Preface

Since a broad range of issues in material science involves multiple scales in space and time, multi-scale modeling and simulation of materials is currently one of the major research topics in material science worldwide. The various levels of material modeling can be roughly grouped into microscopic, mesoscopic, and macroscopic regimes. The microscopic scale refers to atomic level and lattice defect ensembles below the grain scale, from electronic first-principles to atomic molecular dynamics and Monte Carlo methods. Mesoscopic scale refers to lattice defect ensembles at the grain scale, and a typical simulation method at this scale is the phase field. Macroscopic scale refers to the sample geometry represented by a finite element method. These computer simulation methods of different scales have proven to be very useful for the study of fundamental physics, structure and properties of materials, which are not easily accessible via experiment. Moreover, with the advance in computing power, these methods have developed in a remarkable way, not only at the respective space and time scales but also at the couplings between the different scales. They are now becoming increasingly applicable for material processing and performance prediction in advanced engineering and technology applications.

SCIENCE CHINA Physics, Mechanics & Astronomy is publishing this special issue of “Multiscale Modeling & Simulation of Materials” in order to present recent research developments in this important field. The carefully peer-reviewed papers in this special issue comprise modeling and simulation of structure and properties of different materials covering all the scales. In particular, this special issue involves three contributions employing the mesoscopic phase field method to study solidification of materials and void swelling in materials under irradiation. The materials are wide-ranging, from structural materials including metals, metal alloys, and intermetallics to functional materials including multiferroic materials, graphene, nanocoils, as well as HMX and polymer-based composites.

This special issue originated from Symposium T, “Multiscale Modeling and Simulation of Materials”, in the 11th International Conference in Asia of the International Union of Materials Research Societies (IUMRS-ICA2010) that was hosted in Qingdao, China, from 25 to 28 September 2010. Started in 1993 on a ship in the Yangtze River in China, this conference series has been organized subsequently by MRS-T, MRS-K, MRS-J, MRS-India, and MRS-Singapore. IUMRS-ICA2010 is the foremost international forum for scientists, engineers, and students from not only Asia but around the world to exchange their recent achievements in the field of materials research and development. We greatly appreciate the opportunity to host 116 participants from 8 different countries. The success of the meeting was to a large extent made possible by the generous supports from symposium chairs, Prof. Gong Xingao, Prof. Lu Guang-Hong, Prof. Xu Dongsheng, Prof. Ogata Shigenobu, and Prof. Gao Fei, as well as the symposium coordinator, Prof. Shu Xiaolin. We are very grateful for the support received, as well as the efforts provided by the Computational Materials Science Sub-committee of the Chinese Material Research Society. We are also indebted to the teachers and students from Beihang University, who served as conference secretaries and provided great assistance for the meeting.

We are delighted to see the final publication of the achievements in development and application of advanced computer simulation methods and algorithms to achieve fundamental understanding and predictive modeling and simulation of the structure and properties of materials in *SCIENCE CHINA Physics, Mechanics & Astronomy*, and we are looking forward to more special issues which collect further achievements from this field in the near future.

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