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A Journey into Reciprocal Space

A crystallographer's perspective

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ISBN 978-1-6817-4621-0 (ebook)
ISBN 978-1-6817-4620-3 (print)
ISBN 978-1-6817-4623-4 (mobi)

DOI 10.1088/978-1-6817-4621-0

Version: 20171001

IOP Concise Physics
ISSN 2053-2571 (online)
ISSN 2054-7307 (print)

A Morgan & Claypool publication as part of IOP Concise Physics
Published by Morgan & Claypool Publishers, 1210 Fifth Avenue, Suite 250, San Rafael, CA, 94901, USA

IOP Publishing, Temple Circus, Temple Way, Bristol BS1 6HG, UK

Dedicated to all those undergraduates who have had to suffer my tutorials for the last 40 years!

Contents

Preface

The concept of reciprocal space is over 100 years old, and has been made particular use of by crystallographers in order to understand the patterns of spots when x-rays are diffracted by crystals. However, it has a much more general use, especially in the physics of the solid state. In order to understand what it is, how to construct it and how to make use of it, it is first necessary to start with the so-called real or direct space and then show how reciprocal space is related to it. Real space describes the objects we see around us, especially with regards to crystals, their physical shapes and symmetries and the arrangements of atoms within: the so-called crystal structure. Reciprocal space on the other hand deals with the crystals as seen through their diffraction images. Indeed, crystallographers are accustomed to working backwards from the diffraction images to the crystal structures, which we call crystal structure solution. In solid state physics, one usually works the other way, starting with reciprocal space to explain various solid-state properties, such as thermal and electrical phenomena.

In this book, I start with the crystallographer's point of view of real and reciprocal space and then proceed to develop this in a form suitable for physics applications. Note that while for the crystallographer reciprocal space is a handy means of dealing with diffraction, for the solid-state physicist it is thought of as a way to describe the formation and motion of waves, in which case the physicist thinks of reciprocal space in terms of momentum or wave-vector **k**-space. This is because, for periodic structures, a characteristic of normal crystals, elementary quantum excitations, e.g. phonons and electrons, can be described both as particles and waves. The treatment given here, will be by necessity brief, but I would hope that this will suffice to lead the reader to build upon the concepts described. I have tried to write this book in a suitable form for both undergraduate and graduate students of what today we call 'condensed matter physics'.

Acknowledgements

I was fortunate to learn all about crystallography from two great scientists, Kathleen Lonsdale, my PhD supervisor, and Helen D Megaw at the Cavendish Laboratory, Cambridge, who introduced me to the world of perovskites. Although I had started out as a chemist, I soon appreciated from them the value of condensed matter physics and how it related to crystallography. Thus, when I was appointed to the Clarendon Laboratory, Oxford in 1976 I was in a good position to teach undergraduates and graduates about the solid state, sometimes from a unique point of view. The topics described in this book owe much to hours of discussions, sometimes quite heated, with many of my tutees at Jesus College Oxford. There is nothing like teaching students to make one realize how little one really understands about a subject, and how to relearn something that you thought was already done and dusted. Despite retirement, I continue to learn.

Author biography

A M Glazer

Mike Glazer is Emeritus Professor of Physics at the University of Oxford and Jesus College Oxford, and Visiting Professor at the University of Warwick. From 2014 to 2017 he was also Vice-President of the International Union of Crystallography. His PhD research between 1965 and 1968 was under the supervision of Kathleen Lonsdale at University College London, working on the crystallography of organic mixed crystals. In 1968–1969, he was a Fellow at Harvard University, and then from 1969 to 1976 he was at the Cavendish Laboratory, Cambridge. In 1976, he was appointed Lecturer in Physics at the Clarendon Laboratory Oxford and as an Official Fellow and Tutor at Jesus College Oxford. Mike Glazer's research has mainly been in understanding the relationship between physical properties of crystals and their structures. He is perhaps best known for his classification system for tilted octahedra in perovskites. He is also one of the co-founders of Oxford Cryosystems Ltd, which supplies the world market in low-temperature apparatus for crystallographers.