	643
9.2.4	Generalized Ellipsometry Acquisition Techniques	647
9.3	Theory of Generalized Ellipsometry	650
9.3.1	Birefringence in Stratified Media.....	650
9.3.2	4 × 4 Maxwell's Equations in Matrix Form.....	652
9.3.3	Transmission and Reflection GE.....	656
9.4	Special Generalized Ellipsometry Solutions	657
9.4.1	Biaxial Films (Symmetrically Dielectric Materials)	657
9.4.2	Bi-Biaxial or Magneto-Optical Films (Non-Symmetrically Dielectric Materials).....	661
9.4.3	Chiral Biaxial Films (Axially Twisted Symmetrically Dielectric Materials).....	663
9.4.4	Isotropic Dielectric Films	669
9.4.5	Further Solutions: [1 1 1] Superlattice Ordering in III-V Compounds (CuPt-Ordering)	671
9.5	Strategies in Generalized Ellipsometry	675
9.5.1	Data Acquisition Strategies for Anisotropic Samples.....	676
9.5.2	Strategies for Treatment of Sample Backside Effects	679
9.5.3	Model Strategies	682
9.6	Generalized Ellipsometry Applications	683
9.6.1	Anisotropic Bulk Materials	684
9.6.2	Anisotropic Films	693
9.7	Conclusions	710
	Acknowledgements	710
9.8	Further Reading and References	711
9.8.1	General Reading	711
9.8.2	Numbered References	712

Part 4: Emerging Areas in Ellipsometry	719
10 VUV Ellipsometry	721
10.1 Introduction	721
10.2 Historical Review of Short Wavelength Ellipsometry	722
10.2.1 BESSY Ellipsometer	722
10.2.2 EUV Ellipsometer	724
10.3 VUV Ellipsometry Today	726
10.3.1 Current VUV Instrumentation	726
10.4 Importance of VUV Ellipsometry	732
10.5 Survey of Applications	737
10.5.1 Lithography	740
10.5.2 Gate Dielectrics	748
10.5.3 High-energy Optical Constants	749
10.6 Future of VUV Ellipsometry	757
10.7 Acknowledgments	757
10.8 References	757
11 Spectroscopic Infrared Ellipsometry	763
11.1 Experimental Tools	763
11.1.1 Two Kinds of Instruments	763
11.1.2 Optical Equipment for the Infrared-Ellipsometry ..	768
11.1.3 The Degree of Polarization	771
11.1.4 Linearity of the Detection System	775
11.1.5 Infrared Synchrotron Radiation	775
11.2 Applications	776
11.2.1 Optics of Absorbing Media	776
11.2.2 Vibration Modes – the Concept of Weak and Strong Oscillators	778
11.2.3 Inversion of Infrared Ellipsometric Measurements ..	781
11.2.4 Anisotropy Features in the Infrared Ellipsometric Spectra	786
11.3 References	797
12 Ellipsometry in Life Sciences	799
Poem and Dedication	799
12.1 Introduction	800
12.2 Historical Background	802
12.3 The Interfaces Under Study	802
12.4 From Optics to Biology	804
12.4.1 The Unique Possibilities	804
12.4.2 Verification of Ellipsometric Results	805

12.5	Methodology for Data Evaluation – from ψ and Δ to Biologically Related Parameters	806
12.5.1	A Thin Biolayer on a Flat Ideal Substrate.....	806
12.5.2	A Thick Biolayer on a Flat Ideal Substrate	817
12.5.3	Adsorption of Biomolecules into Porous Structures	817
12.5.4	Surface Roughness	819
12.5.5	Use of Dispersion Models	820
12.5.6	Anisotropy	820
12.6	Methodology – Experimental	821
12.6.1	Instrumentation	821
12.6.2	Cell Designs.....	822
12.6.3	<i>In situ</i> Considerations for Biological Interfaces	824
12.6.4	Some Model Surfaces.....	825
12.6.5	Studies on Real Biological Surfaces	827
12.6.6	Complementary and Independent Information	828
12.6.7	Experimental Design	828
12.7	Applications.....	829
12.7.1	Introduction	829
12.7.2	Adsorption of Biomolecules to Model Surfaces	830
12.7.3	Spectroscopy.....	839
12.7.4	Imaging.....	841
12.7.5	Biological Surfaces.....	843
12.7.6	Biosensors Based on Ellipsometric Readout.....	844
12.7.7	Engineering Applications	845
12.8	Outlook	846
	Acknowledgements	847
12.9	References	847