Proceedings of the International Symposium on Advanced Mechanical Engineering between Pukyong National University (Korea), University of Fukui (Japan) and University of Shanghai for Science and Technology (China), November 23-26, 2005, hosted by the School of Mechanical Engineering, Pukyong National University, Busan, Korea.

FULL GEOMETRIC DESCRIPTION OF ALL SYMMETRY ELEMENTS OF CRYSTAL SPACE GROUPS BY THE SUITABLE CHOICE OF ONLY THREE VECTORS FOR EACH BRAVAIS CELL OR CRYSTAL FAMILY

Eckhard Hitzer and Christian Perwass*

910-8507 Fukui, 3-9-1 Bunkyo, Dep. of Phys. Eng., Univ. of Fukui, Japan
URL: <http://sinai.mech.fukui-u.ac.jp/>, Email: hitzer@mech.fukui-u.ac.jp
*Department of Computer Science, Christian-Albrechts-University Kiel, Kiel 24103, Germany
URL: <http://www.perwass.de/>, Email: chp@ks.informatik.uni-kiel.de

ABSTRACT

This paper focuses on the symmetries of crystal cells and 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. The sets of vectors necessary are illustrated in drawings. We then extend this treatment to 2D and 3D space groups by including translations, glide reflections and screw rotations. For 3D space groups we focus on the monoclinic case as an example. A companion paper [15] describes corresponding interactive visualization 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 is internationally represented by the International Union of Crystallography (IUCr), which periodically edits, expands and updates the International Tables for Crystallography, Vol. A (ITC) [10].

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 intruduces 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, Sir W. Hamilton, Ireland) with the Theory of Extension (1844, Grassmann algebra, H. Grassmann, Germany) in 1872 by the talented British mathematician W. Clifford. Geometric algebra has been developed into a comprehensive geometric calculus for all areas of physics, and for the applied sciences, including computational geometry [3,6].

Traditionally three and four dimensional coordinate vectors and matrices in non-cartesian coordinate systems make it hard to relate to the constituting physical vectors and their relative orientations. Yet, 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 compares well with

matrix algebra, though rotation matrixes e.g. cannot distinguish between angles α and $2\pi-\alpha$. 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.

Theoretical research in this area has begun nearly 10 years ago in the thesis of J.D.M. Gutierrez (UNAM, Mexico 1996, supervised by J. Keller), who made a first approach to unify the disciplines of geometric algebra and crystal symmetry. We base our work on the successful attempt of D. Hestenes in [4]. He clearly showed how the 2D and 3D crystallographic point symmetries can be fully described in the geometric algebra of 3D Euclidean space. It is sufficient to select only three vectors for each elementary type of crystal cell. These vectors describe elementary reflections and their geometric products describe all other operations: rotations, rotary reflections, inversions, and rotary inversions. These symmetries can be combined without the need for a coordinate system or matrices, thus achieving a close match of mathematical description and geometric nature of crystals. He indicated that 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).

2. MULTIPLYING VECTORS

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

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

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

$$a \cdot b = (ab+ba)/2 = |a||b| \cos a, \qquad (2)$$
$$a \wedge b = (ab-ba)/2 = |a||b| \mathbf{i} \sin a. \qquad (3)$$

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 $c^{-1}=c/c^2$, $c^{-1}c=1$.)

$$x' = -c^{-1}xc \qquad (6)$$

is the reflected vector as detailed in [11]. To do a sequence of two reflections with unit normal vectors c,d simply results in

$$x'=d^{-1}c^{-1}\ x\ cd = (cd)^{-1}x\ cd, \qquad (7)$$

etc. From elementary geometry we know that two reflections at planes with normal vectors c,d enclosing the angle $\theta/2$ result in a rotation by the angle θ. A general *rot*ation operat*or* (*rotor*) is therefore the product of two vectors $R=cd$ enclosing half the angle of the final rotation.

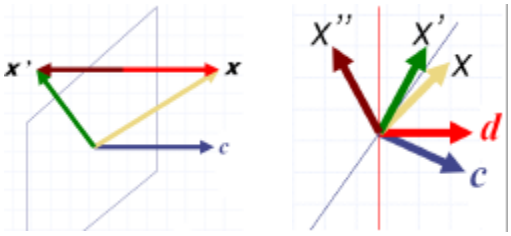

Fig 1. Left: Reflection at plane normal to a. Right: 2 reflections make 1 rotation.

A sequence of three reflections at planes with normal vectors c,d,e gives a *rotary-reflection*:

$$x'=(-1)(cde)^{-1}x\ cde, \qquad (8)$$

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 ($cde=i$), then (8) describes an *inversion:*

$$x' = (-1)(-i)\ x\ i = -x. \qquad (9)$$

The general point group transformation law is

$$x' = (-1)^p\ S^{-1}\ x\ S, \qquad (10)$$

with p = parity (even or odd) of the vector products in S. Because both S^{-1} and S are factors in (10), 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. TWO-DIMENSIONAL POINT GROUPS

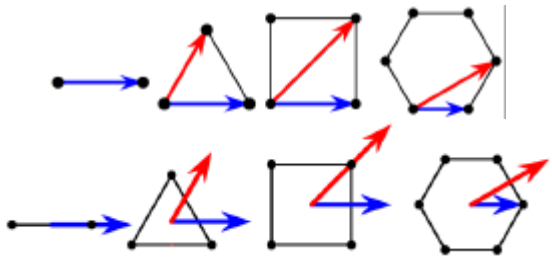

Fig. 2. Top: Regular polygons (n=2,3,4,6) with vectors *a,b*. Bottom: *a,b* shifted to centers.

Fundamental are the two-dimensional symmetries of regular polygons with n=1,2,3,4,6 corners.[4] (With n=5, no lattice can be built.) For an interactive online visualization see [8].
In general the point symmetry group of a regular polygon with n corners is generated by a side vector *a* and a vector *b* pointing to a next neighbor corner as illustrated in Fig. 2. *a,b* will enclose +180°/n. ($R^n = -1$ is equivalent to this.) Using $R=ba$, instead of $R=ab$ would generate rotations of opposite sense.
All reflections and rotations of the two-dimensional symmetry groups of regular polygons with n=1,2,3,4,6 can thus be fully and compactly represented by:

n=1: identity ±1
n=2: reflection ***a***, identity ±1
n=3: reflections ***a***, ***b***, *bR*
120° rot. $R=ab$, R^2, $R^3 = -1$ (11)
n=4: ref. ***a***, ***b***, aR^2, bR^2
90° rot. $R=ab$, R^2, R^3, $R^4 = -1$
n=6: ref. ***a***, ***b***, aR^2, bR^2, aR^4, bR^4
60° rot. $R=ab$, R^2, R^3, R^4, R^5, $R^6 = -1$.

Based on this knowledge and the notation of table 1 we can now denote the 10 point groups of the five two-dimensional crystal cells as

- Oblique 1 (1), 2 (2)
- Rectangular 1 (m), 2 (mm)
- Trigonal 3 (3m), 3 (3)
- Square 4 (4m), 4 (4)
- Hexagonal 6 (6m), 6 (6)

Where the international symbol is given in brackets. We observe that in 2D the underbar indicates a group of rotations. The group 1 only contains the identity element.

4. THREE- DIMENSIONAL POINT GROUPS

All known three-dimensional crystal lattices can be characterized by their crystal cells shown in

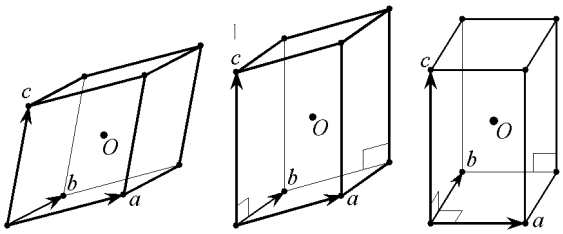

Fig. 3. Triclinic, monoclinic and orthorhombic crystal cells with invariant point centers *O*.

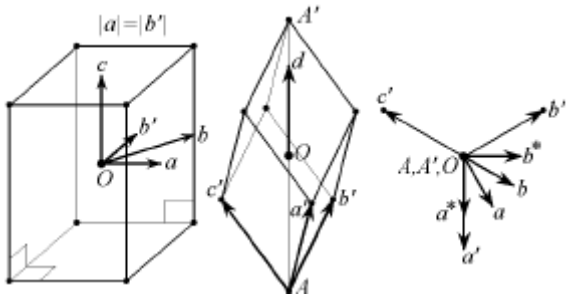

Fig. 4. Tetragonal cell, trigonal ($|a'|=|b'|=|c'|$) cell (side view and top view along *d*-axis A'OA). a^*, *a*, *b*, b^* all in paper plane perpendicular to *d*, containing *O*.

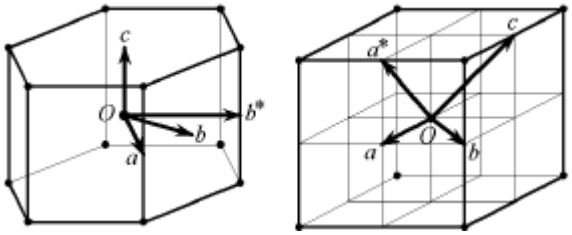

Fig. 5. Hexagonal and cubic cells.

Figs. 3,4 and 5. The symmetry transformations of these cells:

- Simple reflections
- Rotations
- Rotary-Reflections, Inversions
- Rotary-Inversions

which leave the center points *O* invariant, form 32 point groups [11,4,5,6].
For example the *monoclinic* cell of Fig. 3 has three physical edge vectors *a,b,c* of unequal length. Only the angle of *a* and *b* is not 90°. We have the following three groups [11]:

$$1\ (\mathrm{m}) = \{c,\ 1\}, \tag{12}$$
$$\underline{2}\ (2) = \{R=a\wedge b,\ 1\}, \tag{13}$$
$$2\underline{2}\ = (2/\mathrm{m}) = \{c,\ R,\ cR,\ 1\}. \tag{14}$$

where *cR* is a rotary-reflection. The geometric point group symbols 1, $\underline{2}$ and $2\underline{2}$ were introduced in [4]. The second symbol in brackets is the international symbol. In general one or two numbers p, q indicate the angles of the generating vectors (angle of *a,b*: 180?/p, angle of *b,c*: 180?/q). [4] uses overbars instead of underlines. Therefore 1 means a single reflection generating vector (*c*). $\underline{2}$ means a generating rotor *R* formed by the product of two vectors a^*,*b* at 90?

$$a^*=(a\wedge b)b,\ b \qquad (15)$$
$$R= a^*b=(a\wedge b)bb\ ?\ a\wedge b,$$

because $bb=b^2$ is only an unimportant scalar factor. $2\underline{2}$ means three generating vectors a^*,*b,c*, all at right angles (180?/2), two of which are combined to the rotor $R=a^*b$. Compare [11] for a thorough explicit treatment of all 32 point groups. A free attractive interactive visualization of high graphics quality is online available from [13].

Table 1. Geometric point group symbols [4].

Point group symbol	Generators
p	*a, b*
$\underline{\text{p}}$	*ab*
pq	*a,b,c*
$\underline{\text{p}}$q	*ab, c*
p$\underline{\text{q}}$	*a, bc*
$\underline{\text{p}}$ $\underline{\text{q}}$	*ab, bc*
$\underline{\text{pq}}$	*abc*

5. TWO-DIMENSIONAL SPACE GROUPS

The 2D space groups (also known as wallpaper groups) arise from the 2D point groups by including translations *T(a), T(b)* along the vectors *a,b.* As illustrated in Fig. 6, this leads directly to the 11 groups: p$\underline{1}$ (p1), p$\underline{2}$ (p2), p1 (pm), p2 (pmm), p$\underline{4}$ (p4), p4 (p4m), p$\underline{3}$ (p3), p3 (p3m1), p'3 (p31m), p$\underline{6}$ (p6) and p6 (p6m). For the reflection symmetries of p'3 we need to take the dual vectors $a^*=(a?\ b)a$, $b^*=(a?\ b)b$ instead of the translation vectors *a,b.* 'p' stands for *primitive* Bravais lattice. The international notation is given in brackets.

For the rectangular lattice two more groups c1 (cm) and c2 (cmm) stem from adding a general element at the *center* of the rectangle, i.e. by including the translation *T((a+b)/2).*

We obtain further four space groups p_g1 (pg), p_g2 (pmg), p_g2_g (pgg) and p_g4 (p4g) by augmenting reflections by half translations parallel to the line of reflection to become socalled glide reflections. With the geometric notation we followed suggestions of [12]. Fig. 6 shows examples of the 17 two-dimensional space lattices (wallpapers) with asymmetric general elements. It includes all generators, except the lattice translations *T(a), T(b).* The free interactive *Wallpaper Explorer* software is available from [13].

6. THREE-DIMENSIONAL SPACE GROUPS

To give an example of the way geometric algebra represents three-dimensional space groups [4,12,14] we will concentrate on the example of the *monoclinic* lattice space groups. A free, fully interactive and high graphics quality *Spacegroup Visualizer* software is available online from [13]. Its use is described in some detail in a companion paper [15].

Without loss of geometric rigor or generality, we adopt in this section the ITC [10] convention for the labeling of the edge vectors of the monoclinic cell illustrated in Fig. 7. In Fig. 7 the angle of *a,c,* is not 90 ° , whereas the angles of *a,b* and *b,c* are 90 ° angles. In general, the lengths of all three vectors are different.

Then also the labels in equations (12) to (14) need to be changed

$$1\ (\text{m}) = \{b,\ 1\}, \qquad (16)$$
$$\underline{2}\ (2) = \{R=a\wedge c,\ 1\}, \qquad (17)$$
$$2\underline{2}\ =\ (2/\text{m}) = \{b,\ R,\ bR,\ 1\}. \qquad (18)$$

A mathematical remark is, that in (17) and (18)

$$R\ =\ a\wedge c\ ?\ ib, \qquad (19)$$

where *i* represents the *inversion* in geometric algebra. (Taking the inversion to the other side gives a formula for the familiar vector cross product in 3D: $b\ ?\ a\times c\ =\ -ia\wedge c.$) We then recognize the inversion in (18)

$$bR = bib = bbi = |b|^2 i\ ?\ i. \qquad (20)$$

Inserting (19) and (20) in (17) and (18) we get a very elegant form for the monoclinic point group representations in geometric algebra

$$1\ (\mathrm{m}) = \{b,\ 1\}, \qquad (16)$$
$$\underline{2}\ (2) = \{ib,\ 1\}, \qquad (21)$$
$$2\underline{2} = (2/\mathrm{m}) = \{b,\ ib,\ i,\ 1\}. \qquad (22)$$

For constructing the 13 monoclinic space groups we can follow the same strategy as in two dimensions. The only *new* combination of rotations and translations will be the socalled *screw* transformations (in the following: *screws*). *Screws* in the monoclinic case simply consists of a 180 ° rotation around the *b*-axis followed by a half translation in the axis direction. The *screw* generator is therefore because of (19)

$$a?\ c\ T(b/2) = ib\ T(b/2) \qquad (23)$$

The *glide reflection* in the monoclinic case is given by the reflection at the plane normal to *b*, followed by a half translation in *c*. The glide reflection generator is therefore

$$b\ T(c/2). \qquad (24)$$

To find all three dimensional monoclinic space groups starting from the point groups 1, $\underline{2}$, $2\underline{2}$ of (16), (21) and (23) is done by

1. using the translations *T(a), T(b), T(c)*
2. replacing the reflection *b* the glide reflection *b T(c/2)*
3. replacing the rotation $R = a?\ c\ ?\ ib$ by the screw *ib T(b/2)*

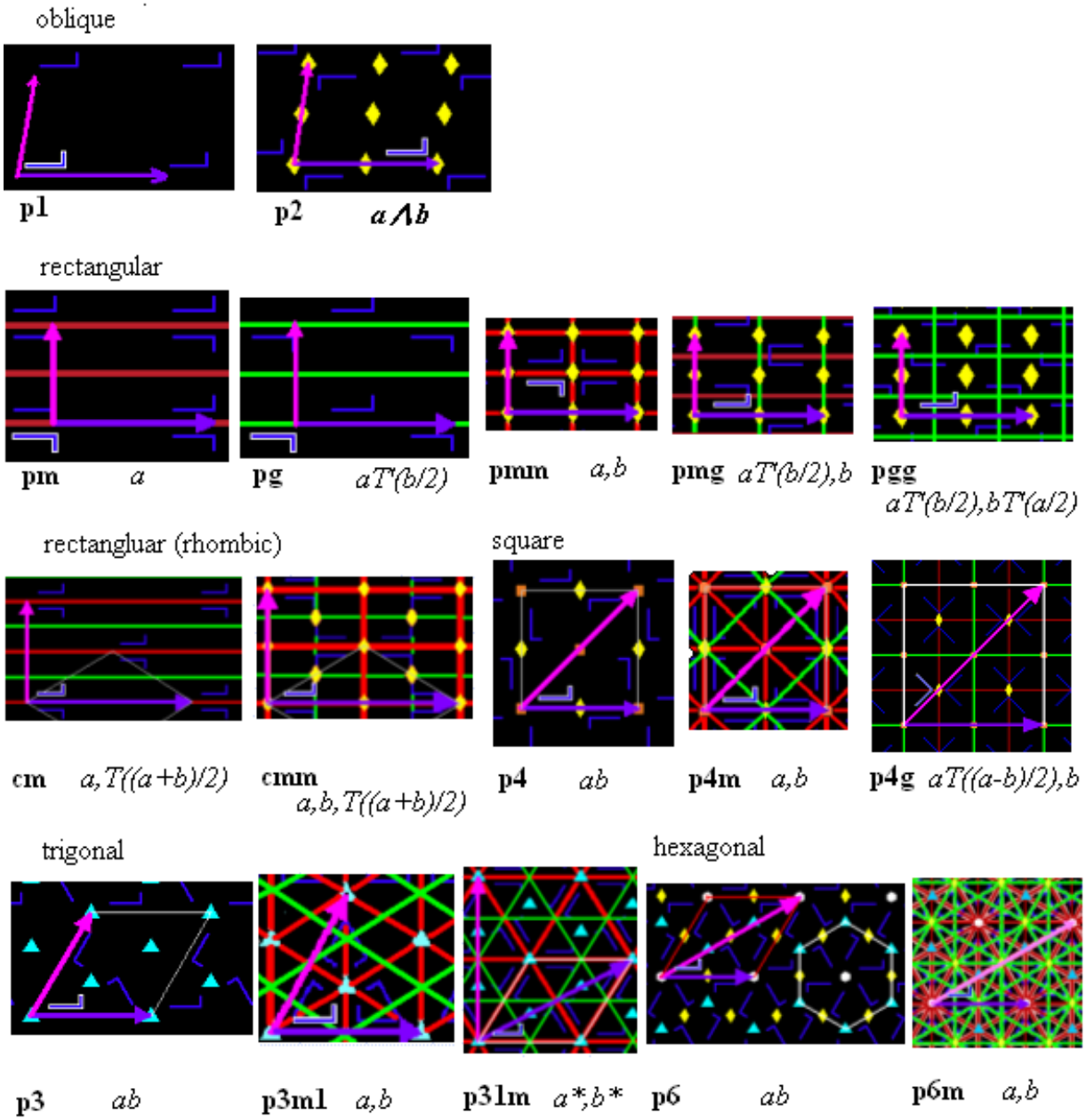

Fig. 6. 17 space group patterns (wallpapers) and generators.

4. 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.

The space groups obtained by 1. have geometric [12] symbols P1, P2, P22. The space groups obtained by 4. have symbols C1, C2, C22. The space groups obtained by 2. have symbols P_c1, P_c22 and C_c1, C_c22. The space groups obtained by 3. have symbols $P2_1$, $P22_1$, P_c22_1. It is obvious, that dropping the initial Bravais letters P or C, the lower screw index number 1 and the lower glide direction index *c* brings us straight back to the original point groups 1, 2, 22. These can be directly interpreted with table 1.

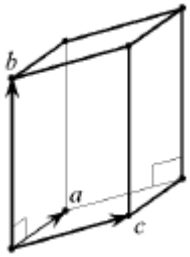

Fig. 7. Monoclinic cell with ITC labeling [10].

All these data are combined in table 2. The first column lists the monoclinic space groups by their ITC number [10]. The second column has the international symbols (abbreviated Hermann-Maugin notation). The third column lists the above explained geometric symbols with a rational geometric interpretation. The fourth column lists the generators of each monoclinic group. These generators can more or less be derived from the geometric symbol.

By convention the ITC tables [10] place the origin at a center of inversion symmetry and the inversion in the space groups derived from point group 22 is taken as generator basis element. Therefore we list in column 5 the geometric algebra generators, that correspond to the generators specified in the ITC table. An alternative set of basis generators based on inversions and reflections is listed in the last column of table 2.

It is an elegant approach to follow the ideas of projective geometry and assign an extra vector to the origin. This can also be done for points at infinity. These vectors are also special in that they square to zero, like light ray vectors in special relativity. This leads to the socalled conformal model of Euclidean space and is very advantageous for computer implementations [4,7,13,15]. Then translations can be represented by translators [16] very similar to the representation of rotations in (10).

7. CONCLUSIONS

In this paper we presented the geometric algebra

Table 2. Monoclinic space group generators represented in geometric algebra (GA). ITC numbers and ITC space group symbols [10], geometric symbols [12,14], 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	$C2/c$	$C_c2\bar{2}$	$bT(\frac{1}{2}c),\ ib,\ T^C$	$i,\ ibT(\frac{1}{2}c),\ T^C$	$i,\ bT(\frac{1}{2}c),\ T^C$

representations of point groups and space groups in two and three dimensions. In three dimensions we focused on the monoclinic space groups.

Both in two and three dimensions it was demonstrated in some detail how to derive the space groups from the corresponding point groups. We also reported suggestions for a new geometric notation for point and space groups [12], which will find a more final form in [14].

An accompanying paper [15] gives details on free, interactive OpenGL visualizations of point and space groups based on the theory introduced in the present paper.

After the completion of these basic geometric formulations for all 230 space groups, we hope to show in the future how this geometric approach leads to new insights for the analysis of crystal symmetry structures by physical methods, like diffraction patterns, for polycrystalline solidification models [1], etc.

ACKNOWLEDGEMENTS

E. Hitzer wants to thank God for his creation: “And he carried me away in the Spirit to a mountain great and high, and showed me the Holy City, Jerusalem, coming down out of heaven from God. It shone with the glory of God, and its brilliance was like that of a very precious jewel, like a jasper, clear as crystal.”[9] He further wants to thank his family for their patient support and the Cognitive Systems group of the University of Kiel for their hospitality when doing this research.

REFERENCES

1. R. Kobayashi, J. Warren, *Modeling the formation and dynamics of polycrystals in 3D*, Physica A, **356**, 2005, pp. 127-132.
2. D. Hestenes, *New Foundations for Classical Mechanics*, Kluwer, Dordrecht, 1999.
3. D. Hestenes, G. Sobczyk, *Clifford Algebra to Geometric Calculus*, Kluwer, Dordrecht, 1984.
4. D. Hestenes, *Point Groups and Space Groups in Geometric Algebra* in L. Dorst, C. Doran, J. Lasenby (eds.), Applications of Geometric Algebra in Computer Science and Engineering, Birkhaeuser, Boston, 2002, pp. 3-34.
5. J.D. M. Gutierrez, *Operaciones de simitria mediante algebra geometrica aplicadas a grupos cristalograficos*, Tesis, UNAM, Mexico 1996.
6. D. Hestenes, *Geometric Algebra for Mathematics and Physics – a Unified Language*, in E. Hitzer, R. Nagaoka (eds.), Proc. of Innovative Teaching of Mathematics with Geoemtric Algebra, Kyoto, RIMS **1378**, 2004, pp. 7-32.
7. C. Perwass et al.: *CLUCalc – A Visual Calculator*, available from www.clucalc.info, 2005.
8. E. Hitzer, *interactive Geometric Algebra illustrated by Cinderella*, available from http://sinai.mech.fukui-u.ac.jp/gcj/software/GAcindy-1.4/GAcindy.htm
9. Bible, Revelations 21, verses 10, 11, (NIV).
10. *International Tables for Crystallography*, Vol. A, Editor: T. Hahn, Springer, 2005.
11. E. Hitzer, C. Perwass: *Crystal cells in geometric algebra*, Proc. of ISAME, Fukui, Japan, 2004, pp. 290-295. Also available from sinai.mech.fukui-u.ac.jp/gcj/publications/crystalc/crystalc_abs.html
12. J. Holt, *Honors Thesis*, University of Michigan Flint.
13. C. Perwass and E. Hitzer: *Space Group Visualiser*, available from www.spacegroup.info, 2005.
14. D. Hestenes, J. Holt, in preparation.
15. C. Perwass, E. Hitzer, *Full Geometric Description of All Symmetry Elements of Crystal Space Groups by the Suitable Choice of Only Three Vectors for Each Bravais Cell or Crystal Family*, this Proc. of ISAME 2005, Busan, Korea.
16. D. Hestenes, H. Li, A. Rockwood, *New Algebraic Tools for Classical Geometry*, in G. Sommer (ed.) Geometric Computing with Clifford Algebras, Springer, Berlin, 2001.