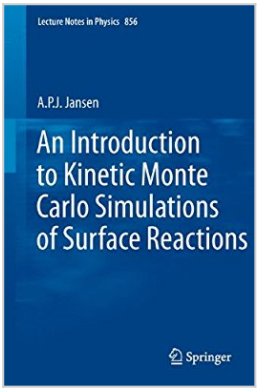

An Introduction to Kinetic Monte Carlo Simulations of Surface Reactions (Lecture Notes in Physics)

By A.P.J. Jansen

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Kinetic Monte Carlo (kMC) simulations still represent a quite new area of research, with a rapidly growing number of publications. Broadly speaking, kMC can be applied to any system describable as a set of minima of a potential-energy surface, the evolution of which will then be regarded as hops from one minimum to a neighboring one. The hops in kMC are modeled as stochastic processes and the algorithms use random numbers to determine at which times the hops occur and to which neighboring minimum they go.
Sometimes this approach is also called dynamic MC or Stochastic Simulation Algorithm, in particular when it is applied to solving macroscopic rate equations.

This book has two objectives. First, it is a primer on the kMC method (predominantly using the lattice-gas model) and thus much of the book will also be useful for applications other than to surface reactions. Second, it is intended to teach the reader what can be learned from kMC simulations of surface reaction kinetics.

With these goals in mind, the present text is conceived as a self-contained introduction for students and non-specialist researchers alike who are interested in entering the field and learning about the topic from scratch.

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Editorial Review

Review

From the reviews:

“This book is a good introduction to the kinetic Monte Carlo (kMC) simulation of surface reactions. … the basic ideas of the kMC method are presented very clearly and understandably for non-specialists. Using simple models and many practical examples makes the book useful not only for specialists but also for those just getting started with the kinetic Monte Carlo method.” (Stefan K. Stefanov, Mathematical Reviews, February, 2013)

“The author uses the kinetic Monte Carlo (kMC) method to examine surface reactions. … The author formulates two goals of this book. The first one is to show that the kMC method can also be applied to phenomena other than surface reactions. Secondly, the reader is informed of what kind of surface-reaction kinetics could be examined with the help of kMC simulations. The book will be of interest to students and newcomers in the field of surface reactions.” (A. V. Fedorov, zbMATH, Vol. 1272, 2013)

From the Back Cover
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