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Nota di contenuto	Front Matter -- Introduction and Fundamentals. Introduction -- Modeling and Simulation in Materials Science -- Fundamentals and Solution of Differential Equations -- Simulation Techniques at the NanoscopicMicroscopic Scale. Fundamentals -- Statistical Mechanics in Atomic-Scale Simulations -- Monte Carlo Simulation and Integration -- Molecular Dynamics -- Simulation Techniques at the MicroscopicMesoscopic Scale. Introduction -- Discrete Dislocation Statics and Dynamics: Sections 9.19.3 -- Discrete Dislocation Statics and Dynamics: Sections 9.49.8 -- GinzburgLandau-Type Phase Field Kinetic Models -- Cellular Automata -- Mesoscale Kinetic Monte Carlo and Potts Models -- Geometrical and Component Models -- Topological Network and Vertex Models -- Simulation Techniques at the MesoscopicMacroscopic Scale. Introduction -- Finite Element and Difference Methods at the Meso -- Macroscale -- Polycrystal Elasticity and Plasticity Models -- Integrated Modeling and Simulation. Fundamentals -- Space and Time Scales in Microstructure Simulation -- Appendices. Appendix A: General Reading -- Appendix B: Computer Classification -- Appendix C: Advanced Empirical Methods -- Appendix D: Percolation Theory -- References -- Index.

Sommario/riassunto

Modeling and simulation play an ever increasing role in the development and optimization of materials. Computational Materials Science presents the most important approaches in this new interdisciplinary field of materials science and engineering. The reader will learn to assess which numerical method is appropriate for performing simulations at the various microstructural levels and how they can be coupled. This book addresses graduate students and professionals in materials science and engineering as well as materials-oriented physicists and mechanical engineers.