# PREFACE

While it is tempting to label computational materials modeling as an emerging field of research, the truth is that both in nature and foundation, it is just as much an established field as the concepts and techniques that define it. It is the recent enormous growth in computing power and communications that has brought the activity to the forefront, turning it into a possible component of any modern materials research program. Together with its increased role and visibility, there is also a dynamic change in the way computational modeling is perceived in such a vast field as materials science with its wide range of length and time scales. As the pace of materials research accelerates and the need for often inaccessible information continues to grow, the demands and expectations on existing modeling techniques have progressed that much faster. Primarily because there is no one technique that can provide all the answers at every length and time scale in materials science, excessive expectations of computational materials modeling should be avoided if possible. While it is apparent that computational modeling is the most efficient method for dealing with complex systems, it should not be seen as an alternative to traditional experimentation.

Instead there is another option, which is perhaps the one that is most likely to become the defining characteristic of computational materials modeling. It is the role of modeling as a tool to connect the different and seemingly unrelated features across the various length scales and types of materials, in synergy with fundamental theory and applied experimentation. As in other areas of evolving modern technology, it is not immediately apparent when we can fully expect to achieve the necessary maturity, coherence, and completeness to fulfill this goal. But until that point is reached, it is necessary to document the progress, acknowledging both successes and limitations, not just with the objective of perfecting the underlying methods and techniques, but also with

the goal of gaining a deeper understanding of the power and essence of the activity. In this regard, the current volume provides a necessarily limited yet broad view of computational materials modeling as applied to metallic materials, and lays the foundation for achieving greater understanding, acceptance, and the proper utilization of computational materials science.

Starting with a detailed description of the fundamental methods for the calculation of electronic structure and their role in the description of complex materials, the first few chapters concentrate on modeling of alloy phase equilibria, emphasizing the connection between first-principles methods and computational thermodynamics. Topics of substantial current interest are examined within this framework, including metallic glass formation and the transition between the nano- to the micro-scale regime by exploring the structure of clusters. The emphasis then shifts to the role of modeling methods in surface science, detailing currently accepted techniques including quantum approximate methods with proven effectiveness in bridging the gap between surface science and bulk solids. New approaches, as well as established techniques are discussed in subsequent chapters, including phase-field simulations, CALPHAD modeling, the quantum approximate BFS method for alloys, and the molecular orbital approach to alloy design. Having established a solid foundation for different modeling approaches, the focus is then on specific materials and properties with current examples and applications, including the intelligent design of age-hardenable aluminum alloys and intergranular modeling of deformation and fracture in metallic materials. The final chapters point to non-traditional areas of materials and surface modeling, with a detailed discussion of current topics in surface analysis, metal-metal interfaces, and nuclear materials.

Needless to say, progress in computational materials modeling is much broader than the contents of this book, but even if every current topic or development could be included, it would not change the fact that in many ways the discipline has come of age, becoming a vital and fundamental part in any modern materials research program. It is our hope that the detailed and comprehensive contributions of our guest authors will help reflect this promising conclusion and provide the proper perspective for the current status and future prospects of computational materials modeling.

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