HANDBOOK OF MATERIALS MODELING

HANDBOOK OF MATERIALS MODELING Part A. Methods

Editor

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PREFACE

This *Handbook* contains a set of articles introducing the modeling and simulation of materials from the standpoint of basic methods and studies. The intent is to provide a compendium that is foundational to an emerging field of computational research, a new discipline that may now be called *Computational Materials*. This area has become sufficiently diverse that any attempt to cover all the pertinent topics would be futile. Even with a limited scope, the present undertaking has required the dedicated efforts of 13 Subject Editors to set the scope of nine chapters, solicit authors, and collect the manuscripts. The contributors were asked to target students and non-specialists as the primary audience, to provide an accessible entry into the field, and to offer references for further reading. With no precedents to follow, the editors and authors were only guided by a common goal – to produce a volume that would set a standard toward defining the broad community and stimulating its growth.

The idea of a reference work on materials modeling surfaced in conversations with Peter Binfield, then the Reference Works Editor at Kluwer Academic Publishers, in the spring of 1999. The rationale at the time already seemed quite clear – the field of computational materials research was taking off, powerful computer capabilities were becoming increasingly available, and many sectors of the scientific community were getting involved in the enterprise. It was felt that a volume that could articulate the broad foundations of computational materials and connect with the established fields of computational physics and computational chemistry through common fundamental scientific challenges would be timely. After five years, none of the conditions have changed; the need remains for a defining reference volume, interest in materials modeling and simulation is further intensifying, the community continues to grow.

In this work materials modeling is treated in 9 chapters, loosely grouped into two parts. Part A, emphasizing foundations and methodology, consists of three chapters describing theory and simulation at the electronic, atomistic, and mesoscale levels, and a chapter on analysis-based methods. Part B is more concerned with models and basic applications. There are five chapters describing basic problems in materials modeling and simulation, rate-dependent phenomena, crystal defects, microstructure, fluids, polymers and soft matter. In

addition this part contains a collection of commentaries on a range of issues in materials modeling, written in a free-style format by experienced individuals with definite views that could enlighten the future members of the community. See the opening Introduction for further comments on modeling and simulation and an overview of the *Handbook* contents.

Any organizational undertaking of this magnitude can only be a collective effort. Yet the fate of this volume would not be so certain without the critical contributions from a few individuals. My gratitude goes to Liesbeth Mol, Peter Binfield's successor at Springer Science + Business Media, for continued faith and support, Ju Li and Xiaofeng Qian for managing the websites and manuscript files, and Tim Kaxrias for stepping in at a critical stage of the project. To all the authors who found time in your hectic schedules to write the contributions, I am deeply appreciative and trust you are not disappointed. To the Subject Editors I say the *Handbook* is a reality only because of your perseverance and sacrifices. It has been my good fortune to have colleagues who were generous with advice and assistance. I hope this work motivates them even more to continue sharing their knowledge and insights in the work ahead.

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