Computational Design of Engineering Materials

Successful computational design of engineering materials requires a combination of multiscale computational methods such as the CALPHAD method, first-principles calculations, phase-field simulation, and finite element analysis, covering the atomic–meso–macro scale ranges. Written jointly by a team of recognized experts in these fields, this book provides unique insights in both the fundamentals and case studies for a variety of materials. The fundamentals of computational thermodynamics, thermophysical properties, first-principles calculations, mesoscale simulation methods, and crystal plasticity finite element method are introduced. The nonspecialist reader with a general science or engineering background should understand these tools deeply enough to consider their applicability and assess the results. In particular, the important role of CALPHAD and its scientific databases in materials design and the integration of simulation tools at different levels are highlighted. Case studies for designing a wide range of materials, including steels, light alloys, superalloys, cemented carbides, hard coating, and energy materials, are demonstrated in detail through a step-by-step methodology. Ancillary materials provide the reader with hands-on experience in simulation tools. This book is intended for professionals in design of engineering materials and other materials, being also an invaluable reference to graduates, undergraduates, researchers, and engineers who use various computational tools in their study, research, and/or development of materials.

Yong Du received his PhD from Central South University (CSU) of China in 1992. From 1993 to 2003, he continued his research at the Tokyo Institute of Technology, University of Barcelona, Clausthal University of Technology, University of Vienna, and University of Wisconsin at Madison. Since 2003, Du has been a professor at CSU. His research fields are thermodynamics, thermophysical properties, and materials design. His recognitions and honors include the National Outstanding Youth by the National Natural Science Foundation of China (NSFC), the Cheung Kong Chair Professorship by the Ministry of Education of China, the Leader of the Innovative Research Team by the NFSC, and the Leader of 973 National Basic Research Program of China. Du is an associate editor for both *CALPHAD* and the *Journal of Phase Equilibria and Diffusion*. He has been awarded one First-Class Prize of Hunan Provincial Natural Science Award, one Third-Class Prize of National Natural Science Award of China, and one best paper prize of the Alloy Phase Diagram International Committee (APDIC).

Rainer Schmid-Fetzer received his PhD from Clausthal University of Technology (TU Clausthal) in 1977. With background in metallurgy and physics he earned merits in thermodynamics, solidification, interface reactions and applications to designing alloys. His career comprised research at the University of Wisconsin at Madison between 1982 and 1984, as lecturer, and professor at TU Clausthal and also in 1994 at the Microelectronics and Microsystems section of the Daimler Benz Corporate Research Institute, Frankfurt, and in 1997 as Visiting Professor at the University of Wisconsin at Madison. He retired in 2015. Schmid-Fetzer is an associate editor of the *Journal of Phase Equilibria and Diffusion* and a member of the advisory board of the *International Journal of Materials Research* (formerly *Zeitschrift für Metallkunde*). He is a fellow of ASM International since 2003. He has been awarded the most prestigious honors and awards, including the Tammann Award and Werner-Köster Prize from the German Society of Materials, the Hume-Rothery Prize of British IoM3, the William Hume-Rothery Award from the Minerals, Metals, and Materials Society (TMS) of USA, and the Lee Hsun Lecture Award from the Institute of Metal Research of the Chinese Academy of Sciences.

Jincheng Wang received his PhD from Northwestern Polytechnical University of China in 2001. He did postdoctoral work at the National Institute for Materials Science of Japan from 2002 to 2004. Since 2005, Wang has been working at the State Key Laboratory of Solidification Processing at the Northwestern Polytechnical University as lecturer, associate professor, and professor. From 2009 to 2010, he worked at the Institute of Space and Astronautical Science of Japan as a visiting professor for six months. His major research fields include solidification; modeling and simulation of microstructure evolution; alloy design; additive manufacturing; and high-entropy alloys. His awards include two Second-Class Prizes of Shaanxi Provincial Natural Science Award.

Shuhong Liu received her PhD from Central South University (CSU) in 2010. Then she did postdoctoral work for one year at the Materials Chemistry Institute of RWTH Aachen University. Since 2010, Liu has been working at the Research Institute of Powder Metallurgy of CSU as lecturer, associate professor, and professor. She is an editorial member of the *Journal of Mining and Metallurgy B*. Her awards include the best paper prize of APDIC and the First-Class Prize of Hunan Provincial Natural Science Award. Her research interests include phase diagram, CALPHAD-type calculations of thermodynamic and thermophysical properties, as well as corrosion and precipitation simulation.

Jianchuan Wang received his PhD from Central South University (CSU) in 2012, being a visiting PhD student in 2011 at Max-Planck-Institut für Eisenforschung GmbH. Since 2013, he has been working at the State Key Laboratory of Powder Metallurgy of CSU as lecturer and associate professor. His major research focuses on using first-principles calculation and molecular dynamics to study defect properties, diffusion, thermodynamics, interface in condensed matter, especially in hydrogen storage materials, and Li-ion batteries. He has (co)authored more than 60 peer-reviewed publications.

Zhanpeng Jin received his master's degree from the Central South Institute of Mining and Metallurgy of China in 1963. He continued his teaching and research there from 1964 until he retired in 2018. From 1978 to 1980, Jin worked at the Royal Institute of Technology of Sweden as a visiting scholar. He was an associate editor of *CALPHAD* and a member of the Asia Pacific Materials Academy. In 2006, Jin became an academician of the Chinese Academy of Sciences. He received one Third-Class Prize of National Natural Science Award of China.

Computational Design of Engineering Materials

Fundamentals and Case Studies

YONG DU
Central South University

RAINER SCHMID-FETZER
Clausthal University of Technology

JINCHENG WANG
Northwestern Polytechnical University

SHUHONG LIU
Central South University

JIANCHUAN WANG
Central South University

ZHANPENG JIN
Central South University

CAMBRIDGE
UNIVERSITY PRESS

MATERIALS RESEARCH SOCIETY
Advancing materials. Improving the quality of life.

CAMBRIDGE
UNIVERSITY PRESS

Shaftesbury Road, Cambridge CB2 8EA, United Kingdom

One Liberty Plaza, 20th Floor, New York, NY 10006, USA

477 Williamstown Road, Port Melbourne, VIC 3207, Australia

314–321, 3rd Floor, Plot 3, Splendor Forum, Jasola District Centre, New Delhi – 110025, India

103 Penang Road, #05–06/07, Visioncrest Commercial, Singapore 238467

Cambridge University Press is part of Cambridge University Press & Assessment, a department of the University of Cambridge.

We share the University's mission to contribute to society through the pursuit of education, learning and research at the highest international levels of excellence.

www.cambridge.org
Information on this title: www.cambridge.org/9781108494106

DOI: 10.1017/9781108643764

First published 2023

A catalogue record for this publication is available from the British Library.

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

ISBN 978-1-108-49410-6 Hardback

Y. Du wishes to dedicate this book to Professor Peiyun Huang, who received his PhD from MIT in 1945 and was one of the two supervisors (along with Professor Zhanpeng Jin) for Du's research.

Cambridge University Press & Assessment
978-1-108-49410-6 — Computational Design of Engineering Materials
Yong Du , Rainer Schmid-Fetzer , Jincheng Wang , Shuhong Liu , Jianchuan Wang , Zhanpeng Jin
Frontmatter
More Information

Contents

Colour plates are to be found between pages 460 and 461.

Foreword

A revolution has been under way for several decades, transforming materials engineering from a much-discredited slow and costly process of trial-and-error experimental "materials by discovery" to one of true *design* enabled by predictive science inverted to exploit the system of CALPHAD fundamental databases now known as the materials genome. Driven by a systems approach to control of hierarchical microstructure, university research initiated in the 1980s integrated materials science, quantum physics, and continuum mechanics to bring materials into a new age of computational engineering design. Moving beyond the reductionist philosophy of traditional academic research, these efforts tested the accuracy limits of density functional theory (DFT)-based quantum mechanical methods in demonstrating particular utility in the prediction of surface thermodynamics, while continuum micromechanics of heterogeneous systems brought new insights to the unit processes of fracture and fatigue where quantitative structure–property relations had previously been lacking. Paramount to the achievements was a synthetic philosophy that can be traced back to the founding of the international CALPHAD collaboration by the work of Kaufman and Cohen in 1956. Rather than the "calculation of phase diagrams," as implied by the CALPHAD acronym, their work actually entailed the opposite – reducing the information in the Fe–Ni equilibrium diagram to its underlying thermodynamics for the specific purpose of controlling behavior far from equilibrium, as represented by martensitic transformations. It is this recognition of the importance of thermodynamics in defining the forces driving dynamic systems, and the attendant expansion of CALPHAD data to incorporate kinetic parameters, that has given CALPHAD such power in enabling the application of our fundamental knowledge of materials dynamics in a quantitative and system-specific form. Just as the human genome functions as a database directing the assembly of the structures of life, the CALPHAD genome embodies the fundamental parameters driving the dynamic assembly of multiscale materials microstructures – the defining concept of the materials genome metaphor.

Successful demonstrations of efficient CALPHAD-based parametric materials design in the 1990s led to the founding of QuesTek Innovations as the first computational materials design company. This was soon followed by the US Defense Advanced Research Projects Agency–Accelerated Insertion of Materials (DARPA-AIM) initiative aiming to accelerate the full materials development and qualification cycle. Here full simulation of microstructural evolution in complex processing enabled a probabilistic science approach to accurately forecast manufacturing variation with minimal test data. Ultimately, that was applied to full flight qualification of two computationally designed aircraft landing gear steels. Achievements of the DARPA-AIM program were highlighted in a 2004 US National Research Council report *Accelerating Technology Transition*, which outlined a national initiative to promulgate this technology, ultimately undertaken in 2011.

The rare event of a speech by a US president announcing this materials research initiative immediately attracted the attention of apex corporations, which brought their resources to its efficient implementation, enabling for the first time the incorporation of materials design and development into concurrent engineering. Here, a historic milestone was the announcement of four new alloys with the Apple Watch in 2014, designed concurrently with the product in less than two years of acquiring the design technology that enabled it. Further migration of the technology led to Elon Musk's announcement of the novel SpaceX SX500 fire-resistant Superalloy as a vital enabler of the Raptor engine of the Mars Starship, integrated at an early stage of development into a highly accelerated concurrent engineering process. A major innovation in automotive technology was Tesla's rapid development of aluminum structure Giga-Casting technology enabled by a novel Al casting alloy designed through tight control of eutectic phase fractions, also delivered concurrently with its casting pilot plants in under a two-year cycle, now in production in the Tesla model Y. With the efficiency and efficacy of CALPHAD-based materials design clearly established by these major successes, Tesla announced the formation of a materials applications group to accelerate the replacement of legacy alloys with designed alternatives to enable a higher level of full-system optimization. We thus find ourselves at the start of another technology revolution whereby the rest of engineering is being retrained to embrace the new opportunity of materials concurrency.

Written by Rainer Schmid-Fetzer and Yong Du (both world-level outstanding scientists) along with four Chinese scientists, this unique book offers a compendium of the full computational toolset enabling this revolution.

Choose wisely.

G. B. Olson
Massachusetts Institute of Technology
Cambridge, MA

Preface

Recently, with the rapid development of computational techniques at different scales and various materials databases, materials design has become a research hotspot in different disciplines, including materials science, metallurgy, physics, chemistry, geology, biotechnology, and more. The most important trend is the integration of multiscale computational techniques for materials design, such as the CALPHAD technique, first-principles calculations in atomistic scale, mesoscale phase-field simulation, and finite element analysis in macroscale. However, most of the relevant books published so far do not reflect this important trend. Moreover, contributors of previously published books have focused on only one or two computational tools and, therefore, could not cover the tools in different scales. Thus, there is a need to publish a new book on this topic.

About half of this book presents for the first time a wide spectrum of various computational methods used in the design of engineering materials. An important feature of this part of the book is the methodology to establish thermodynamic and thermophysical databases for multicomponent and multiphase systems. Such databases are critical for an effective design of various engineering materials, which are usually multicomponent and multiphase alloys. This theoretical part of the book should be very useful for researchers, engineers, and students from materials sciences, metallurgy, physics, mathematics, and chemistry.

The other half of this book features a step-by-step demonstration of the design of engineering materials. This demonstration covers a very wide range of materials, including steels, light alloys, superalloys, cemented carbides, hard coatings, and energy materials.

The major motivation to write this book originated from a long-term cooperation between Professor R. Schmid-Fetzer and Professor Yong Du, which dates back to November 1994, when Dr. Du joined Professor Schmid-Fetzer's group as Alexander von Humboldt Research Fellow. Subsequently, they have established a close collaboration through several channels, such as mutual visits, attending conferences simultaneously, supervising PhD students together, and publishing papers jointly. Through many discussions and their individual experiences, both Professor Schmid-Fetzer and Professor Du have wondered why there is no book on the market that introduces the design of engineering materials via a step-by-step methodology. This book tries to fill that gap.

Figure 0.1 Five authors (Jianchuan Wang, Jincheng Wang, Rainer Schmid-Fetzer, Yong Du, and Shuhong Liu, from left to right) discussing the overall structure of the book in Changsha on September 21, 2018. A black and white version of this figure will appear in some formats. For the colour version, please refer to the plate section.

We believe that researchers, engineers, and graduate and undergraduate students in materials science and engineering, including ceramics, metallurgy, and chemistry, will find the book to be of great value. Moreover, we feel that even other fields, including computational biomaterials science, where modeling approaches have been used extensively for the research and development of various engineering materials, might substantially benefit from the methods and design methodology presented in this book.

Computational techniques and software have developed rapidly in recent times, and new concepts such as machine learning and artificial intelligence have emerged in the past few years. Consequently, it has been a tremendous challenge to keep the content of the book up to date. In addition, we do not expect the book to be error-free. Your comments and feedback on the book are highly appreciated and will enable us to address any shortcomings through the book's website or during the book's next revision.

Acknowledgments

The authors are grateful to many colleagues for inspiration, reading some chapters of the book, contributing some text, giving valuable comments, and producing a number of diagrams. Thanks to Professors Weibin Zhang, Keke Chang, and Wei Xiong; Doctors Yuling Liu, Lianchang Qiu, Yafei Pan, Shiyi Wen, Peisheng Wang, Yingbiao Peng, Yuxiang Xu, Haixia Tian, Kaiming Cheng, Cong Zhang, Peng Zhou, Dongdong Zhao, Dandan Liu, Ying Tang, Fan Zhang, Dandan Huang, Huixin Liu, Fangyu Guo, Shaoqing Wang, Chong Chen, Jinghua Xin, Mingjun Yang and Yinping Zeng; as well as our PhD students Xiaoyu Zheng, Peng Deng, Qianhui Min, Bo Jin, Han Li, Qiang Lu, Baixue Bian, Fengyang Gao, Yiqi Guan, Fangfang Zeng, Huaqing Zhang, Qi Huang, Liying Wu, Ya Li, Tong Yang, Shiwei Zhang, and many others.