ERIC A LORD, ALAN L MACKAY AND
S RANGANATHAN

New Geometries for New Materials

Recent advances in materials science have given rise to novel materials with unique properties, through the manipulation of structure at the atomic level. Elucidating the shape and form of matter at this scale requires the application of mathematical concepts. This book presents the geometrical ideas that are being developed and integrated into materials science to provide descriptors and enable visualisation of the atomic arrangements in three-dimensional (3D) space. Emphasis is placed on the intuitive understanding of geometrical principles, presented through numerous illustrations. Mathematical complexity is kept to a minimum and only a superficial knowledge of vectors and matrices is required, making this an accessible introduction to the area. With a comprehensive reference list, this book will appeal especially to those working in crystallography, solid state and materials science.

Dr Eric A. Lord is a Visiting Scientist in the Department of Metallurgy at the Indian Institute of Science.

Prof. Alan L. Mackay retired in 1991 as a Professor Emeritus in the School of Crystallography at the University of London; however, he continues to pursue several research collaborations. He is a Fellow of the Royal Society.

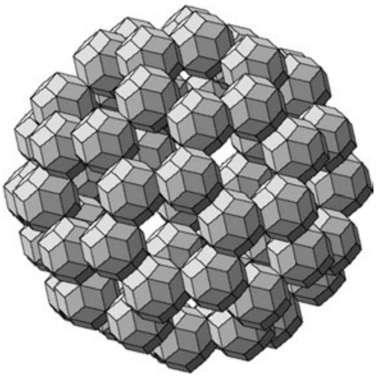
Prof. S. Ranganathan is an Honorary Professor in the Department of Metallurgy at the Indian Institute of Sciences and has contributed to some 250 papers in scientific journals.

NEW GEOMETRIES FOR NEW MATERIALS

ERIC A LORD
Department of Metallurgy, Indian Institute of Science, Bangalore, India

ALAN L MACKAY
School of Crystallography, Birkbeck College, University of London, London, UK

S RANGANATHAN
Department of Metallurgy, Indian Institute of Science, Bangalore, India



CAMBRIDGE
UNIVERSITY PRESS

CAMBRIDGE UNIVERSITY PRESS
Cambridge, New York, Melbourne, Madrid, Cape Town,
Singapore, São Paulo, Delhi, Mexico City

Cambridge University Press
The Edinburgh Building, Cambridge CB2 8RU, UK

Published in the United States of America by Cambridge University Press, New York

www.cambridge.org
Information on this title: www.cambridge.org/9781107411609

First published 2006
First paperback edition 2012

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

Library of Congress Cataloguing in Publication Data

ISBN 978-0-521-86104-5 Hardback
ISBN 978-1-107-41160-9 Paperback

Additional resources for this publication at www.cambridge.org/9781107411609

Contents

* Plates available for download in colour from www.cambridge.org/9781107411609

Cambridge University Press
978-1-107-41160-9 - New Geometries for New Materials
Eric A Lord, Alan L Mackay and S Ranganathan
Frontmatter
More information

Preface

Over the past few decades unprecedented and far-reaching discoveries have been taking place in the materials sciences – in solid state physics, crystallography, metallurgy, nanotechnology, microbiology… These discoveries have given rise to new materials with unusual and valuable properties and have led to a deeper understanding of how nature works – of how atoms combine to build the world. At the most basic level the study of the kinds of patterns and structures that can arise from the combination of subunits in three-dimensional (3D) space reveals a metastructure of underlying general principles. We are essentially dealing here with a *language*, the language of shape and form, the language of the geometry of 3D space.

The range of shapes and patterns that are possible in 3D space is independent of scale. Thus, for example, the C_{60} molecule has been named 'Buckminsterfullerene' or, colloquially, the 'Bucky ball' because the uniform spherical arrangement of its 60 atoms corresponds to the icosahedral geometry underlying Buckminster Fuller's geodesic dome constructions. Only the scale is different. Thus, though the majority of the structures that we have chosen to describe and to exemplify general principles are taken mainly from the literature of the materials sciences, and though it is to the materials scientist that our work is principally addressed, it is our hope that our presentation will not be without interest to a wider readership.

In seeking inroads into the problem of understanding how complex structures arise in nature, some of the more exotic geometries have been employed as an aid to thinking about structures. For example, much of the theoretical investigation of quasicrystals has made forays into 6D space; Stephen Hyde's work has shown how non-Euclidean geometry can throw light on the structure of networks; the real and hypothetical materials investigated by Terrones and his co-workers bring in the geometry of curved surfaces, and so on. As materials science has become increasingly mathematically oriented, mathematicians have in turn been stimulated to new investigations by discoveries in materials science. An exciting dialogue is emerging.

The field is vast, and growing. Clearly, a review such as this needs to be selective. What makes the study of structure fascinating is its appeal to the imagination. We have placed the emphasis on the intuitive feeling for 3D shapes and structures. That is the foundation on which any such study is built. We have, accordingly, attempted to keep mathematical details to a minimum. In the places where a mathematical technique or demonstration seemed unavoidable we hope the uninitiated reader will bear with us. Extensive citations of our sources will, we trust, be helpful for the curious reader who wishes or needs to pursue further some of the more esoteric aspects of our theme.

We have aimed to bring out clearly the interconnections among the topics dealt with in the various chapters – to emphasise tha unity of our subject matter. Hence, the reader will sometimes find the same structures occurring in different contexts, described from different viewpoints.

The writing of this book was undertaken as part of the project ‘New Geometries for New Materials’ sponsored by the Defence Research and Development Organisation, Ministry of Defense, Government of India (project reference DRDO/MMT/SRG/526). Their support and encouragement is gratefully acknowledged. SR is grateful to the Homi Bhabha Fellowship Council for support. Some additional material related to this project can be found on our website http://met.iisc.ernet.in/~lord. Almost all the figures (not just those in Chapter 9) were produced using Ken Brakke’s remarkable software Surface Evolver. We are indebted to him for making Surface Evolver freely available for downloading from the Internet.

Eric A. Lord
Alan L. Mackay
S. Ranganathan