Preface

Materials are one of the bases for human existence and development. From 70s, twentieth century, human began to take information, materials and energies as pillars of social and economic developments. During 80s, twentieth century, with developments of high-tech groups, new materials, information technology and biological technology are in parallel regarded as important signs of the new technological revolution. Nowadays, materials science has become an important part of national economic construction, national defense construction and people's life. To design materials with computer technology is now a very important method to develop new materials. Materials design is usually divided into 3 levels. First is nano level, which is to study the collective behavior of atoms and molecules by using statistical mechanics and quantum mechanics. The second level is micro level, which means above micron size, to study average properties of many atoms or molecules in a certain range, for example deformation, magnetic etc., and are described by Continuous statistical equation usually. And the third level is macro level, such as the relationships among macroscopic properties, production processes and utility performances, and material fracture and microstructure formation, etc. Computer technology can take 3 levels of factors into accounts altogether, get the best composition, best structure, and most reasonable technological process in accordance with the predicted material characters through establishment of model and computer simulation.

When computers' high-speed computing power, huge storage capacity and ability to judge the logic are combined with human creativity, creative schemes could be brought out in material designs. Retrieve and comparison of the large amounts of record data could be finished. Large amounts of complicated mathematics and mechanics calculations could be realized in the total and partial designs. And design schemes could be comprehensively analyzed and optimized, so that to determine the design drawings and provide vital information for manufactures. This design method has improved design qualities, decreased design cycle, and created the conditions for the development of new materials and new technology.

The papers in this book are selected from more than 2000 papers submitted to 2014 International Conference on Materials Science and Computational Engineering (ICMSCE 2014) held in May, 20th, 2014 in Qingdao. The book is separated into 14 chapters, includes subjects such as Material sciences, Computational Science Technology, Algorithms, Biological engineering and chemistry, Manufacturing and industrial technology, Electronics and information technology, Environmental protection and resource development, Operations research and management science, etc.

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