JOURNAL OF APPLIED CRYSTALLOGRAPHY
ISSN 1600-5767

Structures on Different Time Scales. Edited by T. Woike and D. Schaniel. De Gruyter, 2018. Pp. 272. Hardcover, price EUR 99.95, USD 114.99, GBP 91.00. ISBN 978-3-11-044209-0.

Thomas Elsaesser*

Max-Born-Institute, Berlin, 12489, Germany. *Correspondence e-mail: elsasser@mbi-berlin.de

Keywords: book reviews; diffuse scattering; density functional theory; structural dynamics; photocrystallography.

Functional processes in condensed matter are frequently connected with changes of atomic arrangement and electronic structure. A direct mapping of structure changes in space and time is essential for determining dynamics and intermediate structures, and for identifying the underlying driving mechanisms and interactions. Experimental methods based on X-ray scattering in combination with density functional theory and charge-density analysis have played a key role in establishing this research field. Novel X-ray sources providing ultrashort and/or ultrabrilliant X-ray pulses which are synchronized with pulses from ultrafast optical lasers generate exciting perspectives for following structural dynamics at atomic length and time scales.

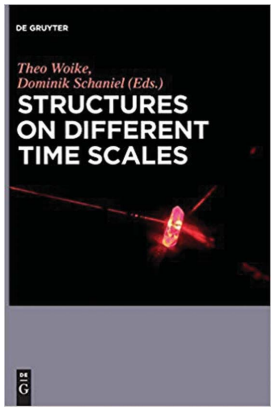
The book edited by T. Woike and D. Schaniel presents theory and experimental methods of time-resolved structure research with X-rays. It consists of six mainly independent chapters which cover a broad range of topics. Experimental and theoretical concepts of static structural analysis are combined with a thorough discussion of density functional theory and time-resolved structural analysis on time scales from femtoseconds to seconds.

The short introductory chapter by D. Schaniel and T. Woike gives a motivation for time-resolved structural analysis and puts it into a historic context. The basic physics of X-ray structure factors is introduced with the help of the independent atom model and complemented by a brief discussion of the multipolar model. The chapter concludes with an overview of the material covered in the book.

The second chapter, by R. B. Neder, deals with static structure analysis by Bragg diffraction and diffuse scattering. The chapter starts with an introduction of the elementary physics of X-ray scattering, followed by a discussion of Laue classes, reflection patterns from Bravais lattices and the Debye–Waller factor. Aspects of time-dependent scattering and temporal averaging are addressed with the help of the Patterson function. The second part of the chapter considers disordered structures and diffuse scattering. The final part of the chapter discusses pair distribution functions from a conceptual point of view, in combination with experimental results for ZnSe nanoparticles. The selected material is well chosen and the presentation clear.

In the third chapter, K. Schwarz and P. Blaha combine an introduction to density functional theory (DFT) for calculating electronic structure with a thorough discussion of the underlying approximations, in particular regarding Coulomb-mediated many-body effects. After a short section on computer codes, DFT results are presented for prototypical examples. The atomic and electronic structure of the perovskite $BaBiO_3$ serves for an in-depth discussion of lattice stability, band structure and electronic densities of state. A brief section on excitations in the single-electron picture and an outlook on DFT beyond the ground state conclude this excellent chapter, which places DFT in a broader physics context.

The fourth chapter, by V. Olevano, gives an overview of time-dependent density functional theory (TDDFT) in the context of transient electronic structure. The theoretical foundation of TDDFT and the relevant approximations are introduced in a clear and tutorial way. Photoexcited ethylene is chosen to illustrate the potential of TDDFT for calculating charge and nuclear dynamics on a few-femtosecond time scale. Electron energy-loss spectra of bulk silicon serve for a comparison of different levels of theory, while local field effects are addressed by calculations for graphite and graphene. This is



followed by an analysis of optical absorption spectra of a number of model systems and a discussion of ongoing methodological developments. The text is nicely focused, fully reflects the state of the art, and points to open questions and future trends.

The fifth chapter, by S. Pillet, discusses structural dynamics of crystalline materials and – to a lesser extent – solution-phase scattering in a time range from femtoseconds to seconds. The text is written from an experimental perspective and gives a high-class introduction to concepts and methods of time-resolved X-ray scattering, including a systematic account of how structure changes manifest in diffraction patterns. This is followed by a description of pump–probe methods and related experimental issues. The main part of the chapter presents judiciously chosen examples of time-resolved structure analysis, ranging from metastable and photostationary states and transient crystallography of the photoexcited photoactive yellow protein to femtosecond charge densities in polar crystalline materials. The material includes structure changes of ferroelectrics driven by external electric fields and dynamics of long-range ordering in manganites. This chapter stands out because of the excellent selection of material, the tutorial character of presentation and the exceptional clarity of text.

The final chapter, by B. D. Patterson, deals with ultrafast structure research and addresses diffraction studies of coherent phonons in bismuth, correlated X-ray scattering from molecules in solution, nonlinear X-ray optics and the operation principle of X-ray free-electron lasers. The phonon section represents a summary of work by a single research group, without covering the broader developments and literature in this area, for example towards soft-mode dynamics and other lattice excitations. The discussion of nonlinear orders in Raman scattering is somewhat misleading, as is the distinction between Raman and displacive excitation mechanisms of vibrational wavepackets. The section on free-electron lasers is very clear and concise. Overall, this chapter fails to reflect the current state of the art in ultrafast X-ray structure research, which covers a much wider range than presented here.

The book is well structured and the content of the different chapters sufficiently distinct and complementary. For newcomers in the field, the book offers a highly tutorial introduction to concepts and methods, augmented by a selection of recent prototypical results of research. The combination of theoretical and experimental chapters is convincing and makes use of consistent definitions of physical quantities and mathematical symbols. Unfortunately, the state of the art and the potential of ultrafast X-ray science with free-electron lasers are covered only in part. Important topics such as resonant X-ray diffraction and ultrafast studies of noncrystalline matter are not addressed. From a practical point of view, the lack of a detailed table of contents makes a quick search for particular content somewhat cumbersome. Nevertheless, the book conveys important knowledge to a broad audience and provides a very good introduction to an exciting new field of X-ray science.