

Contents

Editor's Preface	xii
Author's Preface—Reflections on Some Transformations	xiii
About the Author	xvi
Part 1 Martensite	1
Introduction to Part I—Martensite	3
<i>Harry Bhadeshia</i>	
CHAPTER 1	
Dislocation Theory of Martensitic Transformations	7
Introduction	7
Crystallography and Interfacial Structure	7
Kinematic Approach to Transformation Crystallography	8
Orientation Relations	10
Strain-Energy Minimization	10
Interfacial Dislocations	13
Martensitic Interfaces	18
Interfacial Mobility	30
Conservative versus Nonconservative Motion	30
Interfacial Driving Force	31
Continuous Motion	32
Thermally Activated Motion	32
Strain Interaction	36
Modulus Interaction	39
Short-Range Interactions	41
Multiparticle Interactions	42
Coupled Diffusional/Displacive Transformation	45
Classical Nucleation Theory	47
Heterogeneous Nucleation by Defect Dissociation	48
Dissociation at Fixed Thickness	49
Thickness Fluctuations	52
Nonclassical Nucleation	57
Surface Nucleation	60
Nucleation Kinetics	62
Martensitic Growth	65
Thermoelastic Behavior	65
Thermoelastic–Nonthermoelastic Transition	67
Nonthermoelastic Growth	70
Overall Kinetics	73

Some Special Applications	74
Transformation Plasticity	74
Biological Martensitic Transformations	79
Conclusions	81
CHAPTER 2	
On the Hierarchy of Interfacial Dislocation Structure	86
Abstract	86
Introduction	86
Grain Boundaries	87
Primary Interfacial Dislocations	87
Secondary Interfacial Dislocations	93
Translational Interfacial Dislocations	96
Interphase Boundaries	97
Coherency Interfacial Dislocations	97
Primary Interfacial Dislocations	99
Secondary Interfacial Dislocations	101
Final Remarks	102
CHAPTER 3	
Martensitic Nucleation	105
Historical Perspective	105
Current Theory of Martensitic Nucleation	108
Parameters of Nucleation Theory	108
Strain Path—Classical versus Nonclassical Nucleation	109
Strain Relaxation—States of Coherency	113
Heterogeneity—Homogeneous versus Heterogeneous Nucleation	116
Future Directions	122
CHAPTER 4	
Statistical Aspects of Martensitic Nucleation	126
Abstract	126
Introduction	126
The Nucleation-Site Potency Distribution	126
Small Particle Behavior	126
Bulk Polycrystal Behavior	129
Effect of Applied Stress	130
The Mechanical Driving-Force Distribution	130
Applications to Transformation Plasticity	132
Closure	135
CHAPTER 5	
New Directions in Martensite Theory	136
Abstract	136
Systems—Dynamic Hierarchy	136
Physics of Lattice, Deformations, and Interfaces	138
Nucleation	140
Growth	142
Defect Hierarchy—Distributed Systems	143
Constrained Systems	145
Biological Systems—Molecular Martensite?	146
Chapter 6	
Distributed-Activation Kinetics of Heterogeneous	
Martensitic Nucleation	149
Abstract	149
Introduction	149

Preexisting Defect Size Distribution	150
Singly Activated Kinetic Model	151
Experimental	152
Experimental Results	152
Discussion	154
Critical Defect Size for Martensitic Nucleation	154
Autocatalytic-Defect Size Distribution	155
Distributed Activation Kinetics of Nucleation	158
Range of Kinetic Behaviors	159
Conclusions	161
CHAPTER 7	
Coupled Diffusional/Displacive Transformations (Part II)—	
Solute Trapping	164
Abstract	164
Introduction	164
The Interface Response Functions	165
The Interface Mobility	165
The Diffusion Field Velocity	166
Solute Trapping Law	166
Results and Discussion	168
Conclusions	169
Nomenclature and Abbreviations	169
CHAPTER 8	
Kinetics of Martensite Transformations in Steels	171
Abstract	171
Introduction	171
Mechanism and Kinetics of Martensitic Transformation	171
Heterogeneous Nucleation by Defect Dissociation	172
Mechanically Induced Transformations	173
Mechanism of Stress-Assisted Transformations	174
Mechanism of Strain-Induced Transformations	175
Transformation Plasticity Constitutive Relations and Applications	175
Constitutive Flow Relations of Transformation Plasticity	175
Stability of Plastic Flow	179
Applications of Transformation Plasticity to Ductility	180
Applications of Transformation Plasticity to Fracture Toughness	181
Conclusions	184
CHAPTER 9	
Spinodal Decomposition during Aging of Fe-Ni-C Martensites	187
Abstract	187
Introduction	187
Experimental Procedures	188
Materials and Processing	188
Electron Microscopy	189
Atom-Probe Field-Ion Microscopy	189
Electrical Resistivity Measurements	189
Results	190
Electron Microscopy	190
Atom-Probe Field-Ion Microscopy	192
Electrical Resistivity	200
Discussion	201
Decomposition Morphology	201
Structure of the High-Carbon Phase	202

Thermodynamics of Decomposition	204
Kinetics of Aging	205
Substructural Effects	206
Properties of Aged Martensites	206
Conclusions	207
Part 2 Materials Design	211
Introduction to Part II—Materials Design	213
<i>Charles Kuehmann</i>	
CHAPTER 10	
Computational Design of Hierarchically Structured Materials	215
Abstract	215
Introduction	215
Materials as Systems	215
Subsystem Modeling	218
Strength Subsystems	218
Toughness Subsystems	219
Embrittlement Resistance Subsystems	219
Design Examples	221
CHAPTER 11	
Overview—Science of Steel	225
Introduction—Steels and Materials Design	225
Property Objectives	225
Materials as Systems—An Approach to Design	227
Strengthening	229
Toughening and Shear Localization	237
Shear Instability and Particle Dispersions	237
Transformation Toughening	244
Hydrogen Resistance and Interfacial Cohesion	249
Materials Design—Stainless Bearing Steel	256
Summary	258
CHAPTER 12	
Designing a New Material World	264
Materials as Systems	264
The Materials Discipline Comes of Age	266
Materials by Design—Efficient Innovation	267
Structure of Education	269
Materials by Design	270
Virtualizing Materials to Create Real Ones	271
CHAPTER 13	
Charge Transfer Mechanism of Hydrogen-Induced Intergranular Embrittlement of Iron	277
Abstract	277
Introduction	277
CHAPTER 14	
Influence of Alloying Additions on Grain Boundary Cohesion of Transition Metals—First-Principles Determination and Its Phenomenological Extension	283
Abstract	283
Introduction	283

Phenomenological Model	285
Volume Effect	285
Bonding Character	288
Heat of Formation for Solid Solutions—Macroscopic Atom Model	290
Confirmation of the Model	291
Summary	291
CHAPTER 15	
Strong Interface Adhesion in Fe/TiC	294
Abstract	294
Introduction	294
Computational Details	295
Results and Discussion	296
Bulk Properties of Fe and TiC, Interface Orientation, and Site Preference	296
Interface Properties of Fe/TiC	297
Equilibrium Properties	297
Rigid Separation	298
Separation with Relaxation	301
Summary	302
CHAPTER 16	
Systems Design of High-Performance Stainless Steels—I. Conceptual and Computational Design	305
Abstract	305
Introduction	305
Conceptual Design	307
Property Objectives	307
Design Approach	308
Case Subsystem	309
Core Subsystem	310
Model Development	311
Martensitic Transformation Behavior	312
Precipitation of Coherent M_2C Carbides	313
Aqueous Corrosion Resistance	314
Solidification Microsegregation	315
Computational Design Integration	316
Matrix Optimization	316
Strengthening Dispersion Optimization	317
Aqueous Corrosion	318
Castability	318
Reoptimization	320
Discussion	321
Conclusions	322
CHAPTER 17	
Systems Design of High-Performance Stainless Steels—II. Prototype Characterization	325
Abstract	325
Introduction	325
Materials and Methods	326
Materials	326
Experimental Methods	326
Characterization of Prototype (Results)	328
Core Material	328
Case Material	333

Discussion	337
Conclusions	339
CHAPTER 18	
Computer-Aided Design of Transformation Toughened Blast-Resistant Naval Hull Steels—Part I	341
Abstract	341
Introduction	341
Design Objectives	342
Design Approach	342
Strength Design	346
Quantitative Strengthening Contributions	346
M ₂ C Carbide Strengthening	347
Copper Precipitation Strengthening	349
Transformation Toughening Design	350
Composition Integration	352
Processing Considerations	353
Solution Treatment Temperature and Allotropic Transformations	353
Scheil Simulation for Microsegregation Behavior	353
Selection of Tempering Temperature	354
Summary and Conclusions	354
CHAPTER 19	
Prototype Evaluation of Transformation Toughened Blast-Resistant Naval Hull Steels—Part II	359
Abstract	359
Introduction	360
Material and Experimental Procedures	360
Material	360
Experimental Procedures	360
Heat Treating	360
Metallographic Sample Preparation	360
Dilatometry	361
Microhardness Testing	361
Impact Toughness Testing	361
Tensile Testing	361
Scanning Electron Microscopy	362
3D Atom Probe/Field Ion Microscopy (AP-FIM)	362
Prototype Evaluation Results	363
Primary Processing Behavior	363
Microsegregation and Hot-Working Behavior	363
Evaluation of Allotropic Kinetics	364
Thermal Process Optimization	365
Isochronal Tempering Response	365
Toughness Optimization by Multistep Tempering	367
Mechanical Properties	370
Evaluation of Tensile Properties	370
Toughness-Temperature Dependence	371
Microstructural Validation	372
Three-Dimensional Atom Probe (3DAP) Microscopy	373
Summary and Conclusions	378
CHAPTER 20	
Design of Heusler Precipitation Strengthened NiTi- and PdTi-Base Shape Memory Alloys for Cyclic Performance	382
Abstract	382
Introduction	382

Motivation and Background	382
Design Objectives	384
Systems Design of SMAs	385
Design Chart	385
Models	385
Strengthening Models	385
Kinetic Models	386
Composition Trajectory Models	386
Misfit Model	387
A _f Model	387
Radiopacity Model	388
Experimental Methods	388
Process Optimization	389
NiTi-Base Systems	389
NiTiAl-X (X = 5 at.% Pd, Pt, Zr, Hf) Systems	389
Ni(Ti,Zr,Al) System	390
PdTi-Base Systems	392
Low-Ni (Pd,Ni)(Ti,Al) System	392
Ni-Free (Pd,Fe)(Ti,Al) System	392
Structure/Property Relations	393
Calibrating Strength Models	393
Transformation Temperature	394
Cyclic Stability Validation	396
Low-Ni Hybrid (Pd,Ni)(Ti,Zr,Al)	396
Nonmetallic Inclusions	397
Conclusions and Recommendations	398

CHAPTER 21

Integrated Computational Materials Engineering—Success Stories and Cultural Barriers

	402
Introduction	402
Computational Design Successes—Flying Cyber Steel	402
Extending Computation Design to Qualification and Implementation	404
Integrated Computational Material Engineering Cultural Barriers	405

CHAPTER 22

Computer Simulations for the Prediction of Microstructure/Property Variation in Aeroturbine Disks

	407
Abstract	407
Introduction	407
Multicomponent Precipitation Models	407
Continuity Equation	409
Growth Model	409
Homogeneous and Transient Nucleation Models	410
Isothermal Nucleation	410
Nonisothermal Nucleation	411
Mass Conservation	411
Software Implementation	412
Numerical Schemes	412
CALPHAD Tool Integration	412
Software Engineering and AIM Integration	412
Applications to IN100 Aeroturbine Disk Alloy	413
Simulations for the Disk Center Location	414
Spatial Calculations for IN100 Disk	416
Additional Applications of PrecipiCalc in AIM Program	416
Conclusions	417

CHAPTER 23	
Precipitation Model Validation in Third-Generation Aeroturbine Disc Alloys	419
Abstract	419
Introduction	419
PrecipiCalc Calibration and Validation Protocol	420
Thermodynamics	421
Alloy 10/ME3 Equilibrium Studies	421
Ni-Al-Cr(-X) (X=Re,W) Model Alloys	422
Misfit Estimates	423
Mobility	424
Nonisothermal Precipitation	425
Nucleation Onset Temperatures and SSDTA	425
γ' Microstructure in SSDTA Samples	427
γ' Microstructure in ME3 Water-Quenched Samples	428
γ' Microstructure in Furnace-Cooled Samples	429
Coarsening Experiments	430
Conclusion and Summary	431
CHAPTER 24	
Multiscale Ductile Fracture Integrating Tomographic Characterization and 3D Simulation	433
Abstract	433
Introduction	433
Experimental Reconstruction of a Crack	435
Simulation of Ductile Fracture	435
Integration of Experiment with Simulation	436
Metrics of Fracture	438
Crack Opening Displacement	438
Shear Localization Wavelength	440
Void Growth Ratio	440
Conclusion	442
CHAPTER 25	
3D-Modeling of Subsurface Fatigue Crack Nucleation Potency of Primary Inclusions in Heat-Treated and Shot Peened Martensitic Gear Steels	444
Abstract	444
Introduction	445
Experimental Observations of Fatigue in Case-Hardened Steel	447
Characterization of Mechanical Properties of Matrix and Inclusions	448
General Outline of Elasto-Plastic Framework	448
Imposition of Initial Residual Stress: Modeling the Effect of Shot Peening Process	449
Fatigue Crack Nucleation Analysis under Cyclic Loading	451
Results and Discussion	453
Cracked Inclusion Analyses	453
Partially Debonded Inclusion Analyses	457
Summary	460
CHAPTER 26	
Genomic Materials Design—The Ferrous Frontier	465
Abstract	465
Introduction	465
Background—Emergence of a Design Discipline	466

The Predictive Science Foundation	467
Computational Design Successes—Flying Cybersteel	470
Extending Computational Design to Qualification and Implementation	472
Research/Education Integration	474
Conclusions	475
CHAPTER 27	
Materials Genomics—From CALPHAD to Flight	479
Abstract	479
Introduction	479
Background—Emergence of a Materials Genome Infrastructure	480
Computational Design Successes—Flying Cybersteels	481
Extending Computational Design to Qualification and Implementation	482
Materials Genome Future	483
Conclusions	484
CHAPTER 28	
Cybermaterials—Materials by Design and Accelerated Insertion of Materials	487
Abstract	487
Background—ICMD Blueprint	487
Materials by Design—Design Engine	489
Process—Structure Relation and Design Models	489
Structure—Property Relation and Design Models	493
Structure-Strength	493
Structure-Toughness	495
Structure-Creep/Fatigue	498
AIM—Accelerating Technology Transition	499
Summary—Cybermaterials Innovation Based on Materials Genome	502
CHAPTER 29	
Hierarchical Model for Coaching Technical Design Teams	509
Abstract	509
Coaching Model	509
Model Implementation	510
Design Projects	511
Method	512
Results	512
Mentoring to Achieve a High Technical Level	512
Motivation	513
Discussion	514
Conclusions and Future Work	515
Appendix—Patents and Publications	517
Index	531