STRUCTURAL SCIENCE
CRYSTAL ENGINEERING
MATERIALS

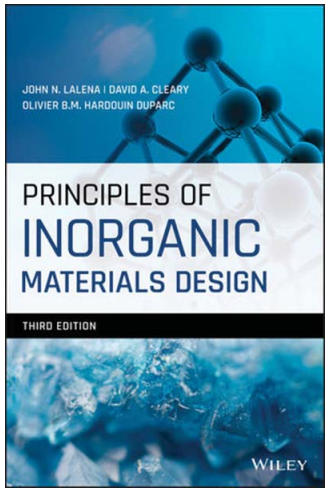
ISSN 2052-5206

Principles of Inorganic Materials Design, third edition. By John N. Lalena, David A. Cleary, Olivier B. M. Hardouin Duparc. Wiley, 2020. Hardcover, pp. 720. Price EUR 166.70. ISBN 978-1-119-48683-1

Claude Lecomte*

Université de Lorraine, CNRS, CRM2, Nancy, France. *Correspondence e-mail: claude.lecomte@univ-lorraine.fr

Keywords: book review; inorganic materials; crystallography; micro structures; solid state physics; nanomaterials.



At 685 pages, this material sciences book is a very pedagogic initiation to the synthesis, macroscopic and microscopic physical properties of materials for physics, chemistry and material science students and teachers. It is augmented, compared to the previous editions, by an excellent introduction to crystallography for materials and microstructures. Most properties of inorganic materials are discussed in 14 chapters: crystallographic considerations, microstructures, crystal structures and binding forces, band theory, transport properties, metal-insulators transitions, magnetic and dielectric properties, optical properties, mechanical properties, phase diagrams, synthetic strategies, introduction to nanomaterials and a discussion on modern computing material science. One originality of this book is that two case studies (TiO_2, GaN) are discussed at the end of the book, nicely illustrating all chapters. Each chapter finishes with selected problems. Four appendices cover crystallographic point and space groups, mathematics of tensors and solution to problems. In all chapters an historical development of the ideas driving the physics of materials is nicely presented with a biography of some scholars who were influential in the field. A table (four pages!) of the – too many – acronyms is given.

In this third edition, three chapters (165 pages) introduce the basic topics of crystallography.

Chapter 1, entitled *Crystallographic Considerations*, deals with geometric crystallography (lattices, groups, twins) and diffraction. Geometric crystallography topics are clearly described including the necessary mathematics; they are selected in accordance with the needs of the book. Diffraction is reduced to Bragg's law, space groups and systematic absences. This part could be more developed as X-ray, electron and neutron diffraction are essential tools to solve and understand the structure and properties of materials. Introducing the scattering and structure factors formalism is essential to understand the nature of wave-matter interactions (electrostatic, magnetic) and structure solution. *On page 22 an error occurs: $CaTiO_3$ is centrosymmetric in its cubic m3m phase.*

Chapter 2 presents microstructures (dislocations, grains, polycrystalline aggregates, thin films, consequences of the physical properties, microstructure design and control).

Chapter 3 is devoted to common crystal structures and cohesive forces in a solid. This chapter carefully selects the concepts needed for understanding the structure of a solid without going into too many details. Ionic, metallic and covalent bonding (including topological properties of the electron density) are well described together with the empirical Goldschmidt's and Pauling's rules. Then all common structure types are shown with related exercises; *Figure 3.17, spinel structure, is not clear.*

Chapters 4 and 5 (80 pages in total) describe the electronic structure of solids, band theory, Bloch's theorem, Fermi energy and surfaces, Brillouin zones, Linear Combination of Atomic Orbitals (LCAO), Density Functional Theory (DFT) (up to its limitations) (chapter 4) and tight binding electronic structure approximation (chapter 5); they clearly teach what the reader needs to understand the origin of the physical properties described in the following chapters; starting from Slater determinants is a challenge and the authors have succeeded.

Chapter 5 introduces tight binding approximation with a thorough mathematical development of the well known LCAO–Hückel method and its extension to solids. Applications on perovskites and reduced dimensional systems are given. Although this chapter is well written, this third edition lacks a comparison with DFT methods (chapter 14) which are widely used now.

Transport properties are described in chapters 6 and 7; tensors (*an error occurs on page 254 where the symmetry of the ellipsoid is mmm not m*), point defects are introduced followed by thermal (free electron and phonons contributions) and electric conductivity. The conductivity tensor σ is described with an exercise on an orthorhombic crystal. Then an easy to follow discussion on band structure for insulators conductors, semiconductors, semi-metals and superconductors follows. Applications like thermoelectric (zT figure of merit) photovoltaics, electro-luminescence and magneto transport are described. This very detailed chapter 6 ends with mass and ionic transport. Chapter 7, *Hopping Conduction and Metal Insulator Transitions*, gives an introduction to correlated systems, Mott–Hubbard insulating states and Anderson localization. Examples on charge density waves and Peierls distortions are given at the end of this chapter.

Chapter 8 (75 pages) is devoted to magnetic and dielectric properties; first a phenomenological description of magnetism is given: important formulas and definitions of susceptibility curves where dia-, para-, ferro- and ferrimagnetism are defined; it is followed by an clear chapter on atomic states and term symbols for free atoms (J quantum number, Russell–Saunders coupling); the example on page 360 about Ti^{2+} is very pedagogic. The atomic origin of paramagnetism is extensively described followed by magnetic ordering leading to ferro-, ferri- and antiferromagnetism. This part of the chapter clearly introduces the material scientist to magnetism. It is also constructed using an historical landscape but I regret that biographies for Professors Langevin and Néel were not given. A good overview of dielectric properties ends this chapter: tensorial properties, piezoelectric and pyroelectric materials and ferroelectricity (illustrated with $BaTiO_3$) but few words are given on the important multiferroic materials.

Chapter 9 is a too-short chapter on optical properties, Maxwell equations, linear optics, absorption and nonlinear phenomena. Nonlinearity could have been explained for example with the KTP family ($KTiOPO_4$)

Chapter 10 describes the mechanical properties of materials with an emphasis on mechanical fatigue which reduces the lifetime of a given material. The stress and strain tensors already described in the piezoelectric part of chapter 8 are used in the linear regime of deformation (Hooke law). There is focus on elastic tensors and their reduction via crystal symmetry. Then relations between cohesive forces and elasticity are explained applied to metals, covalent and ionic solids. Plasticity and its mechanisms follow ending with a description of fracture.

Chapter 11 concerns thermodynamic, phase diagrams and phase modelling. After a short but very clear introduction to thermodynamic rules, unary, binary and ternary phase diagrams are described with examples (iron, Pb–Sn, Al–Zn, and Bi_2O_3–CaO–CuO and others). All phase diagrams are well explained and a beginner can learn a lot. Then follows information on phase diagram modelling applied to long-range order, solid solutions (three related examples). The chapter ends with a description of the CALPHAD (CALculation of PHAse Diagrams) method (also described in chapter 14) and the related software available. CALPHAD enables a nonthermodynamic expert to make phase equilibria predictions on multicomponent systems.

Some major synthetic strategies are then proposed in chapter 12, for example, direct combination low-temperature methods, sol-Gel, solvo-thermal, intercalation. Specific methods are then given such as spinodal decomposition, thin films, nano and liquid phases synthesis.

A book on inorganic material design cannot end without a description of nanomaterials. Chapter 13 begins with a nice but short introduction to the special properties of nanomaterials [electric magnetic, optic (plasmon resonance), mechanical]. One part of the chapter is devoted to preparative techniques for nanomaterials. A chapter on applications of nanomaterials would have been welcome.

Computational methods (chapter 14) start with a rich historical introduction, Monte Carlo (MC), molecular dynamics (MD), tight binding approaches, the birth of the Fortran programming language . . . ; this paragraph ends with an extensive description of the now widely used Hohenberg–Kohn and Kohn–Sham DFT methods and some related software (*Wien 2K* by Blaha and Schwarz, Technical University Wien) is missing. Car–Parinello and related quantum Monte Carlo (MC) methods and development of MC methods for microstructure calculations are also discussed together with high performance and cloud computing (quantum mechanics calculations up to 10^7 atoms). A discussion on computational time related to basis set then follows. This chapter ends with various and clear illustrative examples on phase diagrams (CALPHAD), magnetic properties of double perovskites (Ising model, MC and quantum MC) and plasticity (finite element method).

All properties described in this textbook are illustrated with examples of two widely used materials:

(i) TiO_2 (rutile and anatase, *the brookite phase is not described*)

(ii) GaN.

I recommend using these two examples for an introduction to material science for physical chemists and physicists.

In conclusion, as discussed above most properties of inorganic materials are described. I highly recommend this book for students and teachers in crystallography, metallurgy, solid state physics, solid state chemistry and material science. This a very well written and pedagogic book which introduces in all chapters the necessary basics for understanding what follows.