Crystal Cell and Space Lattice Symmetries in Clifford Geometric Algebra

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1 Introduction

The structure of crystal cells in two and three dimensions is fundamental for many material properties. Many elements, including Aluminium, Copper and Iron have e.g. cubic unit cells. The nearest neighbors of diamond structures form tetrahedrons. About 30 elements show hexagonal close-packed structure. Important organic molecules like benzene have hexagonal symmetry. Today some 80% of crystal structure analysis is carried out on crystallized biomolecules with huge investments from pharmaceutical companies.

In two dimensions atoms (or molecules) often group together in triangles, squares and hexagons (regular polygons). Crystal cells in three dimensions have triclinic, monoclinic, orthorhombic, hexagonal, rhombohedral, tetragonal and cubic shapes (see Fig. 3.1).

The geometric symmetry of a crystal manifests itself in its physical properties, reducing the number of independent components of a physical property tensor, or forcing some components to zero values. There is therefore an important need to efficiently analyze the crystal cell symmetries.

Mathematics based on geometry itself offers the best descriptions. Especially if elementary concepts like the relative directions of vectors are fully encoded in the geometric multiplication of vectors.

2 Multiplying Vectors with Clifford's Geometric Product

The geometric product [2, 3] of vectors a, b includes sine and cosine of the enclosed angle α:

$$ab = |a||b|(\cos\alpha + i\sin\alpha), \tag{1}$$

where $i = e_1e_2$ is the unit oriented area element of the plane of the vectors a, b. The geometric product has symmetric (inner) and antisymmetric (outer) parts:

$$a \cdot b = (ab + ba)/2 = |a||b|\cos\alpha, \quad a \wedge b = (ab - ba)/2 = |a||b|i\sin\alpha. \tag{2}$$

These properties can already be used to implement reflections across a line (in 2D) or at a mirror plane (in 3D). In both cases the mirror (line or plane) can be given by a normal vector c (with inverse $c^{-1} = c/c^2, c^{-1}c = 1$.) A vector x is reflected by

$$x' = -c^{-1}x\,c. \tag{3}$$

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To do a sequence of two reflections with normal vectors c, d simply results in

$$x' = d^{-1}c^{-1}x\,cd = (cd)^{-1}x\,cd, \tag{4}$$

etc. Two reflections at planes with normal vectors c, d enclosing the angle $\theta/2$ result in a rotation by angle θ. A general rotation operator (rotor) is therefore the product of two vectors $R = cd$ enclosing half the angle of the final rotation. A sequence of three reflections at planes with normal vectors c, d, e gives a rotary-reflection:

$$x' = -(cde)^{-1}x\,cde, \tag{5}$$

because the first two reflections result in a rotation followed by a final reflection. If the three vectors c, d, e happen to be mutually orthogonal $(cde = i = e_1e_2e_3, i^2 = -1)$, then (5) describes an inversion:

$$x' = -(-i)x\,i = -x. \tag{6}$$

The general transformation law is

$$x' = (-1)^p S^{-1}x\,S, \tag{7}$$

with p =parity (even or odd) of the vector products in S. Because both S^{-1} and S are factors in (7), the sign of S and (non-zero) scalar factors of S always cancel. We therefore equate operators S if they only differ by real scalar factors (including positive and negative signs)!

3 Representation and Visualization of Point and Space Groups

3.1 2D Point Groups

Fundamental are the two-dimensional symmetries of regular polygons with $n = 1, 2, 3, 4, 6$ corners [4] of Figure 3.1. (With $n = 5$, no lattice can be built.) For an interactive online visualization see [5]. Tables 1 and 2 show

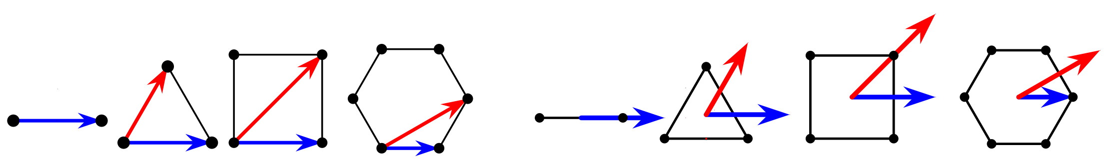

Fig. 1 Left: Regular polygons $n = 1, 2, 3, 4, 6$ with vector generators a, b. Right: a, b attached to polygon centers.

the two-dimensional point groups ($n = 1, 2, 3, 4, 6$). They list the symmetry elements represented by products of the generating vectors a, b, an explicit representation in an orthonormal basis of the two-dimensional Clifford geometric algebra

$$\{1, e_1, e_2, e_1e_2\}, \tag{8}$$

and the conventional matrix representation. The most compact and intuitive representation is certainly by invariant geometric algebra vector products. The geometric algebra basis representation has the advantage that it is immediately seen if a symmetry is a reflection (generator is a vector) or a rotation (generator is scalar plus bivector). The bivector part of the latter immediately represents the rotation plane. The matrix representation seems to be the least intuitive.

3.2 3D Point Groups

All known three-dimensional crystal lattices can be characterized by their crystal cells shown in Fig. 2 . The symmetry transformations of these cells, which leave the center points O invariant, form groups of symmetry operations, called point groups. Altogether there are 32 point groups associated with seven crystal classes. [1, 4]

Table 1 2D point group ($n = 1, 2, 3$) representations: invar. products of crystal vectors, in basis (8), matrices.

invariant	orthon. basis	matrix	invariant	orthon. basis	matrix
n=1					
± 1	± 1	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$			
n=2					
a	e_1	$\begin{pmatrix} \text{-}1 & 0 \\ 0 & 1 \end{pmatrix}$	-1	-1	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$
n=3					
reflections			rotations		
a	e_1	$\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$	ab	$1 + \sqrt{3}e_1e_2$	$\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ +\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$
b	$e_1 + \sqrt{3}e_2$	$\begin{pmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$	$(ab)^2$	$-1 + \sqrt{3}e_1e_2$	$\begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$
bab	$-e_1 + \sqrt{3}e_2$	$\begin{pmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$	-1	-1	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$

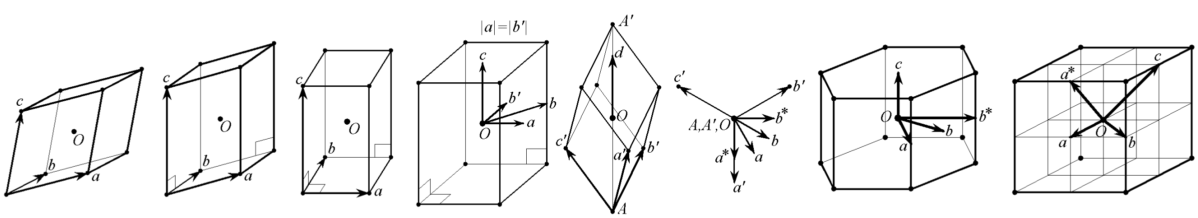

Fig. 2 7 crystal cells with vector generators a, b, c: triclinic, monoclinic, orthorhombic, tetragonal, trigonal (side & top), hexagonal, cubic.

For the visualization of the 3D point groups we used the open source software CLUCalc [6], which supports geometric algebra. Start up opens three windows for script, text output and OpenGL visualization. The latter has three areas: interactive text, bottom control elements, initial and transformed crystal cells. Clicking the blue text links selects a crystal cell type. Next a blue group identifier is chosen. Clicking on highlighted group generators applies the corresponding transformation. Dragging the mouse pointer in the visualization area freely rotates the view.

3.3 2D Space Groups

The two-dimensional space groups (wallpaper groups) can also be elegantly described in Clifford geometric algebra. Using the conformal model of the Euclidean plane in $Cl_{3,1}$ translations can be treated like rotations as multiplicative geometric algebra multivector operators [4].

We also develop free interactive visualization software for the wallpaper groups based on CLUCalc [6]. Our socalled Wallpaper Group Explorer allows the users to freely select a basic cell pattern, decide on reflection and translation generators and combine them to see which wallpaper is generated and what are the conditions for generating a true 2D space group.

Table 2 2D point group ($n = 4, 6$) representations: invariant products of crystal vectors, in basis (8), matrices.

invariant	orthon. basis	matrix	invariant	orthon. basis	matrix
n=4					
reflections			rotations		
a	e_1	$\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$	ab	$1 + e_1e_2$	$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$
b	$e_1 + e_2$	$\begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}$	$(ab)^2$	e_1e_2	$\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$
bab	e_2	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	$(ab)^3$	$-1 + e_1e_2$	$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$
$b(ab)^2$	$e_1 - e_2$	$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$	-1	-1	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$
n=6					
reflections			rotations		
a	e_1	$\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$	$R = ab$	$\sqrt{3} + e_1e_2$	$\begin{pmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}$
b	$\sqrt{3}e_1 + e_2$	$\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}$	R^2	$1 + \sqrt{3}e_1e_2$	$\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$
aR^2	$e_1 + \sqrt{3}e_2$	$\begin{pmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$	R^3	e_1e_2	$\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$
bR^2	e_2	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	R^4	$-1 + \sqrt{3}e_1e_2$	$\begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$
aR^4	$-e_1 + \sqrt{3}e_2$	$\begin{pmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$	R^5	$-\sqrt{3} + e_1e_2$	$\begin{pmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}$
bR^4	$-\sqrt{3}e_1 + e_2$	$\begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}$	$R^6 = -1$	-1	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$

Work is under way on full 3D space group representation in geometric algebra. New ways to describe and analyse crystal symmetries, which are derived straightforward from the physical crystal itself are expected.

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