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.