

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](#)

---

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.

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](#)

---

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](#)

# NEW GEOMETRIES FOR NEW MATERIALS

ERIC A LORD

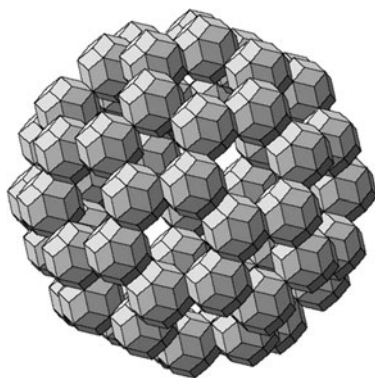
*Department of Metallurgy, Indian Institute of Science, Bangalore, India*

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  
978-1-107-41160-9 - New Geometries for New Materials  
Eric A Lord, Alan L Mackay and S Ranganathan  
Frontmatter  
[More information](#)

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](http://www.cambridge.org)  
Information on this title: [www.cambridge.org/9781107411609](http://www.cambridge.org/9781107411609)

© E. A. Lord, A. L. Mackay and S. Ranganathan 2006

This publication is in copyright. Subject to statutory exception  
and to the provisions of relevant collective licensing agreements,  
no reproduction of any part may take place without the written  
permission of Cambridge University Press.

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](http://www.cambridge.org/9781107411609)

Cambridge University Press has no responsibility for the persistence or  
accuracy of URLs for external or third-party internet websites referred to in  
this publication, and does not guarantee that any content on such websites is,  
or will remain, accurate or appropriate.

## Contents

<i>Preface</i>	<i>ix</i>
1 Introduction	1
1.1 Atoms	1
1.2 Geometry	3
1.3 Crystallography	4
1.4 Generalised Crystallography	5
1.5 Shapes and Structures	6
2 2D Tilings	9
2.1 Kepler's Tilings	10
2.2 Fundamental Regions	11
2.3 Topology of Plane Tilings	13
2.4 Coloured Symmetry	14
2.5 Truchet Tilings	15
2.6 Aperiodic Tilings	16
2.7 Gummelt's Decagon	20
2.8 The Divine Proportion and the Fibonacci Sequence	21
2.9 Random Tilings	23
2.10 Spherical Tilings	23
2.11 Topology of 2D Tilings	27
2.12 Tilings and Curvature	28
2.13 Fullerenes	29
3 3D Tilings	32
3.1 Lattices and Space Groups	32
3.2 Packing of Regular and Semi-regular Polyhedra	35
	v

vi	<i>Contents</i>	
3.3	Voronoi Regions	42
3.4	Fedorov's Parallelohedra	43
3.5	Lattice Complexes	43
3.6	Polytetrahedral Structures	45
3.7	The Polytope {3, 3, 5}	47
3.8	Packings Involving Pentagonal Dodecahedra	47
3.9	Asymmetric Units	49
3.10	Modular Structure	51
3.11	Aperiodic Tilings of $E_3$	55
4	Circle and Sphere Packing	59
4.1	Circle Packing	59
4.2	Cubic Close Packing	61
4.3	Sphere Packings and Nets	62
4.4	Low Density Sphere Packings	62
4.5	The Boerdijk–Coxeter Helix	64
4.6	Random Sphere Packings	65
4.7	Sphere Packings in Higher Dimensions	67
4.8	Packing Circles on a Spherical Surface	68
4.9	Packing of Unequal Spheres	73
4.10	Rod Packings	76
5	Hierarchical Structures	77
5.1	Lindenmayer Systems	77
5.2	Fractal Curves	78
5.3	Inflation Rules	84
5.4	Other Aperiodic Tilings by Iteration	84
5.5	Inflation of 3D-Penrose Tilings	85
5.6	Kramer's Hierarchical Tiling	87
6	Clusters	88
6.1	Clusters of Icosahedra	88
6.2	The Bergman Cluster	91
6.3	The Mackay Icosahedron	95
6.4	The $\gamma$ -Brass Cluster	97
6.5	Clusters of Friauf Polyhedra	99
6.6	Clusters of Tetrahedra and Octahedra	101
6.7	Icosahedra and Octahedra	101
6.8	Triacanthedral Clusters	104
6.9	Crystalloids	107

	<i>Contents</i>	vii
7	Helical and Spiral Structures	110
7.1	Screw Axes	110
7.2	Polyhedral Helices	111
7.3	Polyhedral Rings	112
7.4	Periodic Tetrahelices	114
7.5	A Periodic Icosahelix	115
7.6	Triangulated Cylindrical Polyhedra	117
7.7	Helices and {3, 3, 5}	118
7.8	Nanotubes	119
7.9	Spiral Phyllotaxis	121
7.10	Spiral Distribution of Points on a Sphere	127
8	3D Nets	132
8.1	Infinite Polyhedra	132
8.2	Uniform Nets	133
8.3	Rings and Coordination Sequences	133
8.4	Vertex-Connected Tetrahedra	136
8.5	4-Connected Nets	139
8.6	Crankshafts, Zigzags and Saw Chains	141
8.7	Disclination Networks	144
8.8	Topological Classification of Tilings	145
8.9	Interwoven Nets	149
8.10	Truncation	151
8.11	Polyhedral Nets and Labyrinth Graphs	152
8.12	Polynets Containing Pyrochlore Units	154
8.13	Augmented Nets	159
9	Triply Periodic Surfaces	162
9.1	Minimal Surfaces	162
9.2	Schwarz and Neovius	164
9.3	Schoen's Surfaces	166
9.4	Generating Patches	168
9.5	Fundamental Patches	172
9.6	Orthorhombic, Rhombohedral and Tetragonal Variants	173
9.7	Minimal Surfaces and the Hyperbolic Plane	175
9.8	TPMS with Self-Intersections	177
9.9	Tiling of Triply Periodic Surfaces	181
9.10	Saddle Polyhedra	183
9.11	Other Kinds of Triply Periodic Surfaces	186
9.12	Nodal Surfaces and Level Surfaces	187

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](#)

viii	<i>Contents</i>	
10	Novel Atomic Configurations in Metallics	190
10.1	Geometrical Considerations	190
10.2	Pure Metals	191
10.3	Alloys	193
10.4	Solid Solutions	194
10.5	Intermetallics	194
10.6	Quasicrystals	197
10.7	Structurally Complex Intermetallics	202
10.8	Metallic Glasses	204
10.9	Nanocrystals	206
10.10	Helices	207
10.11	Clathrates	208
10.12	Conclusion	208
	Colour Plates <i>after 150*</i>	
	Appendix: Handling the New Geometry	209
	References	211
	Index	230

\* Plates available for download in colour from [www.cambridge.org/9781107411609](http://www.cambridge.org/9781107411609)



## 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 the 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*