

---

## Contents

---

<b>Preface .....</b>	<b>xi</b>
<b>Chapter 1. Synchrotron Imaging and Diffraction for <i>In Situ</i> 3D Characterization of Polycrystalline Materials .....</b>	<b>1</b>
Henry PROUDHON	
1.1. Introduction .....	1
1.2. 3D X-ray characterization of structural materials .....	3
1.2.1. Early days of X-ray computed tomography .....	3
1.2.2. X-ray absorption and Beer Lambert's law .....	4
1.2.3. X-ray detection .....	6
1.2.4. Radon's transform and reconstruction .....	8
1.2.5. Synchrotron X-ray microtomography .....	10
1.2.6. Phase contrast tomography .....	13
1.2.7. Diffraction contrast tomography .....	14
1.3. Nanox: a miniature mechanical stress rig designed for near-field X-ray diffraction imaging techniques .....	16
1.4. Coupling diffraction contrast tomography with the finite-element method. ....	19
1.4.1. Motivation for image-based mechanical computations. ....	19
1.4.2. 3D mesh generation from tomographic images. ....	20
1.4.3. Toward a fatigue model at the scale of the polycrystal .....	28
1.5. Conclusion and outlook .....	29
1.6. Bibliography. ....	31

---

<b>Chapter 2. Determining the Probability of Occurrence of Rarely Occurring Microstructural Configurations for Titanium Dwell Fatigue . . . . .</b>	<b>41</b>
Adam L. PILCHAK, Joseph C. TUCKER and Tyler J. WEHING	
2.1. Introduction . . . . .	42
2.2. Experimental methods . . . . .	44
2.2.1. MTR quantification metrics . . . . .	44
2.2.2. Synthetic microstructure generation . . . . .	46
2.2.3. Crystallographic analysis for titanium dwell fatigue . . . . .	48
2.2.4. Block maxima . . . . .	50
2.3. Results and discussion . . . . .	51
2.3.1. Probability of occurrence . . . . .	53
2.3.2. “Hard” MTR size distributions . . . . .	57
2.3.3. Block maxima . . . . .	58
2.4. Summary and outlook . . . . .	63
2.5. Bibliography . . . . .	64
<b>Chapter 3. Wave Propagation Analysis in 2D Nonlinear Periodic Structures Prone to Mechanical Instabilities . . . . .</b>	<b>67</b>
Hilal REDA, Yosra RAHALI, Jean-François GANGHOFFER and Hassan LAKISS	
3.1. Introduction . . . . .	68
3.2. Extensible energy of pantograph for dynamic analysis . . . . .	70
3.2.1. Expression of the pantographic network energy . . . . .	70
3.2.2. Dynamic equilibrium equation . . . . .	73
3.3. Wave propagation in a nonlinear elastic beam . . . . .	75
3.3.1. Legendre–Hadamard ellipticity condition and loss of stability . . . . .	77
3.3.2. Supersonic and subsonic modes for 1D wave propagation . . . . .	78
3.3.3. Wave dispersion relation in 2D nonlinear periodic structures . . . . .	81
3.3.4. Anisotropic behavior of 2D pantographic networks versus the degree of nonlinearity . . . . .	84
3.4. Conclusion . . . . .	85
3.5. Appendix . . . . .	86
3.6. Bibliography . . . . .	94

---

<b>Chapter 4. Multiscale Model of Concrete Failure . . . . .</b>	<b>99</b>
Emir KARAVELIĆ, Mijo NIKOLIĆ and Adnan IBRAHIMBEGOVIĆ	
4.1. Introduction . . . . .	99
4.2. Meso-scale model. . . . .	102
4.3. Macroscopic model response . . . . .	106
4.3.1. Uniaxial tests . . . . .	106
4.3.2. Failure surface . . . . .	111
4.4. Conclusions . . . . .	117
4.5. Acknowledgments . . . . .	119
4.6. Bibliography . . . . .	120
<b>Chapter 5. Discrete Numerical Simulations of the Strength and Microstructure Evolution During Compaction of Layered Granular Solids . . . . .</b>	<b>123</b>
Bereket YOHANNES, Marcial GONZALEZ and Alberto M. CUITIÑO	
5.1. Introduction . . . . .	123
5.2. Numerical simulation . . . . .	127
5.2.1. Discrete particle simulations of powder compaction. . . . .	127
5.2.2. Discrete particle simulation of layered compacts. . . . .	129
5.3. Discussion . . . . .	131
5.4. Conclusion . . . . .	137
5.5. Acknowledgements. . . . .	137
5.6. Bibliography . . . . .	137
<b>Chapter 6. Microstructural Views of Stresses in Three-Phase Granular Materials . . . . .</b>	<b>143</b>
Jérôme DURIEZ, Richard WAN and Félix DARVE	
6.1. Microstructural expression of triphasic total stresses . . . . .	145
6.1.1. Stress description within micro-scale volumes and interfaces of triphasic materials . . . . .	145
6.1.2. Total stress derivation. . . . .	146
6.2. Numerical modeling of wet ideal granular materials . . . . .	149
6.2.1. DEM description of fluid microstructure . . . . .	149
6.2.2. DEM description of stress and strains . . . . .	152
6.3. Anisotropy of the capillary stress contribution. . . . .	154
6.3.1. Mechanical loading . . . . .	155
6.3.2. Hydraulic loading . . . . .	157

---

6.4. Effective stress . . . . .	160
6.5. Conclusion . . . . .	162
6.6. Bibliography . . . . .	163

<b>Chapter 7. Effect of the Third Invariant of the Stress Deviator on the Response of Porous Solids with Pressure-Insensitive Matrix . . . . .</b>	167
José Luis ALVES and Oana CAZACU	

7.1. Introduction . . . . .	168
7.2. Problem statement and method of analysis . . . . .	171
7.2.1. Drucker yield criterion for isotropic materials . . . . .	171
7.2.2. Unit cell model . . . . .	173
7.3. Results . . . . .	179
7.3.1. Yield surfaces and porosity evolution . . . . .	179
7.4. Conclusions . . . . .	190
7.5. Bibliography . . . . .	194

<b>Chapter 8. High Performance Data-Driven Multiscale Inverse Constitutive Characterization of Composites . . . . .</b>	197
---	-----

John MICHOPoulos, Athanasios ILIOPOULOS, John HERMANSON,  
John STEUBEN and Foteini KOMNINELI

8.1. Introduction . . . . .	198
8.2. Automated multi-axial testing . . . . .	202
8.2.1. Loading space . . . . .	204
8.2.2. Experimental campaign . . . . .	206
8.3. Constitutive formalisms . . . . .	207
8.3.1. Small strain formulation . . . . .	208
8.3.2. Finite strain formulation . . . . .	209
8.4. Meshless random grid method for experimental evaluation of strain fields . . . . .	209
8.5. Inverse determination of HDM via design optimization . . . . .	211
8.5.1. Numerical results of design optimization . . . . .	214
8.6. Surrogate models for characterization . . . . .	216
8.6.1. Definition and construction of the surrogate model . . . . .	218
8.6.2. Characterization by optimization . . . . .	219
8.6.3. Validation with physical experiments . . . . .	221

---

8.7. Multi-scale inversion . . . . .	221
8.7.1. Forward problem: mathematical homogenization . . . . .	222
8.7.2. Inverse problem . . . . .	224
8.8. Computational framework and synthetic experiments . . . . .	226
8.9. Conclusions and plans . . . . .	230
8.10. Acknowledgments . . . . .	232
8.11. Bibliography . . . . .	232
<b>Chapter 9. New Trends in Computational Mechanics: Model Order Reduction, Manifold Learning and Data-Driven . . . . .</b>	<b>239</b>
Jose Vicente AGUADO, Domenico BORZACCHIELLO, Elena LOPEZ, Emmanuelle ABISSET-CHAVANNE, David GONZALEZ, Elias CUETO and Francisco CHINESTA	
9.1. Introduction . . . . .	240
9.1.1. The big picture . . . . .	240
9.1.2. The PGD at a glance . . . . .	242
9.2. Constructing slow manifolds . . . . .	245
9.2.1. From principal component analysis (PCA) to kernel principal component analysis (kPCA) . . . . .	245
9.2.2. Kernel principal component analysis (kPCA) . . . . .	249
9.2.3. Locally linear embedding (LLE) . . . . .	250
9.2.4. Discussion . . . . .	251
9.3. Manifold-learning-based computational mechanics . . . . .	252
9.4. Data-driven simulations . . . . .	253
9.4.1. Data-based weak form . . . . .	254
9.4.2. Constructing the constitutive manifold . . . . .	254
9.5. Data-driven upscaling of viscous flows in porous media . . . . .	257
9.5.1. Upscaling Newtonian and generalized Newtonian fluids flowing in porous media . . . . .	258
9.6. Conclusions . . . . .	260
9.7. Bibliography . . . . .	261
<b>List of Authors . . . . .</b>	<b>267</b>
<b>Index . . . . .</b>	<b>271</b>