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Three Vector Generation of Crystal Space Groups in Geometric Algebra

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Abstract: This paper focuses on the symmetries of crystal space lattices. All two dimensional (2D) and three dimensional (3D) point groups of 2D and 3D crystal cells are exclusively described by vectors (two in 2D, three in 3D for one particular cell) taken from the physical cells. *Geometric multiplication* of these vectors completely generates all symmetries, including reflections, rotations, inversions, rotary-reflections and rotary-inversions. We then extend this treatment to 3D space groups by including translations, glide reflections and screw rotations. We focus on the monoclinic case as an example. A software demonstration shows the *spacegroup visualizer.*
Keywords: crystal lattice, space group, geometric algebra, OpenGL, interactive software

1. Introduction

Crystallography is one of the oldest scientific occupations of mankind and of pivotal importance for exploiting the symmetry properties of materials. A convenient geometric description of crystal symmetries is e. g. vital for the prediction and description of the grain structure in a material system, which are of primary concern to material engineers [1].

Crystallography deals with the inherent geometric properties of crystals, in particular with their their symmetry transformations, geometric transformations, that consist of reflections, rotations, inversions, translations and their combinations. The classical approach introduces a set of 3D coordinate axis and expresses all positions and symmetry operations by coordinate triplets and matrices. Thus crystallography and its results traditionally become far removed from the inherent geometry of the crystal space lattice.

Our new approach is based on geometric algebra. The origins of geometric algebra go back to the successful union of quaternions (1843, Hamilton) with the Theory of Extension (1844, Grassmann) in 1872 by Clifford. Geometric algebra has been developed into a comprehensive geometric calculus for all areas of physics, and for the applied sciences, including computational geometry [4].

The left and right geometric product with a normal vector (of a mirror plane) in geometric algebra easily produces reflections. Repetition with the normal vector (of a second mirror plane) produces rotations, etc. This way all point symmetries are represented. Like in projective geometry we add two dimensions for the origin and infinity. This permits us an analogous representation of translations. The complete set of infinite geometric algebras (and subalgebras) of translations and reflections of three vectors for each type of crystal cell is in one to one correspondence with the envisaged 230 space groups. This new geometrically motivated approach is fully based on physical crystal vectors and perfectly matches geometric intuition with the powerful multivector computation methods famously invented by Hamilton, Grassmann and Clifford.

It is sufficient to select only three vectors for each elementary type of crystal cell. [3,4] These vectors describe elementary reflections and their geometric products describe all other operations: rotations, rotary reflections, inversions, and rotary inversions. This approach can be expanded to the treatment of the 230 space groups. First work with respect to developing a new fully scientific geometric algebra based space group *notation* has been undertaken by J. Holt (Honors Thesis, Univ. of Michigan Flint, US).

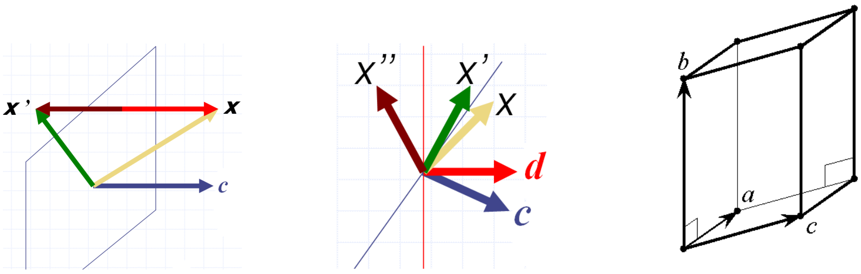

Fig. 1. Reflection and rotation at plane, monoclinic crystal cell.

2. Multiplying Vectors Produces Space Groups

The geometric product [4] of vectors a,b includes sine *and* cosine of the enclosed angle α :

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

The symmetry transformations of these cells: Simple reflections $a,b,c, \ldots$; Rotations $R=ab, \ldots$; Rotary-Reflections $Ra, \ldots$, Inversions i, Rotary-Inversions Ri. All leave the center points O invariant, form 32 point groups [4,5]. For example the *monoclinic* cell of Fig. 1 has three physical edge vectors a,b,c of unequal length. Only the angle of a and c is not 90 deg. We have the following three **point groups** [5]:

$$1\ (\mathrm{m}) = \{b, 1\}, \qquad \underline{2}\ (2) = \{R=a\wedge c= ib, 1\}, \qquad 2\underline{2} = (2/\mathrm{m}) = \{b, R, bR, 1\}. \qquad (2)$$

To find all three dimensional monoclinic **space groups** starting from the point groups 1, $\underline{2}$, $2\underline{2}$ of (2) is done by: using the translations $T(a)$, $T(b)$, $T(c)$; replacing the reflection b the glide reflection $b\ T(c/2)$; replacing the rotation $R = ib$ by the screw $ib\ T(b/2)$; and by placing an additional general element at the center of the a,b base parallelogram of the cell, i.e. using $T^C=T([a+b]/2)$ as additional translation. All these data are combined in table 2.

4. References

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Table 2. Monoclinic space group generators represented in geometric algebra (GA). Int. Tables of Crystallography (ITC) numbers and space group symbols, geometric symbols, GA generators with $T^C=T([a+b]/2)$, ITC generator choices expressed in GA, alternative inversion and reflection generator choice in GA.

No.	IName	GName	Gens.	ITC-Gens.	inv. & refl.
3	$P2$	$P\bar{2}$	$ib = a\wedge c$		
4	$P2_1$	$P\bar{2}_1$	$ibT(\frac{1}{2}b)$		
5	$C2$	$C\bar{2}$	$ib,\ T^C$		
6	Pm	$P1$	b		
7	Pc	P_c1	$bT(\frac{1}{2}c)$		
8	Cm	$C1$	$b,\ T^C$		
9	Cc	C_c1	$bT(\frac{1}{2}c),\ T^C$		
10	$P2/m$	$P2\bar{2}$	$b,\ ib$	$i,\ ib$	$i,\ b$
11	$P2_1/m$	$P2\bar{2}_1$	$b,\ ibT(\frac{1}{2}b)$	$i,\ ibT(\frac{1}{2}b)$	$i,\ bT(\frac{1}{2}b)$
12	$C2/m$	$C2\bar{2}$	$b,\ ib,\ T^C$	$i,\ ib,\ T^C$	$i,\ b,\ T^C$
13	$P2/c$	$P_c2\bar{2}$	$bT(\frac{1}{2}c),\ ib$	$i,\ ibT(\frac{1}{2}c)$	$i,\ bT(\frac{1}{2}c)$
14	$P2_1/c$	$P_c2\bar{2}_1$	$bT(\frac{1}{2}c),\ ibT(\frac{1}{2}b)$	$i,\ ibT(\frac{1}{2}(b+c))$	$i,\ bT(\frac{1}{2}(b+c))$
15	$C2/c$	$C_c2\bar{2}$	$bT(\frac{1}{2}c),\ ib,\ T^C$	$i,\ ibT(\frac{1}{2}c),\ T^C$	$i,\ bT(\frac{1}{2}c),\ T^C$