Preface

By André Authier

The initial idea of having a volume of *International Tables for Crystallography* dedicated to the physical properties of crystals is due to Professor B. T. M. Willis. He submitted the proposal to the Executive Committee of the International Union of Crystallography during their meeting in Vienna in 1988. The principle was then adopted, with Professor Willis as Editor. After his resignation in 1990, I was asked by the Executive Committee to become the new Editor. Following a broad consultation with many colleagues, a nucleus of potential authors met in Paris in June 1991 to define the contents of the volume and to designate its contributors. This was followed by a meeting in 1995, hosted by Theo Hahn in Aachen, of the authors contributing to Part 3 and by another meeting in 1998, hosted by Vaclav Janovec and Vojtech Kopský in Prague, of the authors of the supplementary software.

The aim of Volume D is to provide an up-to-date account of the physical properties of crystals, with many useful tables, to a wide readership in the fields of mineralogy, crystallography, solid-state physics and materials science. An original feature of the volume is the bringing together of various topics that are usually to be found in quite different handbooks but that have in common their tensorial nature and the role of crystallographic symmetry. Part 3 thus confronts the properties of twinning, which traditionally pertains to crystallography and mineralogy, and the properties of ferroelectric or ferroelastic domains, which are usually studied in physics.

The volume comprises three parts and two supplementary computer programs.

The first part is devoted to the tensorial properties of physical quantities. After a presentation of the matrix of physical properties and an introduction to the mathematical notion of a tensor, the symmetry properties of tensors and the representations of crystallographic groups are discussed, with a special treatment for the case of quasiperiodic structures. The first part also includes several examples of physical property tensors developed in separate chapters: elastic properties, thermal expansion, magnetic properties, optical properties (both linear and nonlinear), transport properties and atomic displacement parameters.

The second part is concerned with the symmetry aspects of excitations in reciprocal space. It includes bases of solid-state physics and describes in the first two chapters the properties of phonons and electrons in crystals. The following two chapters deal with Raman and Brillouin scattering.

The third part concerns structural phase transitions and twinning. The first chapter includes an introduction to the Landau theory, a description of the behaviour of physical property tensors at ferroic phase transitions and an approach to the microscopical aspect of structural transitions and soft modes, with practical examples. The second chapter explains the relationship between twinning and domain structures and introduces the group-theoretical tools needed for the analysis of domain structures and twins. In the third chapter, the basic concepts and definitions of twinning are presented, as well as the morphological, genetic and lattice classifications of twins and the properties of twin boundaries, with many examples. The fourth chapter is devoted to the symmetry and crystallographic analysis of domain structures. The relations that govern their formation are derived and tables with useful ready-to-use data on domain structures of ferroic phases are provided.

An innovation of Volume D is the accompanying computer programs. The first, *Ten*χ*ar* (*Calculations with Tensors and Characters*) supports Part 1 for the determination of irreducible group representations and tensor components. The second, *GI*$\star$*KoBo*-1, supports Part 3 on structural phase transitions and enables the reader to find the changes in the tensor properties of physical quantities during ferroic phase transitions.

For various reasons, Volume D has taken quite a long time to produce, from the adoption of its principle in 1990 to its actual printing in 2003, and it is a particular pleasure for me to see the outcome of so many efforts. I would like to take this opportunity to thank all those who have contributed to the final result. Firstly, thanks are due to Terry Willis, whose idea the volume was and who made the initial push to have it accepted. I am very grateful to him for his encouragement and for having translated into English a set of notes that I had written for my students and which served as the nucleus of Chapter 1.1. I am greatly indebted to the Technical Editors who have worked tirelessly over the years: Sue Barnes in the early years and then Nicola Ashcroft, Amanda Berry and the staff of the Editorial Office in Chester, who did the hard work of editing all the chapters and translating them into Standard Generalized Markup Language (SGML); I thank them for their infinite patience and good humour. I am also very grateful to the Research and Development Officer, Brian McMahon, for his successful integration of the supplementary software and for his constant cooperation with its authors. Last but not least, I would like to thank all the authors who contributed to the volume and made it what it is.