



# Computational Materials Engineering: An Introduction to Microstructure Evolution

*Koenraad George Frans Janssens, Dierk Raabe, Ernest Kozeschnik, Mark A Miodownik, Britta Nestler*

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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 for particular material applications. The text displays knowledge of software designers, materials scientists and engineers, and those involved in materials applications like mechanical engineers, civil engineers, electrical engineers, and chemical engineers.

Readers from students to practicing engineers to materials research scientists will find in this book a single source of the major elements that make up contemporary computer modeling of materials characteristics and behavior. The reader will gain an understanding of the underlying statistical and analytical tools that are the basis for modeling complex material interactions, including an understanding of computational thermodynamics and molecular kinetics; as well as various modeling systems. Finally, the book will offer the reader a variety of algorithms to use in solving typical modeling problems so that the theory presented herein can be put to real-world use.

- Balanced coverage of fundamentals of materials modeling, as well as more advanced aspects of modeling, such as modeling at all scales from the atomic to the molecular to the macro-material
- Concise, yet rigorous mathematical coverage of such analytical tools as the Potts type Monte Carlo method, cellular automata, phase field, dislocation dynamics and Finite Element Analysis in statistical and analytical modeling
- Companion web site will offer ample workable programs, along with suggested projects, resources for further reading, and useful classroom exercises

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