

Contents

<i>Preface</i>	<i>page</i> xvi
1 Introduction and Overview	1
1.1 A classification of thin film configurations	2
1.2 Film deposition methods	6
1.2.1 Physical vapor deposition	6
1.2.2 Chemical vapor deposition	9
1.2.3 Thermal spray deposition	10
1.2.4 Example: Thermal barrier coatings	13
1.3 Modes of film growth by vapor deposition	15
1.3.1 From vapor to adatoms	15
1.3.2 From adatoms to film growth	17
1.3.3 Energy density of a free surface or an interface	20
1.3.4 Surface stress	25
1.3.5 Growth modes based on surface energies	27
1.4 Film microstructures	30
1.4.1 Epitaxial films	31
1.4.2 Example: Vertical-cavity surface-emitting lasers	39
1.4.3 Polycrystalline films	40
1.4.4 Example: Films for magnetic storage media	45
1.5 Processing of microelectronic structures	47
1.5.1 Lithography	48
1.5.2 The damascene process for copper interconnects	50
1.6 Processing of MEMS structures	52
1.6.1 Bulk micromachining	52
1.6.2 Surface micromachining	53
1.6.3 Molding processes	55
1.6.4 NEMS structures	55
1.6.5 Example: Vibrating beam bacterium detector	59

viii	<i>Contents</i>	
1.7	Origins of film stress	60
1.7.1	Classification of film stress	60
1.7.2	Stress in epitaxial films	62
1.8	Growth stress in polycrystalline films	63
1.8.1	Compressive stress prior to island coalescence	65
1.8.2	Example: Influence of areal coverage	68
1.8.3	Tensile stress due to island contiguity	69
1.8.4	Compressive stress during continued growth	70
1.8.5	Correlations between final stress and grain structure	72
1.8.6	Other mechanisms of stress evolution	73
1.9	Consequences of stress in films	83
1.10	Exercises	83
2	Film stress and substrate curvature	86
2.1	The Stoney formula	87
2.1.1	Example: Curvature due to epitaxial strain	92
2.1.2	Example: Curvature due to thermal strain	93
2.2	Influence of film thickness on bilayer curvature	93
2.2.1	Substrate curvature for arbitrary film thickness	95
2.2.2	Example: Maximum thermal stress in a bilayer	101
2.2.3	Historical note on thermostatic bimetal	102
2.3	Methods for curvature measurement	104
2.3.1	Scanning laser method	106
2.3.2	Multi-beam optical stress sensor	107
2.3.3	Grid reflection method	109
2.3.4	Coherent gradient sensor method	111
2.4	Layered and compositionally graded films	114
2.4.1	Nonuniform mismatch strain and elastic properties	116
2.4.2	Constant gradient in mismatch strain	120
2.4.3	Example: Stress in compositionally graded films	121
2.4.4	Periodic multilayer film	123
2.4.5	Example: Overall thermoelastic response of a multilayer	124
2.4.6	Multilayer film with small total thickness	125
2.4.7	Example: Stress in a thin multilayer film	126
2.5	Geometrically nonlinear deformation range	127
2.5.1	Limit to the linear range	128
2.5.2	Axially symmetric deformation in the nonlinear range	130
2.6	Bifurcation in equilibrium shape	132
2.6.1	Bifurcation analysis with uniform curvature	134
2.6.2	Visualization of states of uniform curvature	142
2.6.3	Bifurcation for general curvature variation	145

<i>Contents</i>		ix
2.6.4	A substrate curvature deformation map	149
2.6.5	Example: A curvature map for a Cu/Si system	150
2.7	Exercises	151
3	Stress in anisotropic and patterned films	154
3.1	Elastic anisotropy	155
3.2	Elastic constants of cubic crystals	157
3.2.1	Directional variation of effective modulus	158
3.2.2	Isotropy as a special case	161
3.3	Elastic constants of non-cubic crystals	161
3.4	Elastic strain in layered epitaxial materials	163
3.5	Film stress for a general mismatch strain	166
3.5.1	Arbitrary orientation of the film material	166
3.5.2	Example: Cubic thin film with a (111) orientation	169
3.6	Film stress from x-ray diffraction measurement	171
3.6.1	Relationship between stress and d -spacing	172
3.6.2	Example: Stress implied by measured d -spacing	174
3.6.3	Stress-free d -spacing from asymmetric diffraction	174
3.6.4	Example: Determination of reference lattice spacing	179
3.7	Substrate curvature due to anisotropic films	180
3.7.1	Anisotropic thin film on an isotropic substrate	180
3.7.2	Aligned orthotropic materials	182
3.8	Piezoelectric thin film	185
3.8.1	Mismatch strain due to an electric field	186
3.8.2	Example: Substrate curvature due to an electric field	187
3.9	Periodic array of parallel film cracks	188
3.9.1	Plane strain curvature change due to film cracks	190
3.9.2	Biaxial curvature due to film cracks	197
3.10	Periodic array of parallel lines or stripes	201
3.10.1	Biaxial curvature due to lines	201
3.10.2	Volume averaged stress in terms of curvature	206
3.10.3	Volume averaged stress in a damascene structure	209
3.11	Measurement of stress in patterned thin films	212
3.11.1	The substrate curvature method	212
3.11.2	The x-ray diffraction method	213
3.11.3	Micro-Raman spectroscopy	214
3.12	Exercises	216
4	Delamination and fracture	220
4.1	Stress concentration near a film edge	221
4.1.1	A membrane film	223

x	<i>Contents</i>	
	4.1.2 Example: An equation governing interfacial shear stress	226
	4.1.3 More general descriptions of edge stress	227
4.2	Fracture mechanics concepts	232
	4.2.1 Energy release rate and the Griffith criterion	233
	4.2.2 Example: Interface toughness of a laminated composite	237
	4.2.3 Crack edge stress fields	239
	4.2.4 Phase angle of the local stress state	243
	4.2.5 Driving force for interface delamination	243
4.3	Work of fracture	246
	4.3.1 Characterization of interface separation behavior	246
	4.3.2 Effects of processing and interface chemistry	250
	4.3.3 Effect of local phase angle on fracture energy	253
	4.3.4 Example: Fracture resistance of nacre	256
4.4	Film delamination due to residual stress	258
	4.4.1 A straight delamination front	262
	4.4.2 Example: Delamination due to thermal strain	263
	4.4.3 An expanding circular delamination front	264
	4.4.4 Phase angle of the stress concentration field	268
	4.4.5 Delamination approaching a film edge	270
4.5	Methods for interface toughness measurement	272
	4.5.1 Double cantilever test configuration	273
	4.5.2 Four-point flexure beam test configuration	274
	4.5.3 Compression test specimen configurations	277
	4.5.4 The superlayer test configuration	280
4.6	Film cracking due to residual stress	282
	4.6.1 A surface crack in a film	283
	4.6.2 A tunnel crack in a buried layer	290
	4.6.3 An array of cracks	292
	4.6.4 Example: Cracking of an epitaxial film	297
4.7	Crack deflection at an interface	297
	4.7.1 Crack deflection out of an interface	299
	4.7.2 Crack deflection into an interface	302
4.8	Exercises	309
5	Film buckling, bulging and peeling	312
5.1	Buckling of a strip of uniform width	313
	5.1.1 Post-buckling response	314
	5.1.2 Driving force for growth of delamination	319
	5.1.3 Phase angle of local stress state at interface	321
	5.1.4 Limitations for elastic–plastic materials	325

	<i>Contents</i>	xi
5.2	Buckling of a circular patch	327
5.2.1	Post-buckling response	328
5.2.2	Example: Temperature change for buckling of a debond	332
5.2.3	Driving force for delamination	333
5.2.4	Example: Buckling of an oxide film	337
5.3	Secondary buckling	338
5.4	Experimental observations	341
5.4.1	Edge delamination	341
5.4.2	Initially circular delamination	341
5.4.3	Effects of imperfections on buckling delamination	345
5.4.4	Example: Buckling instability of carbon films	348
5.5	Film buckling without delamination	350
5.5.1	Soft elastic substrate	350
5.5.2	Viscous substrate	353
5.5.3	Example: Buckling wavelength for a glass substrate	354
5.6	Pressurized bulge of uniform width	355
5.6.1	Small deflection bending response	355
5.6.2	Large deflection response	357
5.6.3	Membrane response	360
5.6.4	Mechanics of delamination	363
5.7	Circular pressurized bulge	366
5.7.1	Small deflection bending response	367
5.7.2	Membrane response	367
5.7.3	Large deflection response	371
5.7.4	The influence of residual stress	372
5.7.5	Delamination mechanics	374
5.7.6	Bulge test configurations	377
5.8	Example: MEMS capacitive transducer	378
5.9	Film peeling	382
5.9.1	The driving force for delamination	382
5.9.2	Mechanics of delamination	383
5.10	Exercises	385
6	Dislocation formation in epitaxial systems	387
6.1	Dislocation mechanics concepts	388
6.1.1	Dislocation equilibrium and stability	388
6.1.2	Elastic field of a dislocation near a free surface	391
6.2	Critical thickness of a strained epitaxial film	396
6.2.1	The critical thickness criterion	397
6.2.2	Dependence of critical thickness on mismatch strain	400
6.2.3	Example: Critical thickness of a SiGe film on Si(001)	402

xii	<i>Contents</i>	
	6.2.4 Experimental results for critical thickness	403
	6.2.5 Example: Influence of crystallographic orientation on h_{cr}	404
6.3	The isolated threading dislocation	406
	6.3.1 Condition for advance of a threading dislocation	406
	6.3.2 Limitations of the critical thickness condition	411
	6.3.3 Threading dislocation under nonequilibrium conditions	413
6.4	Layered and graded films	416
	6.4.1 Uniform strained layer capped by an unstrained layer	418
	6.4.2 Strained layer superlattice	422
	6.4.3 Compositionally graded film	423
6.5	Model system based on the screw dislocation	424
	6.5.1 Critical thickness condition for the model system	424
	6.5.2 The influence of film–substrate modulus difference	426
	6.5.3 Example: Modulus difference and dislocation formation	429
6.6	Non-planar epitaxial systems	430
	6.6.1 A buried strained quantum wire	432
	6.6.2 Effect of a free surface on quantum wire stability	437
6.7	The influence of substrate compliance	441
	6.7.1 A critical thickness estimate	442
	6.7.2 Example: Critical thickness for a compliant substrate	444
	6.7.3 Misfit strain relaxation due to a viscous underlayer	445
	6.7.4 Force on a dislocation in a layer	448
6.8	Dislocation nucleation	451
	6.8.1 Spontaneous formation of a surface dislocation loop	453
	6.8.2 Dislocation nucleation in a perfect crystal	455
	6.8.3 Effect of a stress concentrator on nucleation	458
6.9	Exercises	461
7	Dislocation interactions and strain relaxation	464
7.1	Interaction of parallel misfit dislocations	465
	7.1.1 Spacing based on mean strain	466
	7.1.2 Spacing for simultaneous formation of dislocations	467
	7.1.3 Spacing based on insertion of the last dislocation	469
7.2	Interaction of intersecting misfit dislocations	470
	7.2.1 Blocking of a threading dislocation	472
	7.2.2 Intersecting arrays of misfit dislocations	477
7.3	Strain relaxation due to dislocation formation	480
	7.3.1 Construction of a relaxation model	480
	7.3.2 Example: Dislocation control in semiconductor films	484
7.4	Continuum analysis of ideally plastic films	488
	7.4.1 Plastic deformation of a bilayer	488
	7.4.2 Thin film subjected to temperature cycling	494

	<i>Contents</i>	xiii
7.5	Strain-hardening response of thin films	496
7.5.1	Isotropic hardening	499
7.5.2	Example: Temperature cycling with isotropic hardening	501
7.5.3	Kinematic hardening	502
7.5.4	Proportional stress history	505
7.6	Models based on plastic rate equations	508
7.6.1	Thermally activated dislocation glide past obstacles	510
7.6.2	Influence of grain boundary diffusion	512
7.7	Structure evolution during thermal excursion	515
7.7.1	Experimental observation of grain structure evolution	515
7.7.2	Experimental observation of threading dislocations	517
7.7.3	Strain relaxation mechanisms during temperature cycling	520
7.8	Size-dependence of plastic yielding in thin films	527
7.8.1	Observation of plastic response	527
7.8.2	Models for size-dependent plastic flow	531
7.8.3	Influence of a weak film–substrate interface	534
7.9	Methods to determine plastic response of films	535
7.9.1	Tensile testing of thin films	535
7.9.2	Microbeam deflection method	537
7.9.3	Example: Thin film undergoing plane strain extension	539
7.9.4	Substrate curvature method	542
7.9.5	Instrumented nanoindentation	543
7.10	Exercises	547
8	Equilibrium and stability of surfaces	550
8.1	A thermodynamic framework	551
8.2	Chemical potential of a material surface	553
8.2.1	An evolving free surface	553
8.2.2	Mass transport along a bimaterial interface	558
8.2.3	Migration of a material interface	560
8.2.4	Growth or healing of crack surfaces	564
8.3	Elliptic hole in a biaxially stressed material	567
8.3.1	Chemical potential	568
8.3.2	Shape stability	570
8.4	Periodic perturbation of a flat surface	573
8.4.1	Small amplitude sinusoidal fluctuation	573
8.4.2	Example: Stability of a strained epitaxial film	578
8.4.3	Influence of substrate stiffness on surface stability	578
8.4.4	Second order surface perturbation	582
8.4.5	Example: Validity of the small slope approximation	586
8.5	General perturbation of a flat surface	588
8.5.1	Two-dimensional configurations	588

xiv	<i>Contents</i>	
	8.5.2 Three-dimensional configurations	589
	8.5.3 Example: Doubly periodic surface perturbation	590
8.6	Contact of material surfaces with cohesion	592
	8.6.1 Force–deflection relationship for spherical surfaces	592
	8.6.2 Example: Stress generated when islands impinge	597
8.7	Consequences of misfit dislocation strain fields	598
	8.7.1 Surface waviness due to misfit dislocations	599
	8.7.2 Growth patterning due to misfit dislocations	602
8.8	Surface energy anisotropy in strained materials	604
	8.8.1 Implications of mechanical equilibrium	605
	8.8.2 Surface chemical potential	608
	8.8.3 Energy of a strained vicinal surface	610
	8.8.4 Example: Stepped surface near (001) for strained Si	615
8.9	Strained epitaxial islands	615
	8.9.1 An isolated island	618
	8.9.2 Influence of an intervening strained layer	624
	8.9.3 Influence of surface energy anisotropy	626
	8.9.4 Nucleation barrier for islands on stable surfaces	628
	8.9.5 Shape transition for preferred side wall orientations	630
	8.9.6 Observations of island formation	632
8.10	Exercises	638
9	The role of stress in mass transport	641
9.1	Mechanisms of surface evolution	643
	9.1.1 Surface diffusion	643
	9.1.2 Condensation–evaporation	647
9.2	Evolution of small surface perturbations	648
	9.2.1 One-dimensional sinusoidal surface	649
	9.2.2 Example: The characteristic time	650
	9.2.3 General surface perturbations	651
	9.2.4 An isolated surface mound	654
9.3	A variational approach to surface evolution	657
	9.3.1 A variational principle for surface flux	658
	9.3.2 Application to second order surface perturbation	662
9.4	Growth of islands with stepped surfaces	665
	9.4.1 Free energy change	666
	9.4.2 Formation and interaction of islands	668
9.5	Diffusion along interfaces	673
	9.5.1 Stress relaxation by grain boundary diffusion	674
	9.5.2 Diffusion along shear bands during deformation	678

Cambridge University Press

978-0-521-82281-7 - Thin Film Materials: Stress, Defect Formation and Surface Evolution

L. B. Freund and S. Suresh

Table of Contents

[More information](#)

<i>Contents</i>		xv
9.6	Compositional variations in solid solutions	681
9.6.1	Free energy of a homogeneous solution	682
9.6.2	Stability of a uniform composition	685
9.6.3	Example: Elastic stabilization of a composition	689
9.6.4	Evolution of compositional variations	690
9.6.5	Coupled deformation–composition evolution	692
9.7	Stress-assisted diffusion: electromigration	697
9.7.1	Atom transport during electromigration	698
9.7.2	The drift test	704
9.7.3	Effects of microstructure on electromigration damage	706
9.7.4	Assessment of interconnect reliability	709
9.8	Exercises	711
	<i>References</i>	713
	<i>Author index</i>	738
	<i>Subject index</i>	745