

Preface

More than five decades have passed since the young German physicist Rudolf L. Mössbauer discovered the *recoilless nuclear resonance (absorption) fluorescence of γ -radiation*. The spectroscopic method based on this resonance effect – referred to as Mössbauer spectroscopy – has subsequently developed into a powerful tool in solid-state research. The users are chemists, physicists, biologists, geologists, and scientists from other disciplines, and the spectrum of problems amenable to this method has become extraordinarily broad. Up to now, more than 60,000 reports have appeared in the literature dealing with applications of the Mössbauer effect in the characterization of a vast variety of materials. Besides many workshops, seminars, and symposia, a biannual conference series called The International Conference on the Applications of the Mössbauer Effect (ICAME) started in 1960 (Urbana, USA) and regularly brings together scientists who are actively working on fundamental – as well as industrial – applications of the Mössbauer effect. Undoubtedly, Mössbauer spectroscopy has taken its place as an important analytical tool among other physical methods of solid-state research. By the same token, high-level education in solid-state physics, chemistry, and materials science in the broadest sense is strongly encouraged to dedicate sufficient space in the curriculum to this versatile method. The main objective of this book is to assist the fulfillment of this purpose.

Many monographs and review articles on the principles and applications of Mössbauer spectroscopy have appeared in the literature in the past. However, significant developments regarding instrumentation, methodology, and theory related to Mössbauer spectroscopy, have been communicated recently, which have widened the applicability and thus, merit in our opinion, the necessity of updating the introductory literature. We have tried to present a state-of-the-art book which concentrates on teaching the fundamentals, using theory as much as needed and as little as possible, and on practical applications. Some parts of the book are based on the first edition published in 1978 in the Springer series “Inorganic Chemistry Concepts” by P. Gülich, R. Link, and A.X. Trautwein. Major updates have been included on practical aspects of measurements, on the computation of Mössbauer

parameters with modern quantum chemical techniques (special chapter by guest-authors F. Neese and T. Petrenko), on treating magnetic relaxation phenomena (special chapter by guest-author S. Morup), selected applications in coordination chemistry, the use of synchrotron radiation to observe nuclear forward scattering (NFS) and inelastic scattering (NIS), and on the miniaturization of a Mössbauer spectrometer for mobile spectroscopy in space and on earth (by guest-authors G. Klingelhöfer and Iris Fleischer).

The first five chapters are directed to the reader who is not familiar with the technique and deal with the basic principles of the recoilless nuclear resonance and essential aspects concerning measurements and the hyperfine interactions between nuclear moments and electric and magnetic fields. Chapter 5 by guest-authors F. Neese and T. Petrenko focuses on the computation and interpretation of Mössbauer parameters such as isomer shift, electric quadrupole splitting, and magnetic dipole splitting using modern DFT methods. Chapter 6, written by guest-author S. Morup, describes how magnetic relaxation phenomena can influence the shape of (mainly ^{57}Fe) Mössbauer spectra. Chapter 7 presents an up-to-date summary of the work on all Mössbauer-active transition metal elements in accordance with the title of this book. This chapter will be particularly useful for those who are actively concerned with Mössbauer work on noniron transition elements. We are certainly aware of the large amount of excellent Mössbauer spectroscopy involving other Mössbauer isotopes, for example, ^{119}Sn , ^{121}Sb , and many of the rare earth elements, but the scope of this volume precludes such extensive coverage. We have, however, decided to describe and discuss some special applications of ^{57}Fe Mössbauer spectroscopy in Chap. 8. This is mainly based on work from our own laboratories and we include these to give the reader an impression of the kind of problems that can be examined by Mössbauer spectroscopy. In Chap. 8, we give examples from studies of spin crossover compounds, systems with biological relevance, and the application of a miniaturized Mössbauer spectrometer in NASA missions to the planet Mars as well as mobile Mössbauer spectroscopy on earth. Finally, Chap. 9 is devoted to the most recent developments in the use of synchrotron radiation for nuclear resonance scattering (NRS), both in forward scattering (NFS) for measuring hyperfine interactions and inelastic scattering (NIS) for recording the density of local vibrational states.

A CD-ROM is attached containing a teaching course of Mössbauer spectroscopy (ca. 300 ppt frames), a selection of examples of applications of Mössbauer spectroscopy in various fields (ca. 500 ppt frames), review articles on computation and interpretation of Mössbauer parameters using modern quantum-mechanical methods, list of properties of isotopes relevant to Mössbauer spectroscopy, appendices referring to book chapters, and the first edition of this book which appeared in 1978. In subsequent print runs files are available via springer.extra.com (see imprint page).

The authors wish to express their thanks to the *Deutsche Forschungsgemeinschaft*, the *Bundesministerium für Forschung und Technologie*, the *Max Planck-Gesellschaft*

and the *Fonds der Chemischen Industrie* for continued financial support of their research work in the field of Mössbauer spectroscopy. We are very much indebted to Dr. M. Seredyuk, Dr. H. Paulsen, and Mrs. P. Lipp, for technical assistance, and to Professor Frank Berry, for critical reading of the manuscript, and to Dr. B.W. Fitzsimmons for assistance in the proof-reading.

Mainz, Mülheim, Lübeck, November 2010

Philipp Gütlich, Eckhard Bill,
Alfred X. Trautwein

Mössbauer Spectroscopy and Transition Metal
Chemistry

Fundamentals and Applications

Gütlich, P.; Bill, E.; Trautwein, A.X.

2011, XV, 569 p., Hardcover

ISBN: 978-3-540-88427-9