Nanoinformatics

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Editor

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Preface

This book focuses on state-of-the-art ideas and tools in informatics that are currently being used in materials science, or are expected to be used in the future. Collaborative research between materials science and information science is growing actively, creating new trends in materials science and engineering. Areas utilizing "big data," generated by experiments and computations to accelerate the discovery of new materials, key factors, and design rules, have rapidly progressed. Data-intensive approaches are indispensable in advanced materials characterization.

"Material informatics" is the central paradigm in this new trend. An essential subset is "nanoinformatics," which focuses on the nanostructures of materials, such as surfaces, interfaces, dopants, and point defects. Experimental and computational techniques to characterize and gain quantitative information about nanostructures have significantly advanced, enabling nanoinformatics to play a critical role in determining material properties.

Most of this book is derived from the collaborative research projects supported by the Grant-in-Aid for Scientific Research on Innovative Areas "Nano Informatics" from the Japan Society for the Promotion of Science (JSPS). This five-year project, which was launched in 2013, aims to accelerate the exploration of frontiers in materials science and promote the integration of information and utilization of accumulated knowledge regarding nanostructures for the design and innovation of actual materials. Project researchers represent diverse disciplines, such as materials science, applied physics, solid-state chemistry, catalytic chemistry, and information science. In addition to those working in the collaborative program, three research groups actively working on data-centric materials science were invited to contribute to the book. With their participation, the subjects in the book are well balanced.

This book is composed of three parts. The first part reviews the ideas and tools of materials informatics as well as actual applications of machine-learning techniques for materials problems. Chapter 1 shows how compounds in materials datasets can be represented as descriptors and applied to machine-learning models. Chapter 2 focuses on a method to discover the potential energy surface of solid-state ionic conductors via a combination of first principles calculations and machine-learning

techniques. Chapter 3 describes the machine-learning predictions of factors affecting the activity of heterogeneous metal catalysts. Chapter 4 discusses the applications of optimal experimental design algorithms for materials science. Chapters 5 and 6 are dedicated to the topological analyses of the atomic structure data of materials. One method is called persistent homology. The other uses polyhedron and polychoron codes. They have been successfully used to analyze amorphous structures.

In the second part, data-centric approaches used for nanoscale analyses of materials data are described. Chapter 7 shows topological data analyses for atom probe tomography (APT) images. Chapter 8 describes the combined efforts of scanning transmission electron microscopy (STEM) experiments, first principles calculations, and informatics approaches to analyzing the atomic structures of materials interfaces. Chapter 9 is based on nanoscale STEM spectroscopic datasets that are analyzed by machine-learning techniques.

The third part is composed of four chapters. Each chapter focuses on a specific target of nanoinformatics approaches. Chapter 10 describes high-quality epitaxial films of materials called "nanolayers" for a variety of functional applications, including thermoelectrics, batteries, memories, and superconductors. Chapter 11 focuses on the grain boundary engineering of alumina ceramics for use as protective films in the hot-section components of airplane engines, gas turbines, and heat treatment furnaces in combustion environments. Chapter 12 shows the structural relaxation of high-pressure oxide compounds, which is important for quenching high-pressure phases in ambient conditions. Chapter 13 describes the syntheses and structures of novel lithium-ion and hydride-ion conductors for use as solid-state electrolytes in electrochemical devices.

This book is an efficient overview of current progress in emerging and interdisciplinary research areas. It will benefit experimentalists and theorists in both academic and industry sectors. All the authors and steering committee members of the collaborative program "Nano Informatics" are gratefully acknowledged. Without their devoted efforts, this book would not be possible.

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