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5.2 Microscopic Diffusion; 5.3 Macroscopic Diffusion; 5.4 Numerical Solution of the Diffusion Equation; Chapter 6. Modeling Precipitation as a Sharp-Interface Phase Transformation; 6.1 Statistical Theory of Phase Transformation; 6.2 Solid-State Nucleation; 6.3 Diffusion-Controlled Precipitate Growth; 6.4 Multiparticle Precipitation Kinetics; 6.5 Comparing the Growth Kinetics of Different Models; Chapter 7. Phase-Field Modeling; 7.1 A Short Overview; 7.2 Phase-Field Model for Pure Substances; 7.3 Study Case; 7.4 Model for Multiple Components and Phases; 7.5 Acknowledgments

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1 Basics of Discrete Plasticity Models; 8.2 Linear Elasticity Theory for Plasticity; 8.3 Dislocation Statics; 8.4 Dislocation Dynamics; 8.5 Kinematics of Discrete Dislocation Dynamics; 8.6 Dislocation Reactions and Annihilation; Chapter 9. Finite Elements for Mierostructure Evolution; 9.1 Fundamentals of Differential Equations; 9.2 Introduction to the Finite Element Method; 9.3 Finite Element Methods at the Meso- and Macroscale; Index

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#### Sommario/riassunto

Computational Materials Engineering is an advanced introduction to the computer-aided modeling of essential material properties and behavior, including the physical, thermal and chemical parameters, as well as the mathematical tools used to perform simulations. Its emphasis will be on crystalline materials, which includes all metals. The basis of Computational Materials Engineering allows scientists and engineers to create virtual simulations of material behavior and properties, to better understand how a particular material works and performs and then use that knowledge to design improvements

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