

# Preface

This book is the first volume of *SpringerBriefs in the Mathematics of Materials* and a comprehensive guide to the interaction of mathematics with materials science. Until recently, the application of mathematics to materials science has progressed mainly to explain *macroscopic phenomena* by means of partial differential equations (PDE). Mathematics however, plays an important role in describing microscopic systems. Recently, direct observation and control of atoms and molecules have become possible and mathematics is expected to describe how macroscopic properties of materials emerge from *microscopic structure*, in particular, from geometrical structure. Furthermore, along with the development of computer technology, a global trend has developed where researchers are deriving important information from a large amount of accumulated data and are designing materials based on this information and mathematics. A new relationship between mathematics and materials science is required.

In the late twentieth century, the importance of injecting mathematics into a wide range of science and technology fields was recognized. Along with a global change in perspective, initiatives bringing mathematics to materials science were encouraged. Materials science has been since its inception an empirical science founded on the many experiments, results, and intuitions. Recently, some researchers have pointed out that it is crucial to *rationalize design and development of materials*, to tighten the development cycle by creating a predictive framework based on theory, and using big data and powerful computational techniques. This book discusses recent attempts to create a *predictive materials science* based on the systematic interaction and cooperation between mathematics and materials science.

In the opening chapters of this book (Chaps. 1 and 2), a selected history of materials science and some examples of the interaction of mathematics with materials science are described. The emergence of materials science was itself a result of the interdisciplinary integration of materials-related disciplines, which occurred in the 1950s and 1960s. Disciplines related to materials include

metallurgy, polymer science, ceramics, solid-state physics, and semiconductors. That mathematics is involved in materials science is no wonder. We believe that this historical background will help readers understand the importance of collaborations between mathematics and materials science.

In Chap. 3, we describe some attempts performed at the *Advanced Institute for Materials Research (AIMR)*, *Tohoku University*, to which the authors are affiliated, trying to create a predictive materials science based on a mathematics–materials science collaboration at an institutional level. In this chapter, some examples of attempts and results will be described briefly. To provide researchers a shared, concrete idea of the objectives of mathematics–materials science collaborations, three target projects (1) *Non-equilibrium Materials based on Mathematical Dynamical Systems*, (2) *Topological Functional Materials*, and (3) *Multi-Scale Hierarchical Materials based on Discrete Geometric Analysis* are discussed. These projects were tackled by AIMR researchers and details of their work are presented in subsequent volumes of this *SpringerBriefs in the Mathematics of Materials* series.

In the last chapter (Chap. 4), we describe how breakthroughs based on mathematics–materials science collaborations can emerge. Our argument is supported by the experiences at AIMR where many researchers from various fields gathered and tackled interdisciplinary research.

We understand that a systematic attempt at a mathematics–materials science collaboration needs much time to mature. Such attempts would have been almost impossible if not for the long-term continuous financial support by the *World Premier International Research Center Initiative (WPI)*, jointly managed by the Japanese Ministry of Education, Culture, Sports, Science and Technology (MEXT) and the Japan Society for the Promotion of Science (JSPS), and we sincerely appreciate the support under this program. This attempt also required the enthusiastic effort of our institute. We would like to thank all researchers at AIMR. In particular, we are deeply indebted to Dr. Daniel M. Packwood for his assistance in improving some parts in Chap. 3. Critical reading by Prof. Yasumasa Nishiura and Prof. Masaru Tsukada has greatly improved the manuscript and the authors appreciate their advice. The charts showing the evolution of materials used in Fig. 1.3 are mural graphics at the entrance of the new building of the Department of Materials Science and Metallurgy, University of Cambridge. We thank Prof. A. Lindsay Greer and Granta Design Limited in Cambridge for permission to reproduce these graphics. We are deeply grateful to Dr. Paul Tambuyser and Dr. Claude Hootel  for permission to use photographs of goniometers in Fig. 2.2. We are also grateful to Prof. An-Pang Tsai, Prof. Yasumasa Nishiura, and Dr. Akihiko Hirata, Tohoku University, for providing, respectively, a photomicrograph of quasicrystals (Fig. 2.5b), photographs of the BZ reaction patterns (Fig. 2.14), and a schematic explaining the structure analysis of metallic glass (Fig. 3.1). We thank Ms. Miho

Iwabuchi for her wonderful illustration depicting the four steps necessary for achieving interdisciplinary integration used in Fig. 4.4. Finally we wish to thank Mr. Masayuki Nakamura of Springer Japan who helped us with the publication of this book.

We would be very honored if readers of this book were interested in our attempt and join the collaborative network to create new materials science together.

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