

Contents

Section 1

Research significance and background — 1

Section 2

Bulk metallic glasses (BMGs) and bulk metallic glass matrix composites (BMGMCs) — 5

- 2.1 Metallic glasses (MG) and bulk metallic glasses (BMGs)/monoliths — 5
- 2.2 Three laws — 5
- 2.3 Classification – various approaches — 6
 - 2.3.1 Based on elements and their types — 7
- 2.4 Important characteristics — 8
 - 2.4.1 Glass-forming ability — 8
 - 2.4.2 Metastability — 11
- 2.5 Limitations — 11
- 2.6 Ductile BMG — 12
- 2.7 Ductile bulk metallic glass matrix composites — 13
- 2.8 Production methods – mechanisms perspective — 14
 - 2.8.1 Liquid–solid transformation (solidification) — 14
 - 2.8.2 Solid–solid (S–S) transformation (devitrification) — 23
- 2.9 Production method – process perspective — 24
 - 2.9.1 Twin-roll casting — 24
 - 2.9.2 Cu mold (suction) casting — 25
 - 2.9.3 Semisolid processing — 26
 - 2.9.4 High-pressure die casting — 27
 - 2.9.5 Continuous casting — 29
 - 2.9.6 Squeeze casting — 29
 - 2.9.7 Injection molding — 30
 - 2.9.8 Centrifugal casting — 31
 - 2.9.9 Friction stir welding — 31
 - 2.9.10 Joining — 32
 - 2.9.11 Foams — 34
 - 2.9.12 Thin films — 35
 - 2.9.13 Additive manufacturing — 36
- 2.10 Model alloys — 39
 - 2.10.1 Common phases and microstructures — 40
 - 2.10.2 Mechanical properties — 45
- 2.11 Very recent trends, approaches and triumphs — 47

- 2.11.1 Understanding structure — **47**
- 2.11.2 Shear bands — **51**
- 2.11.3 High-entropy metallic glass — **52**
- 2.11.4 Nanoglasses — **52**
- 2.11.5 Corrosion behavior — **53**
- 2.11.6 Shape memory BMG — **53**
- 2.11.7 Limitations/research gap – new findings — **53**
- 2.11.8 Present research – advancement since the first edition — **54**

Section 3

Additive manufacturing (AM) — 57

- 3.1 Why additive manufacturing (AM)? — **57**
- 3.2 A brief history of additive manufacturing — **57**
- 3.3 Principles of additive manufacturing — **58**
 - 3.3.1 Laser processes — **58**
 - 3.3.2 Electron beam melting — **67**
- 3.4 Characteristics of process — **69**
 - 3.4.1 LBL formation — **69**
 - 3.4.2 Rapid cooling — **71**
 - 3.4.3 Assimilation of free volume — **71**
 - 3.4.4 In situ heat treatment — **71**
- 3.5 Bulk metallic glasses by additive manufacturing — **72**
- 3.6 Bulk matrix glass matrix composites by additive manufacturing — **72**

Section 4

Modeling and simulation — 77

- 4.1 Why modeling and simulation? — **77**
- 4.2 Capabilities/powers and limitations — **77**
- 4.3 Types of modeling and simulation — **78**
 - 4.3.1 Energy minimization — **78**
 - 4.3.2 Molecular dynamic simulations — **78**
 - 4.3.3 Monte Carlo simulations — **79**
 - 4.3.4 Miscellaneous methods — **79**
- 4.4 Modeling and simulation of nucleation (microstructural evolution) in solidification — **80**
- 4.5 Large-/part-scale modeling — **81**
 - 4.5.1 Analytical modeling — **82**
 - 4.5.2 Computational modeling — **83**
- 4.6 Atomic-scale (atomistic) modeling — **89**
 - 4.6.1 Classical molecular dynamics — **90**

- 4.6.2 Monte Carlo simulations — 90
- 4.6.3 Ab initio methods/first principle calculations — 91
- 4.6.4 Interatomic potential/force fields — 94
- 4.7 Very recent trends/future outlook — 97

Section 5

Modeling and simulation of solidification phenomena during processing of BMGMC by additive manufacturing (AM) — 99

- 5.1 Introduction — 99
- 5.2 Modeling and simulation of heat transfer in liquid melt pool – solidification — 99
 - 5.2.1 Generation of heat (laser matter interaction) — 100
 - 5.2.2 Assimilation of heat (melting and stage of solidification) — 102
- 5.3 Modeling and simulation of nucleation (heterogeneous) in liquid melt pool – microstructural development — 107
 - 5.3.1 Macroscopic models — 108
 - 5.3.2 Microscopic models of microstructure evolution/formation during solidification — 108
 - 5.3.3 Evolution of probabilistic models — 111
 - 5.3.4 Two-dimensional Cellular Automation (CA) method — 113

Appendix A: Heterogeneous nucleation and growth in very fluid alloys (as per CNT) [1064] — 117

Appendix B: Columnar to Equiaxed Transition (CET) — 121

Comparison — 123

Research gap — 129

Overall aims/research questions — 131

Methodology — 133

References — 139

Exercise — 191

Design problems — 193

Index — 195