

From *SIAM News*, Volume 41, Number 3, April 2008

Geometric Ideas for the Description and Analysis of Complex Crystal Structures

New Geometries for New Materials. By E.A. Lord, A.L. Mackay, and S. Ranganathan, Cambridge University Press, Cambridge, UK, 2006, 238 pages, £70 (\$140).

The rather slim book *New Geometries for New Materials* is a review of geometrical ideas used, or intended to be used, in materials science for description and evaluation of two- and three-dimensional atomic arrays. The authors are specialists working in different areas of the field: mathematical description of shapes and forms (E.A. Lord), multiple and very diversified contributions to the field of generalized crystallography (A.L. Mackay), and quasicrystals and clusters (S. Ranganathan).

BOOK REVIEW

By Emil Makovicky

Individual chapters of the book treat a broad spectrum of well-known and, especially, less well-known approaches to these arrays, as summarized by the chapter headings: filling of plane and space, packing of spheres, clusters, hierarchical and helical structures, nets, and triply periodic (minimal) surfaces. The last chapter of the book differs somewhat from the rest, dealing primarily with metals and intermetallics.

Each topical chapter contains a mixture of theoretical and empirical approaches and observations, based on broad experience and a thorough review of literature sources. For example, the chapter on clusters contains sections on clusters of icosahedra, on the special cases of “Bergman,” “Mackay,” and “ γ -brass” clusters in alloys, as well as on clusters composed of octahedra, tetrahedra, icosahedra, and Friauf polyhedra in different combinations. The authors’ considerable experience and interest in intermetallics transpire from this account.

Configurations/tiling are considered in both two and three dimensions, as well as on a sphere and on triply periodic (minimal) surfaces; in the latter case they are related to those on a hyperbolic plane.

The authors opted for moderately deep treatment, appealing intentionally to the reader’s imagination and keeping mathematical detail to a necessary minimum. Along with the topics that are explained in the book (although in a concise way) are a number of others that are referenced only. This is inevitable for a vast and very heterogeneous field of descriptors and approaches. Refreshing are the occasional historic excursions and a chapter on spiral phyllotaxy.

A drawback of the book is the somewhat uneven treatment of different topics. Some sections are self-explanatory, and the reader has to consult original sources only for details, whereas other sections necessitate excursions to Google or Wikipedia for explanation of the basics. Treatment of coordination polyhedra, important for crystal chemistry, is rather cursory, and the spectrum of approaches developed by diverse authors for the calculation of coordination numbers is not considered. Certain illustrations appear twice, once in black-and-white form inserted in the text and again as a separate colour plate. Stereo figures require a stereoscope; the old free-eye trick cannot be used. References appear to have been forgotten in some sections, e.g., section 5.4.

The number of real-structure examples for the application of abstract geometric concepts varies from one section to another. There is a partial overlap with *Crystal Structures I* by O’Keeffe and Hyde (1996). The earlier authors, however, stay much closer to classical structural science, which is then treated in some detail.

New Geometries for New Materials is a thorough review of advanced concepts to be used in the description and analysis of complex crystal structures or their complex properties. It is highly recommended as a source of inspiration for anyone facing a research problem that goes beyond the ordinary. You may find there an approach you never dreamt of!

Emil Makovicky is a professor and practicing crystallographer in the Department of Geology and Geography at the University of Copenhagen.