THEORY OF INELASTIC SCATTERING AND ABSORPTION OF X-RAYS

This comprehensive, self-contained guide to X-ray spectroscopy will equip you with everything you need to begin extracting the maximum amount of information available from X-ray spectra.

Key topics such as the interaction between X-rays and matter, the basic theory of spectroscopy, and selection and sum rules, are introduced from the ground up, providing a solid theoretical foundation. The book also introduces core underlying concepts such as atomic structure, solid-state effects, the fundamentals of tensor algebra and group theory, many-body interactions, scattering theory, and response functions, placing spectroscopy within a broader conceptual framework, and encouraging a deep understanding of this essential theoretical background.

Suitable for graduate students, researchers, materials scientists and optical engineers, this is the definitive guide to the theory behind this powerful and widely used technique.

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CAMBRIDGE
UNIVERSITY PRESS

Shaftesbury Road, Cambridge CB2 8EA, United Kingdom

One Liberty Plaza, 20th Floor, New York, NY 10006, USA

477 Williamstown Road, Port Melbourne, VIC 3207, Australia

314–321, 3rd Floor, Plot 3, Splendor Forum, Jasola District Centre, New Delhi – 110025, India

103 Penang Road, #05–06/07, Visioncrest Commercial, Singapore 238467

Cambridge University Press is part of Cambridge University Press & Assessment, a department of the University of Cambridge.

We share the University's mission to contribute to society through the pursuit of education, learning and research at the highest international levels of excellence.

www.cambridge.org
Information on this title: www.cambridge.org/9781107033559

First published 2015

A catalogue record for this publication is available from the British Library

ISBN 978-1-107-03355-9 Hardback

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Preface

First thoughts of writing a textbook on X-ray spectroscopy followed the publication of a review article on resonant inelastic X-ray scattering (Ament *et al*., 2011). Jeroen van den Brink and I set up an outline of what basis was necessary to read the review article. The idea was that it should be accessible to graduate students or scientists new to the field with little prior knowledge of spectroscopy with an emphasis on the theoretical background. Since it is impossible to interpret spectroscopy without a model of the system that is being studied, it is also necessary to consider a certain amount of atomic and condensed-matter physics. The focus of the book is predominantly on materials that are strongly correlated, i.e. the interactions between the electrons are usually larger than the bandwidths. The book does not aim for completeness in theoretical approaches, experimental overview, or bibliography. Rather it aims to give the reader a basis for further study and an overview of the necessary ingredients to interpret X-ray spectra.

The book is divided into the following chapters. The first chapter gives a brief overview of what is needed to interpret a spectrum. Since the absorption and scattering of X-rays is, to a first approximation, a local process, Chapters 2–4 look at the local electronic structure starting from atomic physics and introduce solid-state effects by crystal fields. These sections rely heavily on group theory necessary to understand the complex interactions between electrons in the atomic orbitals and the X-ray photons that carry angular momentum through the polarization vectors. Obviously, we can only skim the surface of these topics which are by themselves the subjects of entire books. Chapter 5 then discusses many-body effects, focusing on the description of the Coulomb interactions in terms of linear and angular momentum. The latter in particular is responsible for many characteristic features in the X-ray absorption spectra known as multiplet structures. Chapter 6 describes the interaction between the photons and the electrons. Chapter 7 continues the study of many-body effects, focusing on solid-state effects and demonstrating how a solid responds to the absorption of electrons from deep-lying core-levels.

Chapters 8 and 9 finally deal with spectroscopy. For X-ray absorption, the focus lies on trends and how different interactions can change the spectral lineshapes and the integrated intensities. For resonant inelastic X-ray scattering, the emphasis lies on the excitations that can be created and the excitation mechanisms.

I would like to thank the many colleagues who have helped form my ideas on spectroscopy. First, I would like to thank Jeroen van den Brink, who played a crucial role in getting this project started. I would especially like to mention Peter Abbamonte, Ken Ahn, Massimo Altarelli, Luuk Ament, Mali Balasubramanian, Arun Bansil, Bernardo Barbiellini, Lucio Braicovich, Diego Casa, Jun Chang, Cheng-Chien Chen, Frank de Groot, Tom Devereaux, Yang Ding, Art Fedro, Javier Fernández-Rodríguez, John Freeland, Jim Freericks, Giacomo Ghiringhelli, Jeroen Goedkoop, Thomas Gog, Myung Joon (M.J.) Han, Daniel Haskel, Maurits Haverkort, John Hill, Zahirul Islam, Yasuo Ito, Jungho Kim, Young-June Kim, Clyde Kimball, Jonathan Lang, Bob Markiewicz, Ian McNulty, Brian Moritz, Mike Norman, John Rehr, George Sawatzky, Tsezar Seman, Eric Shirley, Yuri Shvyd'ko, George Srajer, Hao Tjeng, Mary Upton, Gerrit van der Laan, Dick van der Marel, Krzysztof Wohlfeld, and Hasan Yavaş. Finally, my thoughts go out to Theo Thole and Paolo Carra.