E. Hitzer, in K. Tachibana (ed.) Tutorial on Reflections in Geometric Algebra, Lecture notes of the international Workshop for "Computational Science with Geometric Algebra" (FCSGA2007), Nagoya University, Japan, 14-21 Feb. 2007, pp. 34-44 (2007).

Tutorial on Reflections in Geometric Algebra

Eckhard Hitzer

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

ABSTRACT

This tutorial focuses on describing the implementation and use of reflections in the geometric algebras of three-dimensional (3D) Euclidean space and in the five-dimensional (5D) conformal model of Euclidean space. In the latter reflections at parallel planes serve to implement translations as well. Combinations of reflections allow to implement all isometric transformations. As a concrete example we treat the symmetries of (2D and 3D) space lattice crystal cells. All 32 point groups of three dimensional crystal cells (10 point groups in 2D) are exclusively described by vectors (two for each cell in 2D, three for one particular cell in 3D) taken from the physical cell. Geometric multiplication of these vectors completely generates all symmetries, including reflections, rotations, inversions, rotary-reflections and rotary-inversions. The inclusion of translations with the help of the 5D conformal model of 3D Euclidean space allows the full formulation of the 230 crystallographic space groups in geometric algebra. The sets of vectors necessary are illustrated in drawings and all symmetry group elements are listed explicitly as geometric vector products. Finally a new free interactive software tool is introduced, that visualizes all symmetry transformations in the way described in the main geometrical part of this tutorial.

Contents

1. INTRODUCTION

We first describe in section two how to multiply vectors in geometric algebra. This leads to the description of transformations as *versors* (products of vectors). In section three we briefly describe what is a symmetry group. In section four we show how to combine reflections as versors to give the point symmetry groups of 2D cells. These point symmetries form the basis of the socalled wallpaper

groups, i.e. space groups for symmetrically repeating infinite patterns in 2D. Space groups arise by adding translations to point groups.

Section five describes likewise how combinations of reflections into versors describe symmetry in 3D. As a particular example we again look at the 3D cells of crystalls. There are seven types. Each type needs its own choice of 3 vectors, each type has a maximum order point group, where reflections are used without restrictions. Imposing restrictions on the combination of reflections, e.g. that they are only allowed to be used in fixed pairs or fixed triples leads to subgroups. Counting all the point groups in 3D, we have 7 maximal point groups and 25 subgroups.

Section 6 finally describes how in the 5D conformal (and homogeneous) model of 3D Euclidean space translations are implemented also as versors (products of vectors). This allows to proceed from symmetries tied to an invariant point at the origin to symmetries in space. This is very useful in computer vision, robot kinematics, wherever rigid motions are involved. Our particular example are again the symmetries of crystals, now (mathematically: infinitely) extended in space. All regular crystals fall into this category, metals, minarals, semiconductor crystals, (bio-)molecular crystals, etc.

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.[1] 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.

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

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

$$ab = |a||b|(\cos\alpha + \mathbf{i}\sin\alpha), \tag{1}$$
$$(ab)c = a(bc) = abc\,, \tag{2}$$

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

$$a\cdot b = b\cdot a = (ab+ba)/2 = |a||b|\cos\alpha, \tag{3}$$
$$a\wedge b = -b\wedge a = (ab-ba)/2 = |a||b|\,\mathbf{i}\sin\alpha. \tag{4}$$

The inner product (3) yields a scalar. The outer product (4) yields a bivector, which can be pictured as the oriented area spanned by moving b along a, with magnitude $|a||b|\sin\alpha$. In general every unit $\mathbf{i}$ is a combination of the three oriented bivector sides of a unit cube:

$$\mathbf{i} = u_1 e_2e_3 + u_2 e_3e_1 + u_3 e_1e_2\,, \quad u_1^2 + u_2^2 + u_3^2 = 1. \tag{5}$$

The commutation properties of (3) and (4) 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

$$c^{-1} = c/c^2, \qquad c^{-1}c = 1\ . \tag{6}$$

A vector x to be reflected, can be written in components parallel and perpendicular to c: $x = x_{\|}+x_{\perp}$. Now $x_{\|}\wedge c=0$, because parallel vectors span no area, and $x_{\perp}\cdot c = 0$, because of perpendicularity. So we must have

$$x_{\|}c = x_{\|}\cdot c + 0 = c\cdot x_{\|} + 0 = cx_{\|}\ , \tag{7}$$
$$x_{\perp}c = 0 + x_{\perp}\wedge c = -\,0 - c\wedge x_{\perp} = -\,cx_{\perp}. \tag{8}$$

Reflection only changes the sign of $x_{\|}$, compare Fig. 1.

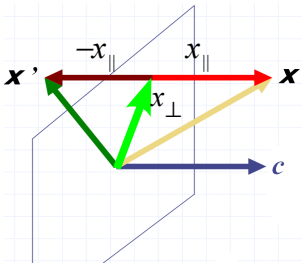

Fig. 1. Reflection of vector x at plane normal to vector c.

Therefore we get for the reflected vector x'

$$x' = -x_{\|}+x_{\perp} = -c^{-1}c(x_{\|}-x_{\perp}) = -\,c^{-1}(cx_{\|}-cx_{\perp}) = -\,c^{-1}(x_{\|}c+x_{\perp}c) = -\,c^{-1}(x_{\|}+x_{\perp})c = -\,c^{-1}xc\ , \tag{9}$$

where (7) and (8) have been applied in the fourth step.

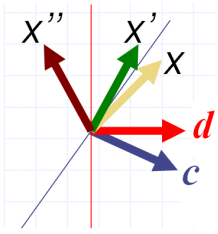

Fig. 2. Sequence of two reflections at lines (planes) with normal vectors c,d .

To do a sequence of two reflections with normal vectors c,d as in Fig. 2 simply results in

$$x' = d^{-1}c^{-1}\,x\,cd = (cd)^{-1}x\,cd = R^{-1}\,x\,R\ ,\ \ R \equiv cd. \tag{10}$$

The two minus signs have canceled.

$$(cd)^{-1} = d^{-1}c^{-1}\ , \tag{11}$$

because with the associativity of the geometric product and with repeated application of (6) we have

$$d^{-1}c^{-1}\,(cd) = \ d^{-1}(c^{-1}c)d = d^{-1}d\ = 1. \tag{12}$$

Equation (12) can indeed be generalized for versors (products of finite numbers of vectors) to

$$(cdef\ldots)^{-1} = \ldots f^{-1}e^{-1}d^{-1}c^{-1}\ . \tag{13}$$

The two reflections at planes with normal vectors c,d enclosing the angle $\theta/2$ result in a rotation by angle θ. To understand this please look at Fig. 2. The angles between the normal vectors c,d and between the lines (planes) of reflection are both equal to $\theta/2$. Let us call the angle between x and x': 2α. We further call the angle between x' and x'': 2β. Observing the figure we see that $\theta/2 = \alpha+\beta$. Hence the total angle between x and x'': $2\alpha+2\beta = \theta$. A general (spinorial) *rot*ation operat*or* (*rotor*) is therefore

the product of two vectors $R=cd$ enclosing half the angle of the final rotation. This description of rotations exactly corresponds to the description by quaternions, because for unit vectors c,d we have

$$c \cdot d = \cos \theta/2 \qquad \text{and} \qquad c \wedge d = \mathbf{i} \sin \theta/2 \tag{14}$$

where **i** is the unit area of the c,d plane, the plane of rotation. $c \cdot d$ corresponds to the scalar part of the quaternion and the bivector $c \wedge d$ corresponds to the pure quaternion part, where the quaternion units $\boldsymbol{i}, \boldsymbol{j}, \boldsymbol{k}$ correspond to e_2e_3 , e_3e_1 , e_1e_2 as in (5).

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

$$x' = (-1)(cde)^{-1} x\, cde, \tag{15}$$

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 ($cde = i = e_1e_2e_3$), then (15) describes an *inversion:*

$$x' = (-1)^3 i^{-1} x\, i = (-1) i^{-1} i\, x = -x. \tag{16}$$

The general transformation law for all orthogonal transformations is therefore

$$x' = (-1)^p S^{-1} x\, S, \qquad S = \lambda S\,, \forall \lambda \in R \setminus 0 \tag{17}$$

with p = parity (even or odd) of the vector products (versors) in S. Because both S^{-1} and S are factors in (17), 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. Symmetry *groups*

A reflection about the diagonal of a square leaves the square as a whole invariant. It is therefore a symmetry (operation) of the square. A reflection about the other diagonal is also a symmetry operation. Combining the two reflections gives a resulting rotation by 180 degrees around the center of the square, as can easily be checked. In general the combination of symmetry operations of an object yields another symmetry operation. We say the set G of all symmetry operations $\{R,S,T, \ldots\}$ of an object is closed:

$$\forall R, S \in G \quad \Rightarrow \quad RS \in G \tag{18}$$

The combination of symmetry operations obeys the following rules:

$$\forall R, S, T \in G \quad \Rightarrow \quad (RS)T = R(ST) \tag{19}$$

For example rotations in two dimensions clearly obey (19). Leaving an object unchanged (e.g. by rotating it with the full angle 360°) we get the identity operation 1, which can always be performed before or after any other symmetry operation

$$\forall S \in G \quad \Rightarrow \quad \exists\ 1 \in G: \quad 1S = S1 = S. \tag{20}$$

Finally when we reflect an object along a line (plane) of symmetry, we can always reflect it back, when we rotate it, we can always rotate it back, ... Every symmetry has an inverse

$$\forall S \in G \quad \Rightarrow \quad \exists_1 S^{-1} \in G: \quad S^{-1}S = S\,S^{-1} = 1. \tag{21}$$

The properties (18) to (21) are needed to define a *group* mathematically. The set G of all symmetry operations of an object is therefore said to to form the *symmetry group* of that object. The set of all translations of a lattice by lattice vectors (connecting lattice points) is such a symmetry group. In the case of a triclinic lattice (angles and lattice cell edges completely free, unsymmetric molecules) this is already the full symmetry group of the lattice, the first socalled 3D *space group*.

Symmetry groups of e.g. crystals are usually represented by matrices, necessitating the introduction of coordinates. Yet an object and its symmetries exist with and without coordinates. Geometric algebra offers an *invariant* way (independent of coordinates) to describe symmetry. In the following we will demonstrate this for crystal cells and crystal lattices.

4. Combinations of reflections in two dimensions (2D)

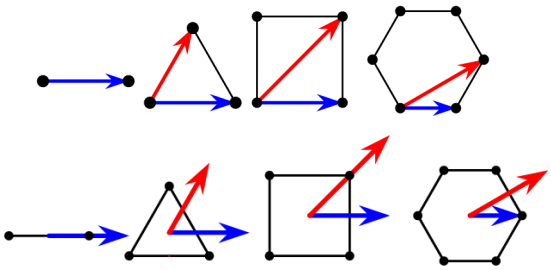

Fig. 3. Top: Regular polygons (n=2,3,4,6) with vectors a,b. Bottom: a,b shifted to centers.

Fundamental are the two-dimensional (2D) symmetries of regular polygons with n = 2,3,4,6 corners.[4] In order to later construct a 2D repetitive pattern (like a wallpaper), of regular polygons we need to exclude other values of n. (With n=5, no lattice can be built without gaps. For n>6 no lattice can be built without overlaps.) 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. 3. a,b will enclose $+180^\circ/n$. (The condition $R^n = -1$ 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 = 2,3,4,6 can thus be fully and compactly represented by:

- general *oblique* figure (cell): identity ±1.

For general oblique figure (cell) with asymmetric unit there is no symmetry apart from the identity.

- n = 2: reflection $\boldsymbol{a}$; identity ±1.

For n=2 we have two points at $x_1=+a$, and $x_2=-a$. The two symmetry operations are the identity and the reflection at the plane perpendicular to a:

$$x' = -a^{-1} x\, a. \tag{22}$$

Instead of the reflection, we can also use a 180° rotation with the help of any vector b perpendicular (+90°=180°/2) to a:

$$x' = b^{-1}a^{-1} x\, ab = (ab)^{-1} x\, (ab) = R^{-1} x\, R\,. \tag{23}$$

Compare Fig. 3.

- n = 3: reflections $\boldsymbol{a}$, $\boldsymbol{b}$, bR ; rotations $R = ab$, R^2, $R^3 = -1$.

For n = 3 we have a regular triangle centered at the origin as in Fig. 3. The two vectors a,b now enclose +60° = 180°/3. The three symmetry rotations (120°, 240°, 360°) in positive sense are:

$$R=ab,\ \ R^2=(ab)^2,\ \ R^3 = (ab)^3 = -1. \tag{24}$$

The three symmetry reflections (6) are at the three lines through the center and the corners:

$$x' = -a^{-1} x\, a, \quad x' = -a^{-1}R^{-1} x\, Ra, \quad x' = -a^{-1}R^{-2} x\, R^2 a. \tag{25}$$

- $n = 4$: ref. ***a***, ***b***, aR^2, bR^2 ; rotations $R = ab$, R^2, R^3, $R^4 = -1$.

For $n = 4$ we have a square centered at the origin (Fig. 1.) Vectors a, b enclose $+45^\circ = 180^\circ/4$. The four symmetry rotations (90°,180°,270°,360°) in positive sense are:

$$R = ab,\ R^2 = (ab)^2,\ R^3 = (ab)^3,\ R^4 = (ab)^4 = -1. \tag{26}$$

The four symmetry reflections (6) are at lines perpendicular to vectors a, b, $R^{-1}aR$, $R^{-1}bR$.

- $n = 6$: ref. ***a***, ***b***, aR^2, bR^2, aR^4, bR^4 ; rotations $R = ab$, R^2, R^3, R^4, R^5, $R^6 = -1$.

For n=6 we have a regular hexagon centered at the origin as in Fig. 1. Vectors a, b enclose $+30^\circ = 180^\circ/6$. The six symmetry rotations (60°,120°,180°,240°,300°,360°) in positive sense are:

$$R=ab,\ R^2,\ R^3,\ R^4,R^5, \text{ and } R^6 = -1. \tag{27}$$

The six symmetry reflections are at lines perpendicular to vectors a,b,aR^2,bR^2,aR^4,bR^4.

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

Symbol	$p=1$	p	$\bar{p}$	pq	$\bar{p}q$	$p\bar{q}$	$\bar{p}\bar{q}$	$\overline{pq}$
Generators	$\vec{a}$	$\vec{a},\vec{b}$	$\vec{a}\vec{b}$	$\vec{a},\vec{b},\vec{c}$	$\vec{a}\vec{b},\vec{c}$	$\vec{a},\vec{b}\vec{c}$	$\vec{a}\vec{b},\vec{b}\vec{c}$	$\vec{a}\vec{b}\vec{c}$

Table 1 gives an overview of the geometric notation (based on versors) for point groups. Based on table 1 we can now denote the 10 point groups of the five two-dimensional crystal cells as in the following table 2.

5. Reflections in three dimensions (3D)

All known three-dimensional crystal lattices can be characterized by seven unit crystal cells shown in Figs. 4, 5 and 6. The symmetry transformations of these cells, which leave the center points O invariant, form groups of symmetry operations, called *point groups* (discrete subgroups of $SO(3)$). Each of the seven unit cells has a highest (cardinality) symmetry group, called holohedry. The other 25 groups are nothing but subgroups of these 7 holohedries. So altogether there are 32 point groups associated with seven crystal classes.[4,5,6]

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	$\bar{3}$	4m	$\bar{4}$	6m	$\bar{6}$

Table 2. Geometric and international notation for point groups. The international symbol is given in brackets. We observe that in two dimensions (2D) the overbar indicates a group of rotations. The group $\bar{1}$ only contains the identity element.

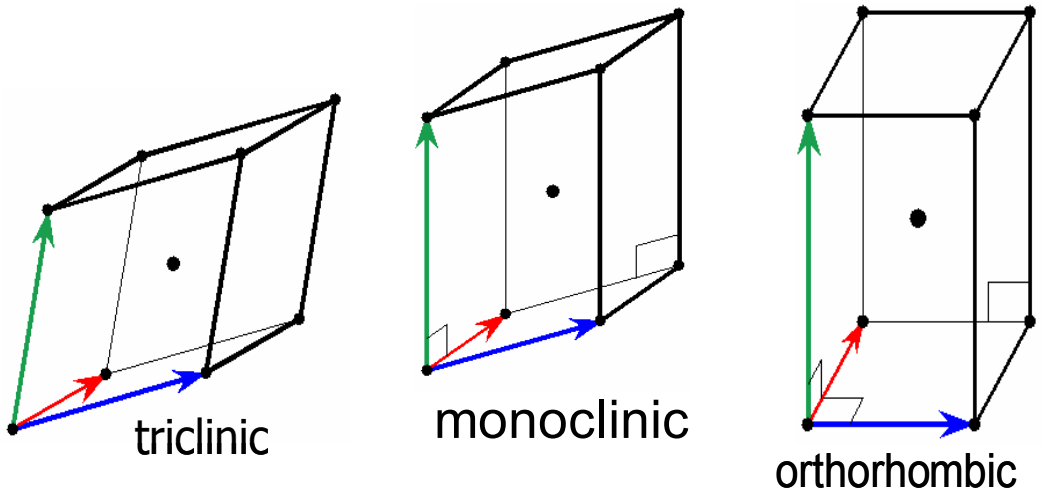

Fig. 4. Triclinic, monoclinic and orthorhombic crystal cells with invariant point centers *O*. The three vectors are actually attached to *O* in order to generate the respective point group symmetries.

As in two dimensions we can find three vectors *a,b,c* in each cell that describe reflection symmetries. The lengths of these vectors will only matter later, when we include translations to fill space and produce 3D lattices. What now matters are their relative directions. The angles are characterized by the index *q* for the angle(*a,b*), and by *q* for the angle(*b,c*). Geometric considerations (positivity of the spherical excess of a sperical triangle) lead to the conclusion that the third angle will always be 90° (index 2 for 90°=180°/2). The geometric symbols of 3D point groups follow table 1: *pq*2, but because the third index 2 is always present, it is mostly omitted: *pq*. These two numbers combined with overbars as in table 1 characterize all 32 point groups. Naturally the holohedries have less overbars, because overbars introduce restrictions to the independent use of reflections. Again the groups will be versor groups, all generators consisting only of products of the vectors *a,b,c*. The geometric meaning and the geometric algebra calculations with these symmetry elements become therefore straightforward and manifestly coordinate independent. A free interactive script for full 3D point group visualization is available for download from www.spacegroup.info .

5.1 Triclinic cell symmetry

The *triclinic* cell of Fig. 4 has three sides of unequal lengths and 3 unequal non-orthogonal angles. The only two symmetry operations are inversion *i* and identity 1, giving the groups:

$$\overline{22} \;= C_i = \{\, i = a\wedge b\wedge c = e_1e_2e_3,\; 1\}, \tag{28*}$$

$$\bar{1} \;= C_1 = \{1\}. \tag{29}$$

With the asterisk in (28*) we indicate that this group is a holohedry (= *). The group symbol $\overline{22}$ of (28*) was introduced in [4], it is equivalent to chosing 3 orthogonal vectors *a, b', c'* (with angles 180°/2) multiplied to give *i*. For using the non-orthogonal edge vectors *a,b,c,* we need to replace $i=a\wedge b\wedge c$ in (16). The second symbol is always the socalled Schoenflies symbol, frequently used in crystallography and solid state physics.

5.2 Monoclinic cell symmetry

The *monoclinic* cell of Fig. 2 has edge vectors *a,b,c* of unequal length. Only the angle between *a* and *b* is not 90°. We have the following three groups:

$$\bar{2} \;= C_2 = \{\, R = a\wedge b,\; 1\}, \tag{30}$$

$$1 = C_S = \{\, c,\, 1 \,\}, \tag{31}$$
$$2\bar{2} = C_{2h} = \{\, c,\, R,\, cR = i,\, 1 \,\}, \tag{32*}$$

where cR is again the inversion i.

5.3 Orthorhombic cell symmetry

The *orthorhombic* cell of Fig. 4 has orthogonal edge vectors a,b,c of generally unequal length. We now get the three symmetry groups:

$$\bar{2}\bar{2} = V = \{\, ab,\, bc,\, ac,\, 1 \,\}, \tag{33}$$
$$2 = C_{2v} = \{\, a,\, b,\, ab,\, 1 \,\}, \tag{34}$$
$$22 = V_h = \{\, a,\, b,\, c,\, ab,\, bc,\, ac,\, abc,\, 1\}. \tag{35*}$$

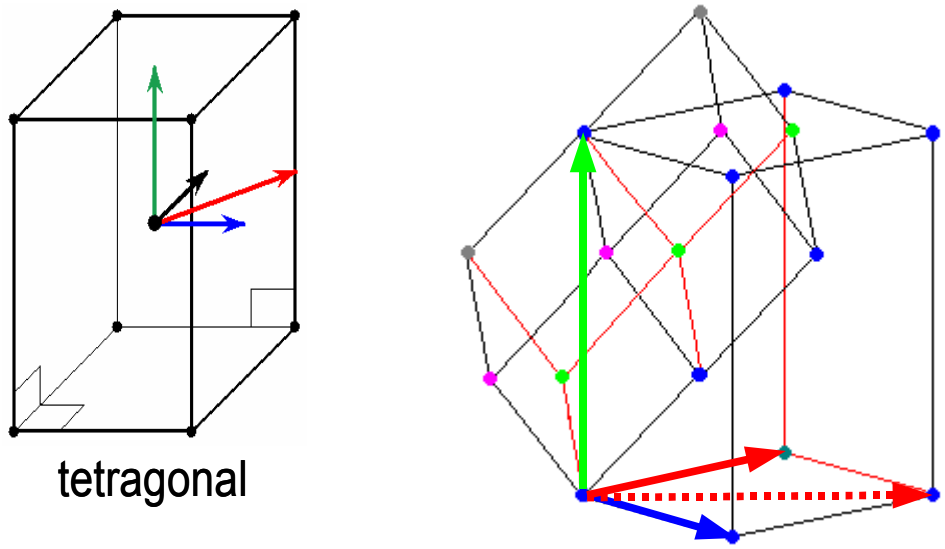

Fig. 5. Tetragonal cell, trigonal lattice cell (rhombohedral in hexagonal R) containing *O*.
(Hexagonal cell: http://www.uwgb.edu/dutchs/symmetry/rhombo-lattice.htm)

5.4 Tetragonal cell symmetry

In the *tetragonal* cell of Fig. 5 two of the orthogonal edge vectors a,b',c have equal length ($|a|=|b'|$), forming the base square. We gain a 4-fold rotation symmetry around the c-axis. To generate the symmetry groups we choose a vector $b=(a+b')/2$ pointing to a corner of the a,b'-square (compare the square in Fig. 3 in 2D). The angle of a and b will therefore be 45°=180°/4. Defining the 90° rotation generator

$$R = ab, \tag{36}$$

the symmetry groups obtained are now:

$$4 = C_4 = \{\, R,\, R^2,\, R^3,\, R^4 = 1 \,\}, \tag{37}$$
$$42 = S_4 = \{\, abc = Rc,\, (Rc)^2 = R^2,\ (Rc)^3 = R^3c,\, (Rc)^4 = 1 \,\}, \tag{38}$$
$$\bar{4}2 = C_{4h} = \{\, R,\, R^2,\, R^3,\, 1,\ c,\, Rc,\, R^2c,\, (Rc)^3 = R^3c \,\}, \tag{39}$$
$$\bar{4}\bar{2} = D_4 = \{\, R,\, R^2,\, R^3,\, 1,\ bc,\, Rbc,\, R^2bc,\, R^3bc \,\}, \tag{40}$$
$$4 = C_{4v} = \{\, a,\, b,\, aR^2,\, bR^2,\, R,\, R^2,\, R^3,\, 1\}, \tag{41}$$
$$4\,2 = V_d = \{\, a,\, bc,\, abc = Rc,\, (Rc)^2 = R^2,\, R^3c,\ aR^2 = bab,\, a(Rc)^3 = bR^2c,\, 1 \,\}, \tag{42}$$
$$42 = D_{4h} = \{\, a,\, b,\, aR^2,\, bR^2,\, c,\ \ R,\, R^2,\, R^3,\, 1,\ \ bc,\, ac,\, aR^2c,\, bR^2c,\ \ Rc,\, R^2c = i,\, R^3c \,\}. \tag{43*}$$

The holohedry 42 of (43*) again contains all other groups (37)-(42) as subgroups. (43*) lists from left

to right: *five* reflections, *four* rotations (90˚,180˚,170˚,360˚), *four* 180˚ rotations and *three* rotary-reflections, with R^2c equal the inversion, altogether the point group 42 has 12 elements. In (37)-(43*) some algebraic identities are inserted, in order to ease the recognition of the subgroup relationships.

5.5 Trigonal cell symmetry

The *trigonal (rhombohedral)* cell of Fig. 5, can be visualized as a cube stretched along one space diagonal *c,* this direction is conventionally called rhombohedral axis. The vectors *a, b* have the same lengths and subtend the able 60°= 180°/3, giving rise to 2×60°= 120° rotations. The holohedry $6\bar{2}$ is actually formed with diagonal vector b^* of the rhombic base of the hexagonal cell indicated in Fig. 5 as dashed vector. Defining the 60° rotary-reflection R_r , and the 120° rotation R as

$$R_r = ab^*c\,, \qquad R = R_r^2 = (ab^*)^2 = ab\,, \tag{44}$$

the holohedry of the trigonal cell is:

$$6\bar{2} = D_{3d} = \{a, aR_r^2, aR_r^4, b^*c, R_r^2b^*c, R_r^4b^*c, R_r, R_r^3=i, R_r^5=(ab^*)^5c, R_r^2=(ab^*)^2, R_r^4=(ab^*)^4, 1\}. \tag{45*}$$

(45*) lists from left to right: *three* reflections, *three* 180˚ rotations, *three* rotary-reflections (the second equals the inversion), and *three* rotations (120˚,240˚,360˚), altogether 12 elements. $6\bar{2} = D_{3d}$ has the following four subgroups:

$$\bar{6}\bar{2} = C_{3i} = \{R_r, R_r^2, R_r^3 = i, R_r^4, R_r^5, 1\}, \tag{46}$$
$$\bar{3}\,2 = D_3 = \{R = ab, R^2, R^3 = -1, bc, Rbc = ac, R^2bc = abac\}, \tag{47}$$
$$3 = C_{3v} = \{a, b, bab, R = ab, R^2, R^3\}, \tag{48}$$
$$3 = C_6 = \{R = ab, R^2, R^3\}. \tag{49}$$

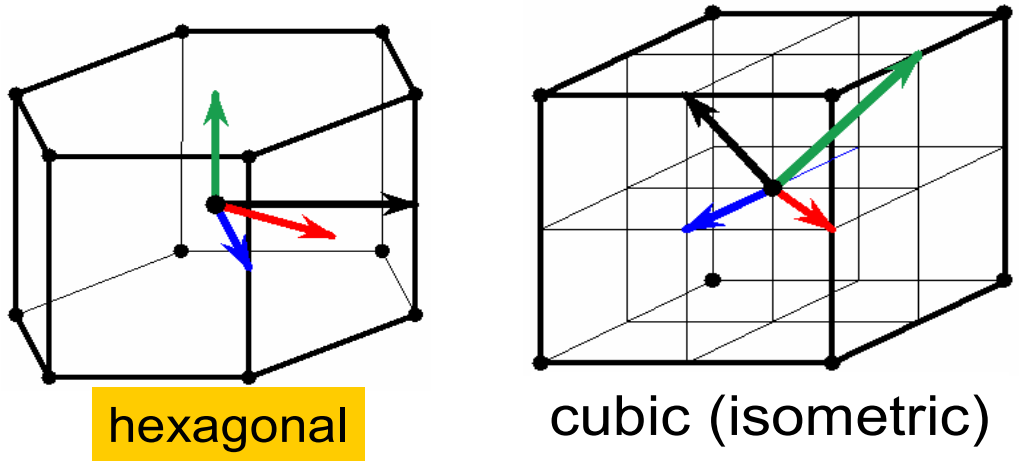

Fig. 6. Hexagonal and cubic cells.

5.6 Hexagonal cell symmetry

For the *hexagonal* cell we define like in Fig. 6 two vectors *a* and *b* (at 30˚=180˚/6 angle) and for convenience an extra vector $b^*=bab$ (at 60˚ angle to *a*). The vertical vector is *c*. With

$$R = ab\,,\ Rc = cR\,,\ R^2 = ab^* \tag{50}$$

The hexagonal holohedry is now

$$\begin{aligned} 62 = D_{6h} = \{&a, b, aR^2, bR^2, aR^4, bR^4,\\ &R, R^2, R^3, R^4, R^5, 1,\\ &c, cR, cR^2, cR^3 = i, cR^4, cR^5,\\ &ac, bc, acR^2, bcR^2, acR^4, bcR^4\}. \end{aligned} \tag{51*}$$

The holohedry 62 of (51) contains line by line: six reflections, six rotations (60˚,120˚,180˚,240˚,300˚, 360˚), six rotary-reflections, and six 180˚ rotations, altogether there are 24 elements. The hexagonal holohedry 62 has the following six subgroups:

$$\bar{6}2 = C_{6h} = \{ R, R^2, R^3, R^4, R^5, 1, \quad c, cR, cR^2, cR^3, cR^4, cR^5 \} , \tag{52}$$
$$\bar{6}\bar{2} = D_6 = \{R, R^2, R^3, R^4, R^5, 1, \quad bc, Rbc, R^2bc, R^3bc, R^4bc, R^5bc \}, \tag{53}$$
$$6 = C_{6v} = \{ R, R^2, R^3, R^4, R^5, 1, \quad a, b, aR^2, bR^2, aR^4, bR^4\} , \tag{54}$$
$$6 \_= C_3 = \{ R, R^2, R^3, R^4, R^5, 1 \} , \tag{55}$$
$$32 = D_{3h} = \{a , b^* = bR = aR^2, aR^4 = b^*R^2 = b^*ab^*, R^2, R^4, 1, \quad c, R^2c, R^4c, ac, b^*c = acR^2 , acR^4 \}, \tag{56}$$
$$\bar{3}2 = C_{3h} = \{ R^2 = ab^* , R^4, 1, \quad c, R^2c, R^4c \} . \tag{57}$$

For the group $\bar{6}\bar{2}$ it is interesting to note that:

$$Rbc = ac, \quad R^2bc = bcR^4, \quad R^3bc = R^2ac = acR^4, \quad R^4bc = bcR^2, \quad R^5bc = R^4ac = acR^2. \tag{58}$$

5.7 Cubic (isometric) cell symmetry

For the *cubic* crystal cell of Fig. 6 we define the three vectors *a,b,c,* such that *a* points to the middle of a side square face, *b* and *c* point to the middle of two edges, and the angles are 45˚ between *a* and *b,* 60˚ between *b* and *c,* and 90˚ between between *c* and *a.* We further define another edge middle vector $a^* = abcba$. a^*,b,c all have mutual angles of 60˚. The cubic holohedry has 48 elements:

$$\begin{aligned} 43 = O_h = \{ & a,b,c, bab, cbabc, \ (ab)^2c(ba)^2, \ bcb, a^* = abcba, aba , \\ & i = (ab)^2cbabc , \ 1, \\ & ab, (ab)^2, (ab)^3, babc, (babc)^2, (babc)^3, a^*a=abcb, \ (a^*a)^2, \ (a^*a)^3, \\ & ic, \ ib, \ ibcb=a^*bab, \ ac, \ ia^*=babcbc, \ iaba=bcbabc , \\ & cbcaba=abci, \ abacbc=(abc)^2, \ (a^*b)^2, \ a^*b, \ acba, \ abca, \ bc, \ (bc)^2 , \\ & abi, \ (ab)^3i, \ babci, \ (babc)^3i, \ a^*ai, \ (a^*a)^3i , \\ & cbcabai=abc, \ abacbci=(abc)^2i, \ (a^*b)^2i, \ a^*bi , \ acbai, \ abcai, \ bci, \ (bc)^2i \ \} . \end{aligned} \tag{59*}$$

The 1st line of (59*) are *nine* reflections, the 2nd line the inversion and identity, the 3rd line *three triples* of rotations by (90˚,180˚,270˚), the 4th line *six* 180˚ rotations, the 5th line *four pairs* of rotations by (120˚,240˚) around the four space diagonals, the 6th line *three pairs* of rotary-inversions, and the 7th line *four pairs* of rotary-inversions around the four space diagonals.

Transformation				
reflections	$\boldsymbol{a} = e_1$, e_2 , e_3	$\boldsymbol{b}=e_1+e_2$, $\boldsymbol{c}=e_2+e_3$, e_1+e_3	e_3-e_2 , e_3-e_1, e_1-e_2	
inversion, identity	$i = e_1e_2\, e_3$	1		
rotations (90˚, 180˚, 270˚)	$1 \pm e_2e_3$, e_2e_3	$1 \pm e_3e_1$, e_3e_1	$1 \pm e_1e_2$, e_1e_2	
180˚ rotations	$e_1e_2 \pm e_3e_1$	$e_2e_3 \pm e_3e_1$	$e_1e_2 \pm e_2e_3$	
120˚, 240˚ space diagonal rots.	$1 \pm (e_{12}+e_{23}+e_{31})$	$1 \pm (e_{12}-e_{23}+e_{31})$	$1 \pm (-e_{12}+e_{23}+e_{31})$	$1 \pm (e_{12}+e_{23}-e_{31})$
90˚, 270˚ rot.-invs.	$i \pm e_1$	$i \pm e_2$	$i \pm e_3$	
120˚,240˚ rot.-invs.	$i \pm (e_1+e_2+e_3)$	$i \pm (-e_1+e_2+e_3)$	$i \pm (e_1+e_2-e_3)$	$i \pm (e_1-e_2+e_3)$

Table 3. Point group 43 in terms of orthonormal basis $\{e_1, \ e_2 , \ e_3\}$. Bivectors specify rotation planes.

It is very revealing to introduce rewrite (59*) in terms of the orthonormal basis $\{e_1,\ e_2\ ,\ e_3\}$, as in table 3, where bivectors specify rotation planes and vectors specify rotation axis.

Table 4 gives the same symmetry operators, emphasizing the use of axis vectors. A rotation plane bivector U and its axis vector u are related by

$$U = iu\ ,\quad u = -iU\ , \tag{60}$$

but because of (17) the minus sign in (60) is not really substantial.

The cubic holohedry 43 of (59*) has the following subgroups:

$$\begin{aligned} 4\bar{3} \;&= T_h = \{a,\ bab,\ cbabc,\ i,\ 1,\ (ab)^2,\ (babc)^2,(a^*a)^2,\\ &\quad abci,\ (abc)^2,\ (a^*b)^2,\ a^*b,\ acba,\ abca,bc,(bc)^2,\\ &\quad abc\ ,(abc)^2i,\ (a^*b)^2i,\ a^*bi,\ acbai,\ abcai,\ bci,\ (bc)^2i\}\\ &= \{e_1,\ e_2\ ,\ e_3\ ,\ i,\ 1,\ e_2e_3,\ e_3e_1,\ e_1e_2,\\ &\quad 1\pm i(e_1+e_2+e_3),\ 1\pm i(-e_1+e_2+e_3),\ 1\pm i(e_1+e_2-e_3),\ 1\pm i(e_1-e_2+e_3),\\ &\quad i\pm(e_1+e_2+e_3),\ i\pm(-e_1+e_2+e_3),\ i\pm(e_1+e_2-e_3),\ i\pm(e_1-e_2+e_3)\}\ , \end{aligned} \tag{61}$$

$$\begin{aligned} \bar{4}\bar{3} \;&= O = \{ab,\ (ab)^2,\ (ab)^3,\ babc,\ (babc)^2,\ (babc)^3,\ a^*a,\ (a^*a)^2,\ (a^*a)^3,\ 1,\\ &\quad ic,\ ib,\ ibcb,\ ac,\ ia^*,\ iaba\ ,\\ &\quad abci,\ (abc)^2,\ (a^*b)^2,\ a^*b,\ acba,\ abca,\ bc,\ (bc)^2\}\\ &= \{\ (1+ie_k)^m,\ \ k,m = 1,2,3\ \}\\ &\quad \cup\ \{\ (e_3\pm e_2)i,\ (e_1\pm e_2)i,\ (e_3\pm e_1)i,\\ &\qquad 1\pm i(e_1+e_2+e_3),\ 1\pm i(-e_1+e_2+e_3),\ 1\pm i(e_1+e_2-e_3),\ 1\pm i(e_1-e_2+e_3)\ \}\ , \end{aligned} \tag{62}$$

Transformation				
reflections	$\boldsymbol{a}\ = e_1,\ e_2\ ,\ e_3$	$\boldsymbol{b}=e_1+e_2,\ \boldsymbol{c}=e_2+e_3,\ e_1+e_3$	$e_3-e_2\ ,\ e_3-e_1,\ e_1-e_2$	
inversion, identity	$i = e_1e_2\ e_3$	1		
90°,180°,270° rotations (m =1,2,3)	$(1+ie_1)^m$	$(1+ie_2)^m$	$(1+ie_3)^m$	
180° rotations	$(e_3\pm e_2)i$	$(e_1\pm e_2)i$	$(e_3\pm e_1)i$	
120°, 240° space diagonal rots.	$1\pm i(e_1+e_2+e_3)$	$1\pm i(-e_1+e_2+e_3)$	$1\pm i(e_1+e_2-e_3)$	$1\pm i(e_1-e_2+e_3)$
90°, 270° rot.-invs.	$i\pm e_1$	$i\pm e_2$	$i\pm e_3$	
120°,240° rot.-invs.	$i\pm(e_1+e_2+e_3)$	$i\pm(-e_1+e_2+e_3)$	$i\pm(e_1+e_2-e_3)$	$i\pm(e_1-e_2+e_3)$

Table 4. Point group 43 in terms of orthonormal basis $\{e_1,\ e_2\ ,\ e_3\}$. Emphasize on *axis* vectors.

$$\begin{aligned} 33 = T_d = \{&b,\ c,\ (ab)^2c(ba)^2,\ cbc,\ a^*,\ aba,\\ &1,\ (ab)^2,\ (babc)^2,\ (a^*a)^2,\\ &abci,\ (abc)^2,\ (a^*b)^2,\ a^*b,\ acba,\ abca,\ bc,\ (bc)^2,\\ &abi,\ (ab)^3i,\ babci,\ (babc)^3i,\ a^*ai,\ (a^*a)^3i\}\\ =\{&e_1\pm e_2,\ e_2\pm e_3,\ e_1\pm e_3\ ,\\ &1,\ e_2e_3,\ e_3e_1,\ e_1e_2,\\ &1\pm i(e_1+e_2+e_3),\ 1\pm i(-e_1+e_2+e_3),\ 1\pm i(e_1+e_2-e_3),\ 1\pm i(e_1-e_2+e_3)\ \}\\ \cup\ \{&i\pm e_k,\ k=1,2,3\}\ , \end{aligned} \tag{63}$$

$\bar{3}\,\bar{3}$ $= T = \{ 1, (ab)^2, (babc)^2, (a^*a)^2,\ \ abci, (abc)^2, (a^*b)^2, a^*b, acba, abca, bc, (bc)^2\}$
$= \{1,\ e_2e_3, e_3e_1, e_1e_2, 1\pm i(e_1+e_2+e_3), 1\pm i(-e_1+e_2+e_3), 1\pm i(e_1+e_2-e_3), 1\pm i(e_1-e_2+e_3)\}.$ (64)

Multivector (versor)	Symmetry transformation
u	reflection at hyperplane normal to U
i	inversion
$i\pm u$	$\mp 90^\circ$ rotary inversion with axis u (plane of rotation: U)
$i\pm d$	$\mp 120^\circ$ rotary inversion with axis u (equiv. to d, plane of rotation: U)
$U = iu, id$	180° rotation around axis u
$1\pm iu$	±90° rotation around axis u (plane of rotation: U)
$1\pm id$	±120° rotation around axis u (equivalent to d, plane of rotation: U)

Table 5. Symmetry transformations expressed by unit vector u, $d = \sqrt{3}\,u$, bivector $U=iu$.

In general we observe for unit vectors u, $u^2 = 1$, bivectors $U=iu$ (60), and vectors $d = \sqrt{3}\,u$ the relationships of table 4. Table 5 summarizes all 48 cubic point group symmetry transformations if the vectors u, d are chosen from the three edge vectors, the six face diagonal vectors, or the four space diagonal (d) vectors respectively.

6. Reflections and translations unified in the conformal 5D model of Euclidean 3D space

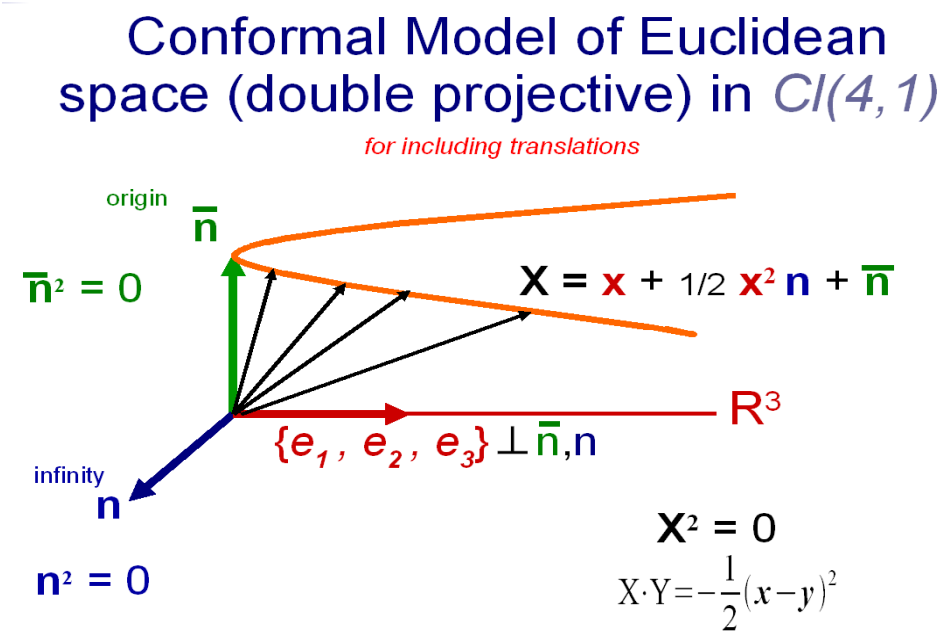

Fig 7. Overview of conformal model of Euclidean space.

6.1 The conformal 5D model of Euclidean 3D space reviewed

The 5D conformal model of Euclidean space adds two dimensions (two linearly independent vectors) to 3D Euclidean space, one for the origin n_0 and one for infinity n_∞ (compare Fig. 7)

$$X = x + \frac{1}{2}x^2 n_\infty + n_0, \tag{65}$$

These vectors seem at first sight somewhat special, because they square to zero

$$n_\infty^2 = n_0^2 = 0. \tag{66}$$

The coefficients in the linear combination (65) ensure that as a consequence every X is also a null-vector

$$X^2 = 0\ . \tag{67}$$

The second condition for X which is guaranteed by (65) is

$$X \cdot n_\infty = -1 \qquad (\Rightarrow n_0 \cdot n_\infty = -1). \tag{68}$$

(67) says that all X are on a null-cone type of surface (a 4D surface in 5D) and (68) cuts out of this surface a 3D subspace that is equivalent (isomorphic) to Euclidean three space $\mathbb{R}^3$:

$$x \in \mathbb{R}^3 \Rightarrow X = x + \frac{1}{2} x^2 n_\infty + n_0. \tag{69}$$

The way from a *conformal* point $X \in \mathbb{R}^{4,1}$ back to $x \in \mathbb{R}^3$ is to simply drop (project out) the origin and infinity parts. But what do we gain by introducing the conformal model? We get

- a new formula for calculating Euclidean distances
- a new description of located planes
- a new operator for expressing translations.

In the geometric algebra of $\mathbb{R}^{4,1}$ the scalar product of two conformal points X and A represents their Euclidean distance according to

$$X \cdot A = -\frac{1}{2}(x-a)^2, \tag{70}$$

where x and a are nothing but the Euclidean position vectors of X and A. (67) is fully in line with (70), because $(x–x)^2 = 0$, i.e. the Euclidean distance of x and x is zero.

Now all the points equidistant from two points A and B form the mid plane between A and B. Such a mid plane is in general position, i.e. it is not bound to contain the origin. An equation for the mid plane is given by

$$X \cdot A = X \cdot B \quad \Leftrightarrow \quad X \cdot (A - B) = 0 \quad \Leftrightarrow \quad X \cdot m = 0, \quad m = A - B. \tag{71}$$

$$\begin{aligned} m \;&=\; A - B \;=\; a - b + \frac{1}{2}(a^2 - b^2) n_\infty \;=\; a - b + \frac{1}{2}(a-b)\cdot(a+b) n_\infty \\ &=\; |a-b| \{ \frac{a-b}{|a-b|} + \frac{a-b}{|a-b|} \cdot \frac{a+b}{2} n_\infty \} \;=\; |a-b| \{ p + d\, n_\infty \}, \end{aligned} \tag{72}$$

where in the last line of (72) we use the abbreviations $p = (a-b)/|a-b|$ for the unit normal vector p of the mid plane represented by m , and $d = p \cdot (a+b)/2$ for the scalar oriented distance d to the origin of the plane m , as depicted in Fig. 8. Because the conformal points are homogeneous m can also simply be written as unit vector (discarding the non-zero factor $|a-b|$)

$$m = p + d\, n_\infty, \qquad m^2 = p^2 + n_\infty^2 + 2\mathrm{p} \cdot n_\infty = p^2 = 1. \tag{73}$$

For the unit plane representing vector m we also have

$$m^{-1} = m. \tag{74}$$

Exactly as before in Euclidean space, we can now use the positioned plane m in order to reflect a vector X (its perpendicular component $x_\perp$) to the other side.

$$X' = -m^{-1} X m = -m X m \tag{75}$$

The second equality holds for the unit m of (73) and (74). To proof (75) algebraically we use (7) and (8) and the following relationships (parallel and perpendicular always to unit vector p of Fig. 8!)

$$n_0 \perp p, n_\infty \perp p \quad \Rightarrow \quad X_\parallel = x_\parallel, \quad X_\perp = -x_\parallel + X \tag{78}$$

This leads with (7), (8) to

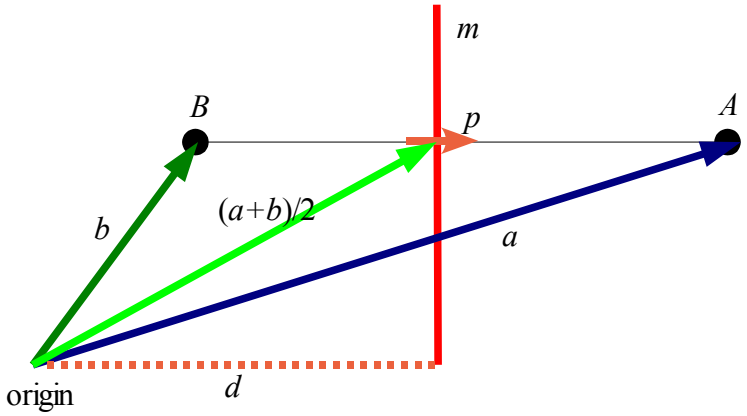

Fig. 8. Mid plane between points A, B, described by $m = A - B \propto p + d n_\infty$.

$$pX = p X_\parallel + p X_\perp = X_\parallel p - X_\perp p = x_\parallel p - (-x_\parallel + X) p = 2 x_\parallel p - X p. \tag{79}$$

We further get with (68) that

$$n_\infty n_0 = n_\infty \cdot n_0 + n_\infty \wedge n_0 = -1 - n_0 \wedge n_\infty = -2 - n_0 \cdot n_\infty - n_0 \wedge n_\infty = -2 - n_0 n_\infty . \tag{80}$$

Because of (7), (8) and (80) we have

$$d\, n_\infty X = d\, n_\infty (x + \frac{1}{2} x^2 n_\infty) + d\, n_\infty n_0 = -(x + \frac{1}{2} x^2 n_\infty) d\, n_\infty - 2d - n_0 d\, n_\infty = -2d - X d\, n_\infty . \tag{81}$$

Taking (79) and (81) together

$$\begin{aligned} X' = -m X m = -(p + d n_\infty) X m = -(2x_\parallel p - 2d) m + X (p + d n_\infty) m \\ = -2(x_\parallel p - d)(p + d n_\infty) + X m^2 \\ = -2 x_\parallel p^2 + 2 dp + 2 d^2 n_\infty - 2 dx_\parallel p n_\infty + x_\parallel + x_\perp + \frac{1}{2}(x_\parallel^2 + x_\perp^2) n_\infty + n_0 \\ = 2 dp - 2x_\parallel + x_\parallel + x_\perp + \frac{1}{2}(4 d^2 - 4 dx_\parallel p + x_\parallel^2 + x_\perp^2) n_\infty + n_0 \\ = 2 dp - x_\parallel + x_\perp + \frac{1}{2}(2 dp - x_\parallel + x_\perp)^2 n_\infty + n_0 . \end{aligned} \tag{82}$$

which according to Fig. 9 is exactly X reflected at m.
No doubt this was not the most elegant way to conduct the proof. But the intention was to only use step by step simple algebraic properties like (7) and (8).

Please note that equation (22) for the reflection at a plane through the origin with normal a and equation (75) for the reflection at a plane m in general position are formally identical. We only need to replace x by X and a by m. The composition of reflections works therefore in the very same way. For non-parallel m and m'

$$X' = m' m X m m' \tag{83}$$

describes therefore a rotation by twice the helical angle between m and m' (i.e. twice the angle between the plane normals p and p') around the line of intersection (the rotation axis perpendicular to both p and p').

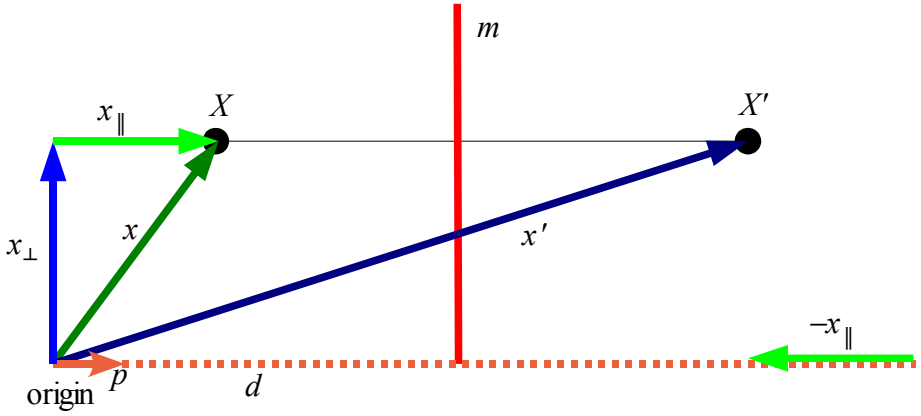

Fig. 9. Reflection of the conformal point X at plane m.

A general rotation operator (rotor) has therefore the form

$$R = m\, m'. \tag{84}$$

But what if the two planes m and m' happen to be parallel? Then the result is a translation perpendicular to the planes by twice the Euclidean distance vector $t/2$ of the planes (compare Fig. 10). In the conformal model we therefore get a translation operator (short: translator)

$$T = m\, m', \tag{85}$$

which is in its algebraic form identical to the rotation operator. What the transformation is (rotation or translation) now only depends on the relative *normal directions* of the planes m and m'. In general the versor $m\, m'$ gives

$$m m' = (p + d\, n_\infty)(p' + d'\, n_\infty) = p\, p' + (d'\, p - d\, p')\, n_\infty. \tag{86}$$

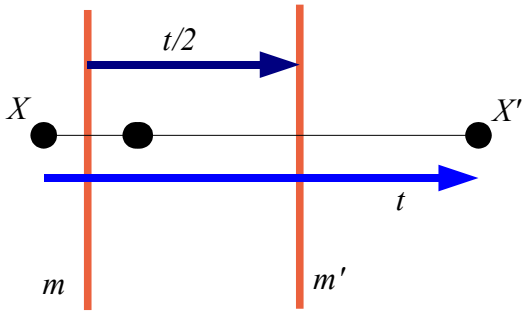

Fig. 10. Reflection at two parallel planes yields a translation by twice the distance.

We can now distinguish three cases:

- Case 1. Parallel planes with $p = p'$. Then we have a pure translation by $t = 2(d'-d)p$. The translator $T(t) = mm'$ then has the form

$$T(t) \;=\; mm' \;=\; 1+(d'-d)\,p\,n_\infty \;=\; 1+\frac{1}{2}t\,n_\infty \;=\; \exp(\frac{1}{2}t\,n_\infty), \qquad t/2 \;=\; (d'-d)\,p. \tag{87}$$

The reverse product gives

$$m'm \;=\; 1+(d-d')\,p\,n_\infty \;=\; 1-\frac{1}{2}t\,n_\infty \;=\; \exp(\frac{-1}{2}t\,n_\infty) \;=\; T(-t). \tag{88}$$

- Case 2. $d = d' = 0$, $p \neq p'$ Pure rotation around the origin. The rotor mm' then has the form

$$mm' \;= p\,p'. \tag{89}$$

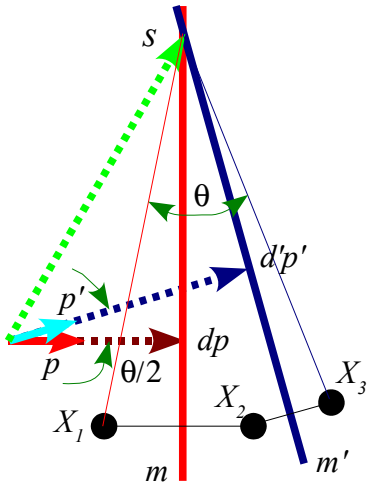

Fig. 11. Two reflections at planes m and m'.

- Case 3. $p \neq p'$, and d, d' not both zero. We call s a location on the intersection line (axis) of m and m'. The the following versor identity holds

$$mm' \;=\; T(-s)\,pp'\,T(s), \tag{90}$$

i.e. a translation of the axis to the origin followed by the pp' rotation about the origin and the back translation with $T(s)$, compare Fig. 11.

We now proof (90). s is on m and on m', therefore

$$s\cdot p = d, \qquad s\cdot p' = d'. \tag{91}$$

We calculate (remember $n_\infty \perp p$, $n_\infty \perp p'$, $n_\infty^2 = 0$)

$$\begin{aligned} T(-s)\,pp'\,T(s) \;&=\; (1-\frac{1}{2}s\,n_\infty)\,p\,p'\,(1+\frac{1}{2}s\,n_\infty) \\ =\; pp' - \frac{1}{2}s\,pp'\,n_\infty + \frac{1}{2}pp'\,s\,n_\infty + 0 \;&=\; pp' + \frac{1}{2}(pp's - s\,pp')\,n_\infty \\ =\; pp' + \frac{1}{2}(p\cdot p's + (p\wedge p')\cdot s + p\wedge p'\wedge s - s\,p\cdot p' - s\cdot(p\wedge p') - s\wedge p\wedge p')\,n_\infty \\ =\; pp' - s\cdot(p\wedge p')\,n_\infty \;&=\; pp' + (-s\cdot p\,p' + s\cdot p'\,p)\,n_\infty \\ =\; pp' + (-d\,p' + d'\,p)\,n_\infty \;&=\; mm', \end{aligned} \tag{92}$$

where we used (87), (88) and $p \wedge p' \wedge s = -p \wedge s \wedge p' = s \wedge p \wedge p'$.

The s (point of intersection of axis with p, p' plane) in the p, p' plane can be calculated as

$$s = [d\,p + d'\,p' - p \cdot p'(d'\,p + d\,p')] \;/\; [1 - (p \cdot p')^2]. \tag{93}$$

6.2 Combinations of point group transformations with lattice translations

In order to combine translations (along the selected lattice edges or in general from one general position in the lattice to another one) we need to know how to combine translators *T(a),* where *a* is the Euclidean 3D translation vector, with reflections *b* in the simplest way possible, i.e. without always calculating full 5D conformal model GA expressions. Combinations fundamentally obey the following formula

$$\mathrm{T}(a)\,b = b\,\mathrm{T}(a'), \qquad a' = -b^{-1}\,a\,b \tag{94}$$

Proof.

$$\mathrm{T}(a)\,b = (1 + \frac{1}{2}\,a\,n_\infty)\,b = b + \frac{1}{2}\,a\,n_\infty\,b = b - \frac{1}{2}\,a\,b\,n_\infty$$
$$= b - \frac{1}{2}\,b\,b^{-1}\,a\,b\,n_\infty = b(1 + \frac{1}{2}\,a'\,n_\infty) = b\,T(a').$$

In table 6 formula (94) is applied repeatedly.

index p	∠(*a*,*b*)	in particular
1	180°	T(a)b = bT(-a)
		T(b)a = aT(-b)
2	90°	T(a)b = bT(a)
		T(b)a = aT(b)
3	60°	T(a)b = bT(a-b)
		T(b)a = aT(b-a)
4	45°	T(a)b = bT(a-b)
		T(b)a = aT(b-2a)
6	30°	T(a)b = bT(a-b)
		T(b)a = aT(b-3a)

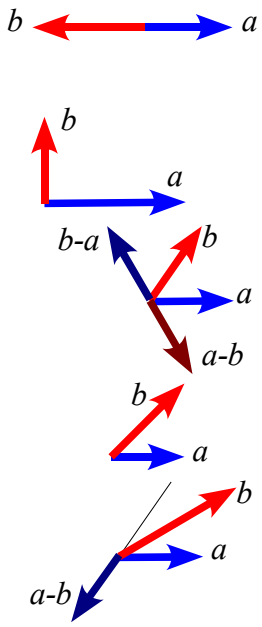

Table 6. Computing with reflections and translations. Index 2 ... rectangular cell, 3 ... equilateral triangle, 4 ... square cell, 6 ... *a* is the blue side vector in the base plane of the right cell of Fig. 5 and *b* is the red dashed line diagonal vector in the same base plane.

6.3 Example of a rectangular 2D lattice spacegroup: c2

Fig. 12 shows a rectangular centered cell with space group symmetry c2. All symmetry elements are

depicted. The generators of spacegroup c2 (ITC-No. 9, see [6]) are:

$$a,\ b,\ \mathbf{T}([a+b]/2),\ \ \mathbf{T}(k a),\ \mathbf{T}(k b) \quad \text{with} \quad k = -1, +1. \tag{95}$$

The centers of 180 degree rotations are given by

$$a b\ \mathbf{T}([a+b]/2) \quad \text{located at} \quad (a+b)/4+(ka+lb)/2, \quad k, l \in \mathbb{Z}. \tag{96}$$

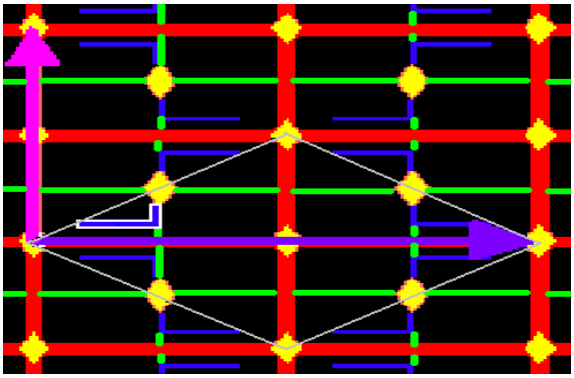

Fig. 12. Planar space group (wallpaper) with ITC-Nr. 9, geometric symbol: c2.

- Red lines: reflection lines
- Green lines: lines of glide reflection
- Yellow dots: Centers of 180 deg. rotation
- Violet and pink vectors: *a,b*
- Blue L: Asymmetric general element representing a molecule.

The glide reflections of c2 have the following generators:

$$b\mathbf{T}([a+b]/2) = \mathbf{T}(-b/4) \quad b\mathbf{T}(a/2) \quad \mathbf{T}(b/4), \quad \text{located at} \quad b/4+lb/2, \quad l \in \mathbb{Z}. \tag{97}$$

The symmetry operators of the other 16 2D spacegroups can be composed of versor operators analogous to the versors given in (95) – (97). The only depend on two vectors a,b characteristic for the associated lattice (oblique, rectangular, square, trigonal and hexagonal). The geometric names of 2D spacegroups are derived from the associated geometric point group symbols of Table 2 by adding a prefix for the type of Bravais lattice (p ... primitive, c ... centered, h ... hexagonally centered) and an index *g* where a simple reflection in the group basis has been replaced by a glide reflection.

6.4 Example of a 3D monoclinic space group

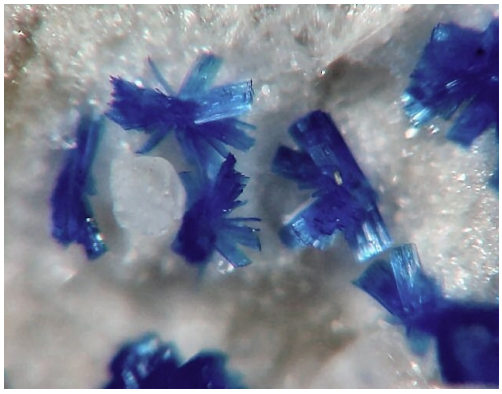

Fig. 13. The mineral Kinoite (Image: http://webmineral.com/data/Kinoite.shtml)

Spacegroup $P\bar{2}2_1$ symmetries from generator products: multiplying *ic*T(*c*/2), *c*T(*c*/2) and T(***a***), *T(**b***), T(***c***):

- Glide reflections are actually square roots of translations:

$$T(c) \simeq [icT(c/2)]^2 \tag{98}$$

- Reflections perpendicular to vector ***c***, located at ***c***/4+*k****c***/2

$$cT(c/2)T(k\,c) \;=\; T^{-1}(\frac{1}{4}c+\frac{1}{2}kc)cT(\frac{1}{4}c+\frac{1}{2}kc), \quad k\in\mathbb{Z} \tag{99}$$

- Family of inversions located at *(ka+lb+mc)*/2

$$icT(c/2)cT(c/2) \;=\; ic^2T(-\frac{c}{2}+\frac{c}{2}) \;\simeq\; i\,, \tag{100}$$
$$iT(ka+lb+mc) \;=\; T^{-1/2}(ka+lb+mc)\,i\,T^{1/2}(ka+lb+mc), \quad k\,,l\,,m\in\mathbb{Z}$$

- Family of screws located at *(ka+lb)*/2

$$icT(c/2)T(ka+lb) \;=\; T^{\frac{-1}{2}}(ka+lb)icT(c/2)T^{\frac{1}{2}}(ka+lb), \quad k\,,l\in\mathbb{Z} \tag{101}$$

Fig. 14 shows a depiction of one monoclinic crystal with spacegroup symmetry $P\bar{2}2_1$ with depictions of all its symmetry elements.

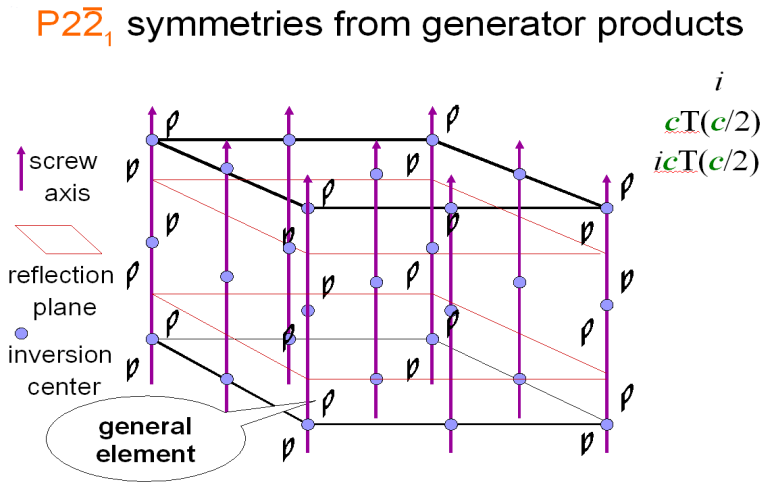

Fig. 14. Schematic (monoclinic) crystal cell (e.g. of Kinoite) with all centers of inversion, reflection planes and screw axis shown. The symbol P represents a general asymmetric unit (e.g. a molecule).

7. VISUALIZATION OF CRYSTAL CELL SYMMETRIES

A visualization of the various space group symmetries can further their understanding considerably. For this purpose we employed the freely available software CLUCalc [7]. CLUCalc is a 3D-visualization tool with an extensive scripting language, which fully supports Geometric Algebra. A fully free *point group* visualization script and a demonstration version of the *Space Group* Visualizer (SGV) script that was developed is also available from www.spacegroup.info . In the following a short introduction to the usage of the scripts is given.

When CLUCalc starts up, it opens three windows: a script window, a text output window and a visualization window (Fig. 15). Through the menu of the script window the script can be loaded. After the point symmetry group script has been loaded, the visualization window is split into three areas: at the left a descriptive text containing interactive links is given, at the bottom control elements are shown and in the remaining space the crystal cell and related elements are visualized. The visualization is best viewed when the visualization window is maximized.

Initially the two crystal cells with a triclinic symmetry are shown. By clicking on the blue text links in the left area with the mouse pointer, one can switch to crystal cells with different symmetries. The left crystal cell is always the initial cell, while the right cell shows the transformed crystal cell. The transformations

performed are shown above the crystal cells. Initially only a '1' is shown, i.e. the identity transformation. In order to perform group transformations on a cell, one first has to select a group by clicking on one of the blue group identifiers. Then the group generators become active, i.e. they become blue links. Clicking on one of the group generators applies the corresponding transformation to the left crystal cell, and the result is shown by the right cell. If a sequence of group generators are selected, one after another, the right cell represents the total transformation. The history of transformations is shown above the cells ... [13].

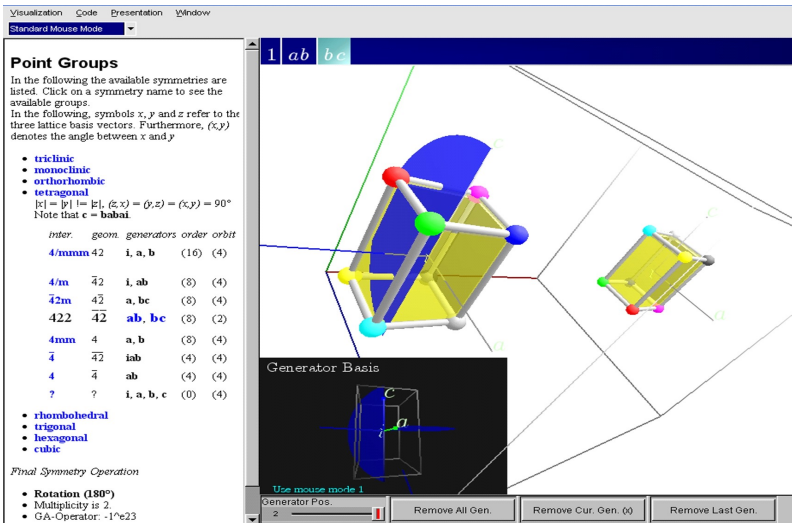

Fig. 15. Example view of point symmetry group visualization script.

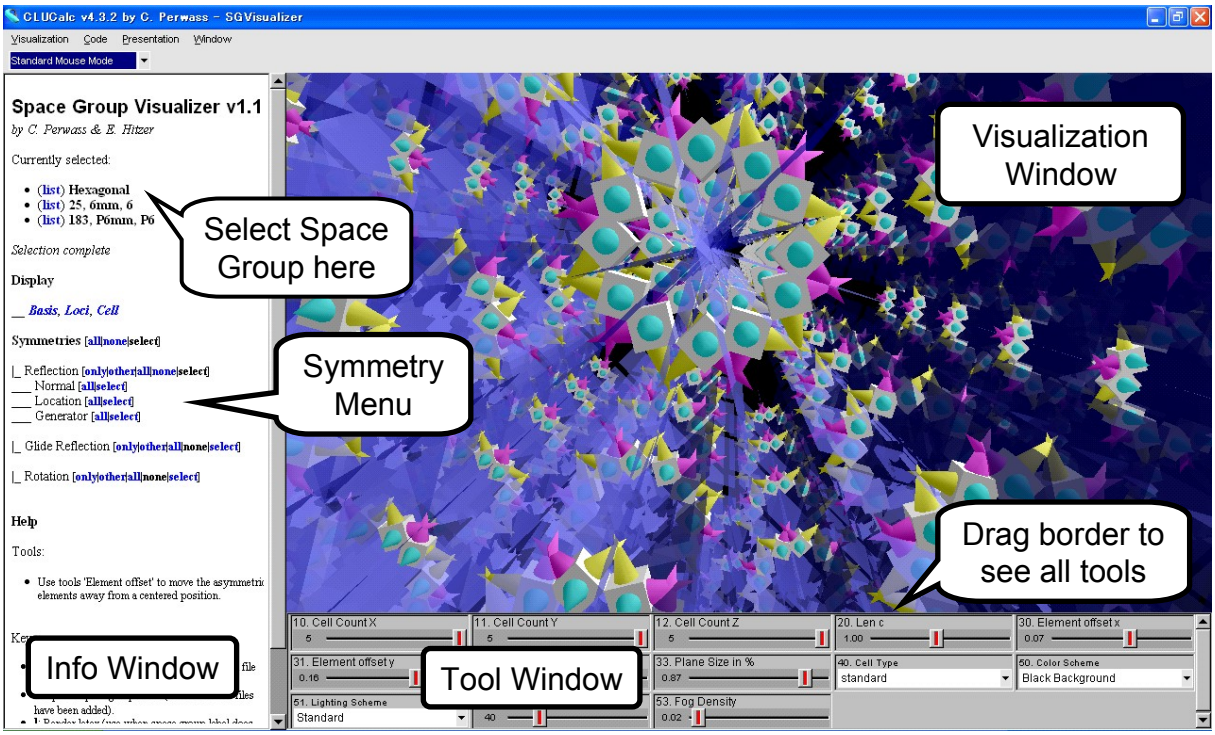

Fig. 16. Example view of Space Group Visualizer (www.spacegroup.info) .

The latest demo version of another CLUCalc script, the space group visualizer (SGV) can be obtained from www.spacegroup.info . Clicking the download link downloads the executable installation file. Executing the installation file installs the space group visualizer in a dedicated program folder and deposits a shortcut to the space group visualizer software on the desktop of the computer. Clicking this desktop icon opens the

visualization window (Fig. 16). On the left this window has a vertical browser panel for selecting a specific space group. To the right we find the actual graphical visualization with a grey pull up tool sector at its bottom. Dragging up the upper border of the tool sector gives access to all available tools ... [17].

8. CONCLUSIONS

We have shown how reflections can be implemented in the GA of Euclidean space and in the 5D conformal model of 3D Euclidean space. Combining reflections allows to generate all isometric transformations. In the conformal model rotations and translations get a unified treatment as double reflection versors. The underlying geometric ideas are contained in [4], but in our example we even treated all elements of all 32 point groups of three dimensional crystal cells explicitly.
The explicit representation of all point symmetry group elements as a geometric product of physical vectors taken from the crystal cell may also serve as both example and reference for future research.
The interactive visualization software tools for point groups (free) and space groups (free demo) constitute a valuable teaching resource for both instruction and self-study. It should be obvious that the versor representation of geometric transformations is universal, it is in no way limited to our domain of examples from crystallography, it especially can be applied to both higher and lower dimensions and to spaces with non-Euclidean signature.

ACKNOWLEDGEMENTS

E. Hitzer wants to thank God for his creation: *It is I who made the earth and created mankind upon it. My own hands stretched out the heavens; I marshaled their starry hosts.*[9] I further want to thank my family for their loving and patient support, C. Perwass excellent cooperation, the Cognitive Systems group of the University of Kiel for their hospitality when doing part of this research, and my students D. Ichikawa, M. Sakai, and K. Yamamoto. A special thanks goes to Ass. Prof. Dr. Kanta Tachibana of the FCS of Nagoya University and his whole group for organizing this tutorial and workshop.

Bibliography

All papers of E. Hitzer are freely available from: http://sinai.mech.fukui-u.ac.jp/gcj/publications/

1. N.W. Ashcroft, N.D. Mermin, *Solid State Physics*, Sounders College, Philadelphia, 1988.
2.D. Hestenes, *New Foundations for Classical Mechanics*, Kluwer Academic Publishers, 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. Free download: http://modelingnts.la.asu.edu/pdf/crystalsymmetry.pdf . D. Hestenes, J. Holt, *The Crystallographic Space Groups in Geometric Algebra*, accepted for publication by JMP, 2007.
5. J.D. M. Gutierrez, *Operaciones de simitria mediante algebra geometrica aplicadas a grupos cristalograficos*, Tesis, UNAM, Mexico 1996.
6. Th. Hahn, *Int. Tables for Crystallography, Volume A: Space-group symmetry,* Kluwer, Dordrecht, 1992.
7. C. Perwass, Homepage of Open Source Software CLUCalc: http://www.clucalc.info/
8. Homepage with Java applets (ca. 100) illustrating fundamental laws of Geometric Algebra.
http://sinai.mech.fukui-u.ac.jp/gcj/software/GAcindy-1.4/GAcindy.htm
9. Bible, Isaiah 45:12 (NIV). http://www.biblegateway.com/
10. E.M.S. Hitzer, L. Redaelli, **Geometric Algebra illustrated by Cinderella,** *Advances in Applied Clifford Algebras*, **13**(2) pp. 157-181 (2003).
http://sinai.mech.fukui-u.ac.jp/gcj/publications/GAbyCindy/GAbyCindy.pdf
11. E.M.S. Hitzer, C. Perwass, **Crystal Cells in Geometric Algebra,** Proceedings of the *International Symposium on Advanced Mechanical Engineering, between University of Fukui (Japan) - Pukyong National University (Korea),* 27 Nov. 2004, pp. 290-295 (2004).
http://sinai.mech.fukui-u.ac.jp/gcj/publications/crystalc/crystalc.pdf
12. E.M.S. Hitzer, C. Perwass, **Crystal Cell and Space Lattice Symmetries in Clifford Geometric**

Algebra, in TE. Simos, G. Sihoyios, C. Tsitouras (eds.), *International Conference on Numerical Analysis and Applied Mathematics 2005*, Wiley-VCH, Weinheim, 2005, pp. 937-941.
http://sinai.mech.fukui-u.ac.jp/gcj/publications/cellspacesym/cellspacesym.pdf
13. E.M.S. Hitzer, C. Perwass, **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,** Proceedings of the *International Symposium on Advanced Mechanical Engineering, between University of Fukui (Japan), Pukyong National University (Korea) and University of Shanghai for Science and Technology (China)*, 23-26 Nov. 2005.
http://sinai.mech.fukui-u.ac.jp/gcj/publications/SGtheory/SGtheory.pdf
14. C. Perwass, E.M.S. Hitzer, **Interactive Visualization of Full Geometric Description of Cyrstal Space Groups,** Proceedings of the *International Symposium on Advanced Mechanical Engineering, between University of Fukui (Japan), Pukyong National University (Korea) and University of Shanghai for Science and Technology (China)*, 23-26 Nov. 2005.
http://sinai.mech.fukui-u.ac.jp/gcj/publications/SGvisual/SGvisual.pdf
15. E.M.S. Hitzer, C. Perwass, **Three Vector Generation of Crystal Space Groups in Geometric Algebra,** *Bulletin of the Society for Science on Form*, **21**(1), pp. 55,56 (2006).
http://sinai.mech.fukui-u.ac.jp/gcj/publications/tvgcsg/tvgcsg.pdf
16. E.M.S. Hitzer, C. Perwass, **Space Group Visualizer for Monoclinic Space Groups,** *Bulletin of the Society for Science on Form*, **21**(1), pp. 38,39 (2006).
http://sinai.mech.fukui-u.ac.jp/gcj/publications/sgvmsg/sgvmsg.pdf
17. E.M.S. Hitzer, C. Perwass, **The Space Group Visualizer,** Proc. of *Int. Symp. on Adv. Mech. Enging, between Univ. of Fukui (Jp.), Pukyong Nat. Univ. (Kor.) and Univ. of Shanghai for Sci. and Techn. (China)*, 26-29 Oct. 2006, pp. 172-181 (2006). http://sinai.mech.fukui-u.ac.jp/gcj/publications/TheSGV/TheSGV.pdf

E. Hitzer, in K. Tachibana (ed.) Tutorial on Reflections in Geometric Algebra, Lecture notes of the international Workshop for “Computational Science with Geometric Algebra” (FCSGA2007), Nagoya University, Japan, 14-21 Feb. 2007, pp. 34-44 (2007).