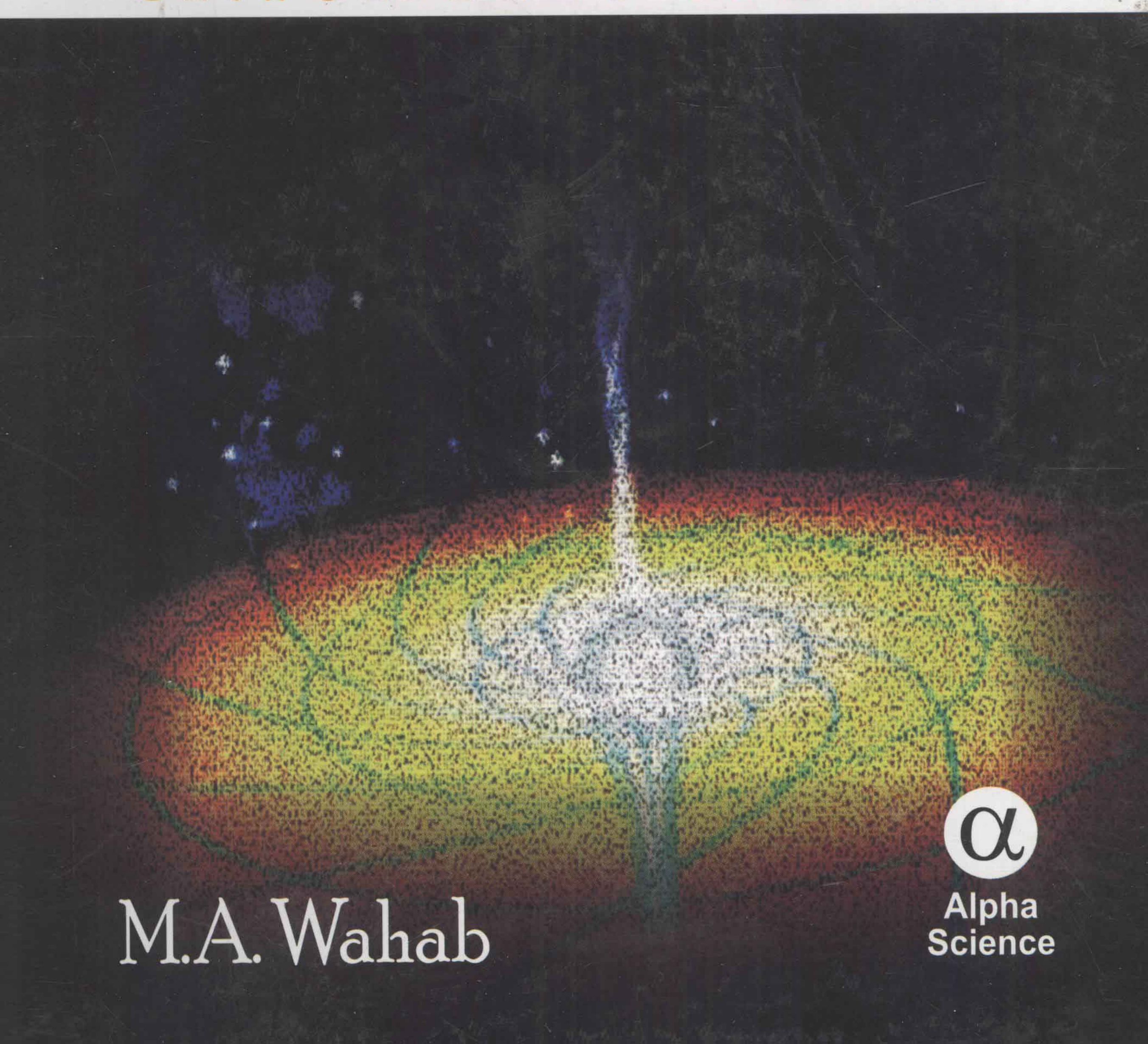
Essentials of CRYSTALLOGRAPHY



M.A. Wahab

Alpha Science

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Alpha Science International Ltd.
Oxford, U.K.

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332 pgs. | 228 figs. | 48 tbls.

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ALPHA SCIENCE INTERNATIONAL LTD.
7200 The Quorum, Oxford Business Park North
Garsington Road, Oxford OX4 2JZ, U.K.

www.alphasci.com

ISBN 978-1-84265-392-0

Printed in India

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PREFACE

As the name indicates this book contains the essential topics needed to understand the crystals from macroscopic and microscopic point of view and the mode of their growth, structure determination and structural refinements from experimental and theoretical point of view. The aim of the present book is to provide a comprehensive introduction to the subject of crystallography in a simplified manner to the students of M.Sc, M.Phil, and Ph.D of Physical, Chemical, Biological, Materials, Engineering Sciences and Faculties in this field. The subject of crystallography is conceptual and imaginative and the students generally find it relatively difficult. However, the author with all his experience in the field and hard work has successfully made it easy for them to understand.

This book contains a total of fourteen chapters, out of which initial seven chapters deal with the basic aspects of crystallography. They include the development of space lattices, description of macroscopic and microscopic symmetries exhibited by crystalline solids and simplified approach to understand the derivation of point groups and space groups. The chapter number eight particularly deals with the basics of theory and experiments of crystal growth while the chapter number nine deals with the imperfections normally encountered in crystalline solids. The chapter number ten deals with the diffraction methods based on both film and counter techniques and for date collection. The last four chapters deal with topics related to crystal structure analyses they are: factors affecting x-ray intensities, structure factors and fourier synthesis,(where the concepts of structure factor have been developed using optical analogue), and important methods of crystal structure analysis and refinements.

The main features of the book are:

1. Solved examples for a better understanding of the text.
2. Matrix representation of symmetry elements and derivation of point group by simple matrix multiplication.
3. Summary and definitions of important terms at the end of each chapter for quick revision.
4. Problems and exercises.

Although proper care has been taken during the preparation of the manuscript, still some errors are expected to creep in. Any omissions, errors, suggestions brought to the knowledge of the author will be gratefully acknowledged.

First of all I sincerely thank our Vice Chancellor Prof. Musheerul Hasan for providing me the timely needed sabbatical leave. This indeed helped me in completing the MS in time. I sincerely express my sense of gratitude to my Research guide, Prof. G.C. Trigunayat, former Head, Deptt. of

Physics, Delhi University. I also thank colleagues of J.M.I from different departments for their encouragement.

I am indeed grateful to all the authors and publishers of Books and Journals mentioned in the bibliography for freely consulting them and even borrowing some ideas during the preparation of the manuscript. I am also grateful to M/s Narosa Publishing House, New Delhi for timely publication of this book.

My special thanks to the members of my family for their continuous support and encouragement during the preparation of the manuscript. I particularly thank my wife Mrs. Raees Begum for making a fair draft of the entire manuscript.

M.A. Wahab

CONTENTS

CHAPTER 1

BRAVAIS LATTICE IN TWO DIMENSIONS

1.1 INTRODUCTION

From our everyday experience, we are familiar with a one dimensional iron chain and two dimensional periodic patterns as in wall papers (Fig. 1.1) and fabrics etc. We find a large variety in design by changing both the forms of the basic motif (or unit of pattern) and the spacing of its periodic repetition. To analyse the nature of the given pattern, a single motif is selected such that the pattern could be obtained by two periodic transformations in two non collinear directions. Thus the essential features of the given pattern are specified by two non parallel translation vectors. Replacing each motif in the pattern with a point, a periodic pattern of points defined by the same translation

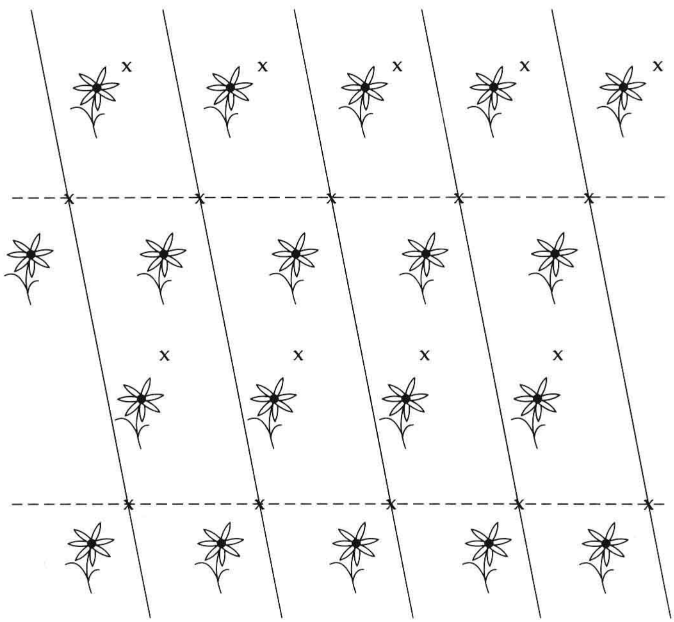

Fig. 1.1 A two dimensional periodic pattern