Foreword

Modern developments in science and technology require the production of new materials and designs. Knowing the material's properties is mandatory to develop and manufacture tailor-made materials for technical applications.

Crystallography is a profoundly interdisciplinary science and focuses nowadays on the investigation of the spatial arrangement of matter in all different types of materials and their changes under external influences like temperature or pressure. The crystal structure itself is very complex: it can be seen as an interplay of static and dynamic structures, it contains imperfections and structural disorder, such as point defects or dislocations, and it has to be distinguished between average and local structures. The crystal structure plays a crucial role in determining the physical properties of a material. A material of certain chemical composition can have different structural parameters and thus have different properties.

But crystallography not only applies to the atomic structure of materials, it is also crucial for the understanding of disordered materials such as glasses and collective quantum phenomena such as superconductivity. Thus, the knowledge about a material's structural characteristics and its correlation with technologically relevant properties is the prerequisite for designing new materials, with tailored properties central to technological needs, and is at the forefront of materials research.

This book shows that crystallography provides the foundation for the understanding of structure-function relationships and bridges the fundamental understanding of materials with applications.

The purpose of this book is twofold: (1) to present an overview on crystallographic techniques and methods to study complex structural material properties and (2) to present exemplarily investigations of structure-function relations in various technologically relevant materials like those for solar energy conversion and for solar-thermal water splitting or batteries. In the book, it is shown that crystallography can also be extremely useful in research areas that are normally not using structure studies such as corrosion research. Finally, the book also pays attention to recent advances in structure modeling as well as structure-property investigations with the help of density functional theory calculations. We have collected chapters written by renowned experts in the different research fields, giving insights into their scientific areas as well as reflecting modern aspects of crystallographic materials research.

This book is addressed to a wide audience of scientists in the field of physics, chemistry, mineralogy, and – of course – crystallography and materials science. It will be also interesting for graduate students in these disciplines. The book is intended to

pique the curiosity of younger students about crystallography and its fascinating insights into materials.

We thank all authors for their valuable contributions which made *Crystallography in Materials Science* possible.

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