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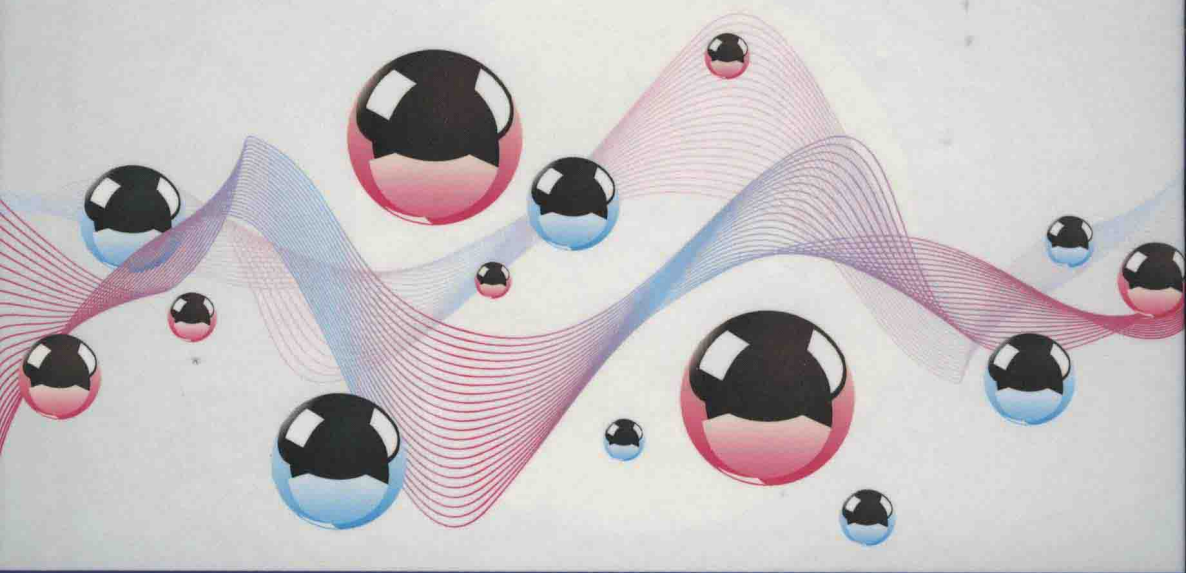

COMPUTATIONAL MATERIALS SCIENCE

SURFACES, INTERFACES, CRYSTALLIZATION

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Computational Materials Science

Surfaces, Interfaces, Crystallization

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Elsevier
32 Jamestown Road, London NW1 7BY
225 Wyman Street, Waltham, MA 02451, USA

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British Library Cataloguing-in-Publication Data
A catalogue record for this book is available from the British Library

Library of Congress Cataloging-in-Publication Data
A catalog record for this book is available from the Library of Congress

ISBN: 978-0-12-420143-9

Computational Materials Science

Acknowledgments

Authors would like to thank Professor O.Yo. Sokolovsky, Department of Theoretical Physics, Dnipropetrovs'k National University; Assistant Professor I.G. Rasin, Department of Chemical Engineering of Technion, Israel; Assistant Professor O.I. Kushnerev, Department of Physics of Metals, Dnipropetrovs'k National University for their fruitful discussion on a number of principal questions.

Authors want to gratefully acknowledge Professor V.F. Bashev, the head of the Department of Physics of Metals for his support of the researches in the field of Computational Materials Science which resulted in this book, and for the wholesome discussions.

Authors are thankful to the reviewers of the book *Computer Simulation of Phase Transitions and Surface Phenomena: textbook* published in Ukrainian language in 2011, which was a precursor to this book: Professor V.V. Maslov* (deceased), the head of the Department of Crystallization, G.V. Kurdyumov Institute for Metal Physics, National Academy of Sciences, Ukraine (Kiev) and Professor V.V. Girson, the head of the Department of Physics of Metals, Zaporozhye National University, Ukraine for their preview of the manuscript and useful advices.

Preface

Simulation is one of the main means for development of our ideas of outward things and theoretical description of various phenomena and processes. History of knowledge clearly shows that new, more complicated models come to replace the old, simple ones to provide a better description of the real processes. Simple models such as ideal gas model are easily analyzable. Complication of models leads to the increase of difficulties in their analysis and expects application of advanced mathematical methods.

Mathematical physics and computational mathematics have evolved due to the need for development of analysis and computer techniques. The latter was "translated" into the language suitable for computers and became a useful instrument for the scientists in different fields of knowledge.

Analysis of the sufficiently realistic models is an extremely hard task, and it is not always possible to reduce results to a form suitable for application of the computational mathematics technique. For example, analytical solutions of the boundary problems of heat and mass transfer could be derived only for bodies of a very simple shape under some certain simplified boundary conditions. At the same time, numerical solution of the initial equations by the finite-difference method (one of the simulation techniques) allows to obtain a full picture of changes in temperature and concentration fields, to take into account movement of the phase boundaries and changes in their shapes. At the same time, simulation program is an analogue of both an analytical solution and its finite expressions. Using calculations provided on computer, it is enough to change the input parameters of the system under consideration in order to obtain corresponding results with complete visualization of the ongoing processes.

An algorithm and a program provided that they are correct and that results of their application are proved at least for simplified models are none the worse for analytical solutions and could be much simpler for usage in practice. For example, now nobody tries to obtain an analytical solution to the many-body problem of celestial bodies, instead appropriate programs for calculations are used.

Hence it is clear why the simulation methods find their place in curricula of famous universities. A good many books are dedicated to the simulation methods at a different level of complexity. Those written by mathematicians are mostly focused on the methods themselves. In textbooks written by theoretical physicists, most attention is given to the phenomenological problems. But those who want to apply simulation methods should bear in mind that in order to be able to do it they need to master the subject itself and to understand the relevant phenomena at the

level of latest advances in science and technology. Therefore, it is better not to separate courses in simulation from the main course.

In this book, we yield to the theoretical basis necessary for understanding atomic surface phenomena and processes of phase transitions, especially crystallization. Theoretical basis for computer simulation by different methods and simulation techniques for modeling of physical systems are also presented, as well as additional information concerning their accuracy. A number of results are discussed concerning modern studies of crystallization: processes of thin film formation, kinetics of crystal growth, stability of crystal shapes including crystallization front, and nanocrystal formation during solidification from the supercooled melts.

In the last chapter of this book, several computer experiments from the list proposed to the students of the Dnipropetrovs'k National University are described. Explicit instructions to contents of these works and detailed explanations of the main procedures of programs (Delphi, C++, Visual C# environments, and the Pascal codes of several programs are also included) should help everyone understand the essence of simulations. Open access to executable files (the website of Elsevier http://booksite.elsevier.com/9780124201439/) makes it possible for everyone to achieve a better understanding of the main phenomena described in this book. A description of programs is sufficient for their reconstruction in any programming environments.

Owing to the specific structure of the book, lists of references to its first chapters are considerably reduced. Some educational stuff is given without source references if it was previously presented in some textbooks and it is hard to figure out where it was published for the first time. The following sources were the most often used for the preparation of the book:

D.W. Heermann, Computer Simulation Methods in Theoretical Physics, second ed., Springer, 1990.

Experiment on a Display, Moscow, Science, 1989, 99 p. (in Russian).

M.P. Allen, D.J. Tildesley, Computer Simulation of Liquids, Clarendon Press, Oxford, 1989, 385 p.

D. Frenkel, B. Smit, Understanding Molecular Simulation. From Algorithms to Applications, Academic Press, New York, London, Tokyo, 2002, 628 p.

D.K. Belashchenko, Computer Simulation of Liquid and Amorphous Matters MISSIS, Moscow, 2005, 407 p. (in Russian).

H. Gould, J. Tobochnik, An Introduction to Computer Simulation Methods: Applications to Physical Systems Parts 1 and 2, Addison-Wesley, Reading, MA, 1988.

H. Gould, J. Tobochnik, W. Cristian, An Introduction to Computer Simulation Methods: Applications to Physical Systems, third ed., Addison-Wesley, Reading, MA, 2007, 813 p.

V.I. Rashchikov, A.S. Roshal, Numerical Methods in Solution of Physical Problems, Lan', St. Petersburg, 2005 (in Russian).

Other editions wherein mathematical fundamentals of simulation methods are described in step-by-step fashion.

The book *Physics of Surface* by A. Zangwill (Cambridge University Press, 1988) remains the most consistent on the subject of surface physics; some materials from this book were used in Chapter 4. More recent researches of the surface structure are represented in the book *Introduction to the Physics of Surface* by K. Our, V.G. Livshitz, A.A. Saranin, A.V. Zotov, G. Katayama (in Russian, Nauka, Moscow, 2006, 490 p.).

Our book does not cover all aspects of simulations in Materials Science. Simulations of mass crystallization that give information on microstructure formation in materials during crystallization, especially in the high and very high supercooling ranges, are not presented here. Another large direction in modeling, which is of a special importance for production and exploitation of engineering materials, is application of computational methods in continuum mechanics. There are some very useful books dealing with the questions of continuum mechanics. Continuum-based simulation approaches in the continuum scale and atomic scale are described in the book by Dierk Raabe (*Computational Materials Science. The Simulation of Materials Microstructures and Properties*, Wiley-VCH, Weinheim, New York, Toronto, 1998, 326 p.) and the book edited by Dierk Raabe, Franz Roters, Frederic Barlat, Long-Qing Chen (*Continuum Scale Simulation of Engineering Materials: Fundamentals—Microstructures—Process Applications*, Wiley-VCH Verlag GmbH & Co. KGaA, 2004, 845 p.). The book of S. Schmauder and L. Mishnaevsky Jr. (*Micromechanics and Nanosimulation of Metals and Composites*, Springer-Verlag, Berlin Heidelberg, 2009, 421 p.) contains descriptions of different experimental and computational analysis methods of micromechanics of damage and strength of materials.

This book will be useful for everyone who has interest in applying modern simulation techniques for development and analysis of more realistic models of physical processes in Materials Science.

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