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Crystallogaphic space groups: Representation and interactive visualization by geometric algebra

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Abstract. We treat the symmetries of crystal space lattices in geometric algebra (GA) [1]. All crystal cell point groups are generated by geometric multiplication of two or three physical cell vectors. Only one or two relative angles subtended by these vectors need to be known. This treatment extends to space groups by including translations. GA helps to identify optimal multivector generators. As example we take the monoclinic case. New free interactive OpenGL and GA based software visualizes these symmetries.

1 Introduction

Crystals are fundamentally periodic geometric arrangements of molecules. The directed distance between two such elements is a Euclidean vector in $\mathbb{R}^3$. Intuitively all symmetry properties of crystals depend on these vectors. Indeed, the geometric product of vectors [2] combined with the conformal model of 3D Euclidean space yield an algebra fully expressing crystal point and space groups [3, 1, 4]. Two successive reflections at (non-) parallel planes express (rotations) translations, etc. This leads to a 1:1 correspondence of geometric objects and symmetry operators with vectors and their products (versors), ideal for creating a suit of interactive visualizations using CLUCalc and OpenGL (free download from: [4]).

2 Cartan and geometric algebra

Clifford's associative geometric product [2] of two vectors simply adds the inner product to the outer product of Grassmann

$$\vec{a}\vec{b} = \vec{a}\cdot\vec{b} + \vec{a}\wedge\vec{b}. \tag{1}$$

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Under this product parallel vectors commute and perpendicular vectors anti-commute

$$\vec{a}\vec{x}_{\|} = \vec{x}_{\|}\vec{a}, \qquad \vec{a}\vec{x}_{\perp} = -\vec{x}_{\perp}\vec{a}. \tag{2}$$

This allows to write the reflection of a vector $\vec{x}$ at a hyperplane through the origin with normal $\vec{a}$ as

$$\vec{x}\,' = -\,\vec{a}^{\,-1}\vec{x}\,\vec{a}, \qquad \vec{a}^{\,-1} = \frac{\vec{a}}{\vec{a}^{\,2}}. \tag{3}$$

The composition of two reflections at hyperplanes whose normal vectors $\vec{a},\vec{b}$ subtend the angle α yields a rotation around the intersection of the two hyperplanes by 2α

$$\vec{x}\,' = (\vec{a}\vec{b})^{-1}\vec{x}\,\vec{a}\vec{b}, \qquad (\vec{a}\vec{b})^{-1} = \vec{b}^{\,-1}\,\vec{a}^{\,-1}. \tag{4}$$

Continuing with a third reflection at a hyperplane with normal $\vec{c}$ according to Cartan yields rotary reflections and inversions

$$\vec{x}\,' = -\,(\vec{a}\vec{b}\vec{c})^{-1}\vec{x}\,\vec{a}\vec{b}\vec{c}, \qquad \vec{x}\,'' = -\,i^{-1}\vec{x}\,i, \qquad i \doteq \vec{a}\wedge\vec{b}\wedge\vec{c}, \tag{5}$$

where $\doteq$ means equality up to scalar factors (which cancel out). In general the geometric product of k normal vectors (the versor S) corresponds to the composition of reflections to all symmetry transformations [1] of 2D and 3D crystal cell point groups

$$\vec{x}\,' = (-1)^k S^{-1}\,\vec{x}\,S. \tag{6}$$

3 Two dimensional point groups

2D point groups [1] are generated by multiplying vectors selected [4] as in fig. 1. The index p can be used to denote these groups as in table 1. For example the hexagonal point group is given by multiplying its two generating vectors $\vec{a},\vec{b}$

$$6 = \{\vec{a},\vec{b},R = \vec{a}\vec{b},R^2,R^3,R^4,R^5,R^6 = -1,\vec{a}R^2,\vec{b}R^2,\vec{a}R^4,\vec{b}R^4\}. \tag{7}$$

The rotation subgroups are denoted with bars, e.g. $\bar{6}$.

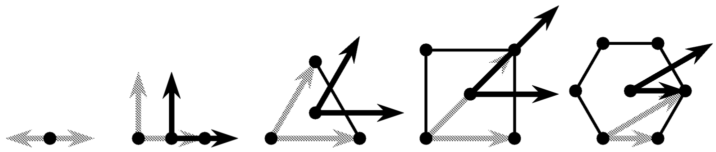

Figure 1. Regular polygons ($p = 1,2,3,4,6$) and point group generating vectors subtending angles π/p shifted to center.

Table 1. Geometric and international notation for 2D point groups.

Crystal	Oblique		Rectangular		Trigonal		Square		Hexagonal	
geometric	$\bar{1}$	$\bar{2}$	1	2	3	$\bar{3}$	4	$\bar{4}$	6	$\bar{6}$
international	1	2	m	mm	3m	3	4m	4	6m	6

4 Three dimensional point groups

The selection of three vectors $\vec{a},\vec{b},\vec{c}$ from each crystal cell [1, 4] for generating all 3D pointgroups is indicated in fig. 2. Using $\angle(\vec{a},\vec{b})$ and $\angle(\vec{b},\vec{c})$ we can denote all 32 3D point groups as in table 2. For example the monoclinic point groups are then (int. symbols: 2/m, m and 2, respectively)

$$2\bar{2} = \{\vec{c}, R = \vec{a}\wedge\vec{b} = i\vec{c}, i = cR, 1\}, \quad 1 = \{\vec{c}, 1\}, \quad \bar{2} = \{i\vec{c}, 1\}. \tag{8}$$

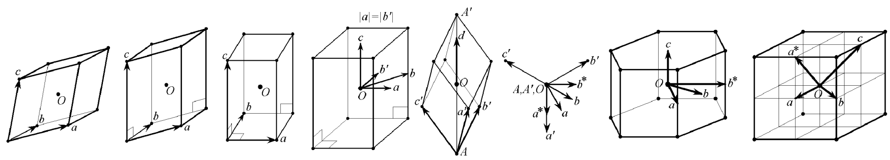

Figure 2. 7 crystal cells with vector generators $\vec{a},\vec{b},\vec{c}$: triclinic, monoclinic, orthorhombic, tetragonal, trigonal (side & top), hexagonal, cubic.

Table 2. Geometric 3D point group symbols [1] and generators with $\theta_{\vec{a},\vec{b}} = \pi/p$, $\theta_{\vec{b},\vec{c}} = \pi/q$, $\theta_{\vec{a},\vec{c}} = \pi/2$, $p,q \in \{1,2,3,4,6\}$.

Symbol	p	$\bar{p}$	pq	$\bar{p}q$	$p\bar{q}$	$\bar{p}\bar{q}$	$\overline{pq}$
Generators	$\vec{a},\vec{b}$	$\vec{a}\vec{b}$	$\vec{a},\vec{b},\vec{c}$	$\vec{a}\vec{b},\vec{c}$	$\vec{a},\vec{b}\vec{c}$	$\vec{a}\vec{b},\vec{b}\vec{c}$	$\vec{a}\vec{b}\vec{c}$

5 Spacegroups

The smooth composition with translations is best done in the conformal model [5] of Euclidean space (in the GA of $\mathbb{R}^{4,1}$), which adds two null-vector dimensions for the origin $\vec{n}_0$ and infinity $\vec{n}_\infty$

$$X = \vec{x} + \frac{1}{2}\vec{x}^2\vec{n}_\infty + \vec{n}_0, \quad \vec{n}_0^2 = \vec{n}_\infty^2 = X^2 = 0, \quad X \cdot \vec{n}_\infty = -1. \tag{9}$$

The inner product of two conformal points gives their Euclidean distance and therefore a plane equidistant from two points A, B as

$$X \cdot A = -\frac{1}{2}(\vec{x} - \vec{a})^2 \;\Rightarrow\; X \cdot (A - B) = 0, \quad m = A - B \propto \vec{p} - d\,\vec{n}, \tag{10}$$

where $\vec{p}$ is a unit normal to the plane and d its signed scalar distance from the origin. Reflecting at two parallel planes m, m' with distance $\vec{t}/2$ we get the *translation* operat*or* (by $\vec{t}$)

$$X' = m'mX\,mm' = T_{\vec{t}}^{-1} X T_{\vec{t}}, \quad T_{\vec{t}} = 1 + \frac{1}{2}\vec{t}\vec{n}. \tag{11}$$

Reflection at two non-parallel planes m, m' yields the rotation around the m, m'-intersection by twice the angle subtended by m, m'.

Group theoretically the conformal group $C(3)$ is isomorphic to $O(4,1)$ and the Euclidean group $E(3)$ is the subgroup of $O(4,1)$ leaving infinity $\vec{n}_\infty$ invariant [1]. Now general translations and rotations are represented by geometric products of vectors (versors). To study combinations of versors it is usefull to know that

$$T_{\vec{t}}\,\vec{a} = \vec{a}\,T_{\vec{t}'}, \qquad \vec{t}' = -\vec{a}^{-1}\vec{t}\,\vec{a}. \tag{12}$$

Applying these techniques we get table 3 listing monoclinic space groups and their versor generators. All this is interactively visualized in [4].

Table 3. Monoclinic space group versor generators (gen.), $T^A = T^{1/2}_{\vec{b}+\vec{c}}$, geo. = geometric, n. = name, alt. = alternative, cols. 3&4: [1]. $T_{\vec{a}}, T_{\vec{b}}, T_{\vec{c}}$ suppressed.

# [6]	Int. n. [6]	Geo. n.	Geo. gen.	Gen. [6]	Alt. gen.
3	$P2$	$P\bar{2}$	$ic = a \wedge b$		
4	$P2_1$	$P\bar{2}_1$	$i\vec{c}T^{1/2}_{\vec{c}}$		
5	$C2$	$A\bar{2}$	$i\vec{c}$, T^A		
6	Pm	$P1$	$\vec{c}$		
7	Pc	P_a1	$\vec{c}T^{1/2}_{\vec{a}}$		
8	Cm	$A1$	$\vec{c}$, T^A		
9	Cc	A_a1	$\vec{c}T^{1/2}_{\vec{a}}$, T^A		
10	$P2/m$	$P2\bar{2}$	$\vec{c}$, $i\vec{c}$	i, $i\vec{c}$	i, $\vec{c}$
11	$P2_1/m$	$P2\bar{2}_1$	$\vec{c}$, $i\vec{c}T^{1/2}_{\vec{c}}$	i, $i\vec{c}T^{1/2}_{\vec{c}}$	i, $\vec{c}T^{1/2}_{\vec{c}}$
12	$C2/m$	$A2\bar{2}$	c, $i\vec{c}$, T^A	iT^A, $i\vec{c}T^A, T^A$	i, $\vec{c}$, T^A
13	$P2/c$	$P_a2\bar{2}$	$\vec{c}T^{1/2}_{\vec{a}}$, ic	i, $i\vec{c}T^{1/2}_{\vec{a}}$	i, $\vec{c}T^{1/2}_{\vec{a}}$
14	$P2_1/c$	$P_a2\bar{2}_1$	$\vec{c}T^{1/2}_{\vec{a}}$, $i\vec{c}T^{1/2}_{\vec{c}}$	i, $i\vec{c}T^{1/2}_{\vec{a}+\vec{c}}$	i, $\vec{c}T^{1/2}_{\vec{a}+\vec{c}}$
15	$C2/c$	$A_a2\bar{2}$	$\vec{c}T^{1/2}_{\vec{a}}$, $i\vec{c}$, T^A	i, $i\vec{c}T^{1/2}_{\vec{a}}, T^A$	i, $\vec{c}T^{1/2}_{\vec{a}}, T^A$

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