

Contents

Introduction — V

Acknowledgments — IX

1 Theory — 1

- 1.1 Coarse graining for fast dynamics of order parameters — **1**
- 1.1.1 Master equations — **1**
- 1.1.2 Coarse-grained concentration, atomic number density — **5**
- 1.2 Fast dynamics for the phase-field models — **10**
- 1.2.1 Approaches to the description of fast transitions — **10**
- 1.2.2 Eckhaus instability — **17**
- 1.3 Traveling waves in phase-field crystals — **28**
- 1.3.1 Analytical solution for traveling waves — **28**
- 1.3.2 Triangle structure — **35**

2 Modeling — 37

- 2.1 Equilibrium diagrams — **37**
- 2.1.1 Two-dimensional structures — **40**
- 2.1.2 Three-dimensional lattices — **44**
- 2.2 Numerical solutions — **50**
- 2.2.1 Two-dimensional structures — **50**
- 2.2.2 Three-dimensional case — **53**
- 2.3 Metastable structures — **54**
- 2.3.1 Marginal stability analysis — **54**
- 2.3.2 Distorted patterns — **67**
- 2.3.3 Effect of the noise — **73**
- 2.4 Stability of the numerical scheme — **75**
- 2.4.1 Eyre theorem — **75**
- 2.4.2 One useful consequence — **80**
- 2.4.3 Unconditionally stable algorithms — **80**
- 2.4.4 Lagrange finite elements — **90**
- 2.4.5 Isogeometric analysis — **98**
- 2.4.6 Influence of computational parameters — **100**

Conclusions and outlook — 105

Definitions and abbreviations — 109

Bibliography — 113

Index — 121