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Interactive 3D Space Group Visualization with CLUCalc and Crystallographic Subperiodic Groups in Geometric Algebra

Eckhard Hitzer, Christian Perwass and Daisuke Ichikawa

Abstract The Space Group Visualizer (SGV) for all 230 3D space groups is a standalone PC application based on the visualization software CLUCalc. We first explain the unique geometric algebra structure behind the SGV. In the second part we review the main features of the SGV: The GUI, group and symmetry selection, mouse pointer interactivity, and visualization options. We further introduce the joint use with the International Tables of Crystallography, Vol. A [7]. In the third part we explain how to represent the 162 socalled subperiodic groups of crystallography in geometric algebra. We construct a new compact geometric algebra group representation symbol, which allows to read off the complete set of geometric algebra generators. For clarity we moreover state explicitly what generators are chosen. The group symbols are based on the representation of point groups in geometric algebra by versors.

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 [4] combined with the conformal model of 3D Euclidean space [1, 5, 16, 21–24, 36] yields an algebra fully expressing crystal point and space

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groups [6, 10, 28–30]. Two successive reflections at (non-) parallel planes express (rotations) translations, etc. [2, 3] This leads to a 1:1 correspondence of geometric objects and symmetry operators [25] with vectors and their products, ideal for creating a suite of interactive visualizations using CLUCalc [34] and OpenGL [28–30].

For crystallographers the subperiodic space groups [42] in 2D and 3D with only one or two degrees of freedom for translations are also of great interest.

We begin in Section 2 by explaining the representation of point and space groups in conformal geometric algebra. Next we explain the basic functions of the software implementation, called Space Group Visualizer [35] in Section 3. Finally in Section 4 we show how to construct a new compact geometric algebra group representation symbol for subperiodic space groups (Frieze groups, rod groups and layer groups), which allows to read off the complete set of geometric algebra generators. For clarity we moreover state explicitly what generators are chosen.

2 Point groups and space groups in Clifford geometric algebra

2.1 Cartan-Dieudonné and geometric algebra

Clifford's associative geometric product [4] of two vectors simply adds the inner product to the outer product of Grassmann

$$\boldsymbol{ab} = \boldsymbol{a}\cdot\boldsymbol{b} + \boldsymbol{a}\wedge\boldsymbol{b}\,. \tag{1}$$

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

$$\boldsymbol{a}\boldsymbol{x}_{\parallel} = \boldsymbol{x}_{\parallel}\boldsymbol{a}\,, \qquad \boldsymbol{a}\boldsymbol{x}_{\perp} = -\boldsymbol{x}_{\perp}\boldsymbol{a}\,. \tag{2}$$

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

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

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

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

Continuing with a third reflection at a hyperplane with normal $\boldsymbol{c}$ according to the Cartan–Dieudonné theorem [38–41] yields rotary reflections and inversions

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

where $\doteq$ means equality up to non-zero scalar factors (which cancel out in (6)). In general the geometric product S of k normal vectors corresponds to the composition of reflections to all symmetry transformations [10] of 2D and 3D crystal cell point

groups

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

where $\widehat{S} = (-1)^k S$ is the *grade involution* or *main involution* in Clifford geometric algebra. We call the product of invertible vectors S in (6) *versor* [10, 11, 22, 25, 26], but the names *Clifford monomial* of invertible vectors, *Clifford group element*, or *Lipschitz group element* are equally in use [22, 37].

2.2 Two dimensional point groups

2D point groups [10] are generated by multiplying vectors selected [28–30] 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 $\boldsymbol{a},\boldsymbol{b}$

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

The rotation subgroups are denoted with bars, e.g. $\bar{6}$. The identities $\boldsymbol{a}^2 = \boldsymbol{b}^2 = 1$ and $R^6 = -1$ directly correspond to relations in the group presentation [8] of 6.

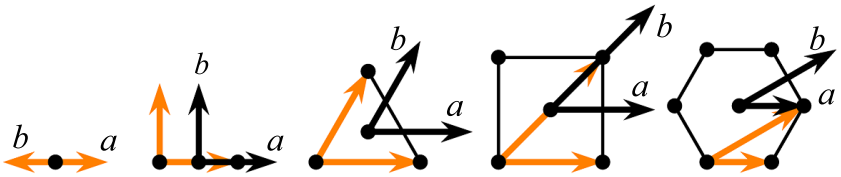

Fig. 1 Regular polygons ($p = 1,2,3,4,6$) and point group generating vectors $\boldsymbol{a},\boldsymbol{b}$ subtending angles π/p shifted to center.

Table 1 Geometric [10, 11] and international [7] notation for 2D point groups.

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

2.3 Three dimensional point groups

The selection of three vectors $\boldsymbol{a},\boldsymbol{b},\boldsymbol{c}$ from each crystal cell [10, 28–30] for generating all 3D point groups is indicated in Fig. 2. Using $\angle(\boldsymbol{a},\boldsymbol{b})$ and $\angle(\boldsymbol{b},\boldsymbol{c})$ we can denote all 32 3D point groups (alias crystal classes) as in Table 2. For example the monoclinic point groups are then (int. symbols of Hermann-Maugin: $2/\mathrm{m}$, m and 2, respectively)

$$2\bar{2} = \{\boldsymbol{c}, R = \boldsymbol{a}\wedge\boldsymbol{b} = i\boldsymbol{c}, i = \boldsymbol{c}R, 1\}, \qquad 1 = \{\boldsymbol{c}, 1\}, \qquad \bar{2} = \{i\boldsymbol{c}, 1\}. \tag{8}$$

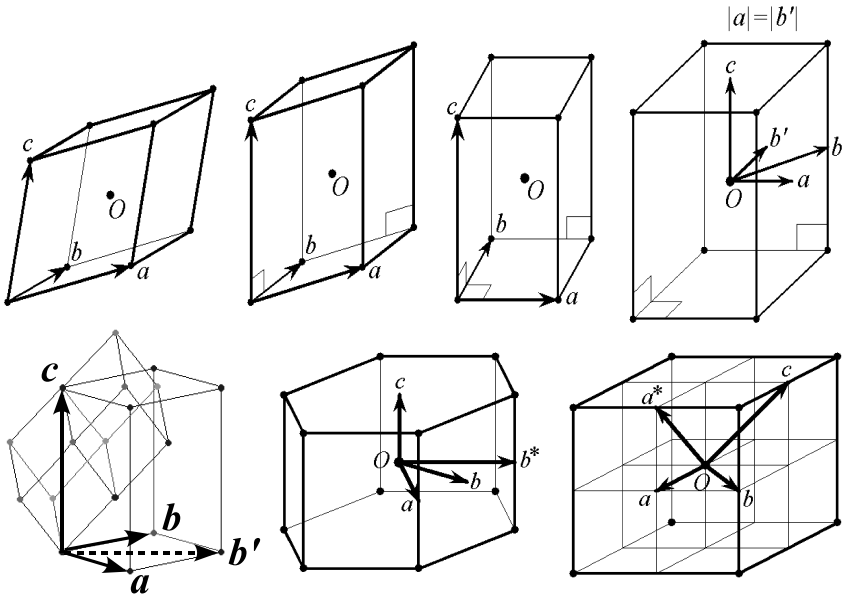

Fig. 2 7 crystal cells with vector generators $\boldsymbol{a},\boldsymbol{b},\boldsymbol{c}$: triclinic, monoclinic, orthorhombic, tetragonal, trigonal (rhombohedral), hexagonal, cubic.

Table 2 Geometric 3D point group symbols [3, 10] and generators with $\theta_{\boldsymbol{a},\boldsymbol{b}} = \pi/p$, $\theta_{\boldsymbol{b},\boldsymbol{c}} = \pi/q$, $\theta_{\boldsymbol{a},\boldsymbol{c}} = \pi/2$, $p,q \in \{1,2,3,4,6\}$.

Symbol	$p=1$	$p\neq 1$	$\bar{p}$	pq	$\bar{p}q$	$p\bar{q}$	$\bar{p}\bar{q}$	$\overline{pq}$
Generators	$\boldsymbol{a}$	$\boldsymbol{a},\boldsymbol{b}$	$\boldsymbol{ab}$	$\boldsymbol{a},\boldsymbol{b},\boldsymbol{c}$	$\boldsymbol{ab},\boldsymbol{c}$	$\boldsymbol{a},\boldsymbol{bc}$	$\boldsymbol{ab},\boldsymbol{bc}$	$\boldsymbol{abc}$

Table 3 Computing with reflections and translations. The vectors $\boldsymbol{a},\boldsymbol{b}$ are pictured in Fig. 1.

$\angle(\boldsymbol{a},\boldsymbol{b})$	180°	90°	60°	45°	30°
$T_{\boldsymbol{a}}\boldsymbol{b} =$	$\boldsymbol{b}T_{-\boldsymbol{a}}$	$\boldsymbol{b}T_{\boldsymbol{a}}$	$\boldsymbol{b}T_{\boldsymbol{a}-\boldsymbol{b}}$	$\boldsymbol{b}T_{\boldsymbol{a}-\boldsymbol{b}}$	$\boldsymbol{b}T_{\boldsymbol{a}-\boldsymbol{b}}$
$T_{\boldsymbol{b}}\boldsymbol{a} =$	$\boldsymbol{a}T_{-\boldsymbol{b}}$	$\boldsymbol{a}T_{\boldsymbol{b}}$	$\boldsymbol{a}T_{\boldsymbol{b}-\boldsymbol{a}}$	$\boldsymbol{a}T_{\boldsymbol{b}-2\boldsymbol{a}}$	$\boldsymbol{a}T_{\boldsymbol{b}-3\boldsymbol{a}}$

2.4 Space groups

The smooth composition with translations is best done in the conformal model [1,5, 12–15, 17–21, 23, 24, 26, 27, 36] of Euclidean space (in the GA of $\mathbb{R}^{4,1}$), which adds two null-vector dimensions for the origin $\boldsymbol{e}_0$ and infinity $\boldsymbol{e}_\infty$

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

The $+\boldsymbol{e}_0$ term integrates projective geometry, and the $+\frac{1}{2}\boldsymbol{x}^2\boldsymbol{e}_\infty$ term ensures $X^2 = 0$. The inner product of two conformal points gives their Euclidean distance and therefore a plane m equidistant from two points A, B as

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

where $\boldsymbol{p}$ 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 $\boldsymbol{t}/2$ we get the so-called *translator* (*transla*tion opera*tor* by $\boldsymbol{t}$)

$$X' = m'mX\,mm' = T_{\boldsymbol{t}}^{-1} X T_{\boldsymbol{t}}, \quad T_{\boldsymbol{t}} = 1 + \frac{1}{2}\boldsymbol{t}\boldsymbol{e}_\infty. \tag{11}$$

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 $\boldsymbol{e}_\infty$ invariant [10,11, 22]. Now general translations and rotations are represented by geometric products of vectors. To study combinations of versors it is useful to know that (cf. Table 3)

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

Applying these techniques one can compactly tabulate geometric space group symbols and generators [11]. Table 4 implements this for the 13 monoclinic space groups. All this is interactively visualized by the Space Group Visualizer [35].

Table 4 Monoclinic space group versor generators, $T^A = T^{1/2}_{\boldsymbol{b}+\boldsymbol{c}}$, int. = international [7], geo. = geometric, alt. = alternative, columns 3 and 4: [11]. $T_{\boldsymbol{a}}, T_{\boldsymbol{b}}, T_{\boldsymbol{c}}$ suppressed.

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

3 Interactive Software Implementation

The realization in software relies on the visual multivector software CLUCalc [34]. The excellent graphics rendering is based on OpenGL graphics. The space group symmetry definitions described in the previous sections are denoted for each space group in the form of an XML input file. The XML files serve as input for a CLUCalc script named Space Group Visualizer (SGV) [35].

3.1 The Space Group Visualizer GUI

Fig. 3 shows the SGV GUI. The SGV toolbar is magnified and annotated in Fig. 4. Depending on the displayed space group, basis vector lengths and (or) angles may be fixed (i.e. they may not be changed by the user). This is indicated by toolbar elements shaded in gray.

3.2 Space group and symmetry selection

Figure 5 shows the interactive (hyperlink like) space group selection. Clicking blue text elements in the browser panel on the left of the GUI allows to access crystal systems, crystal classes (point groups), and individual space groups.

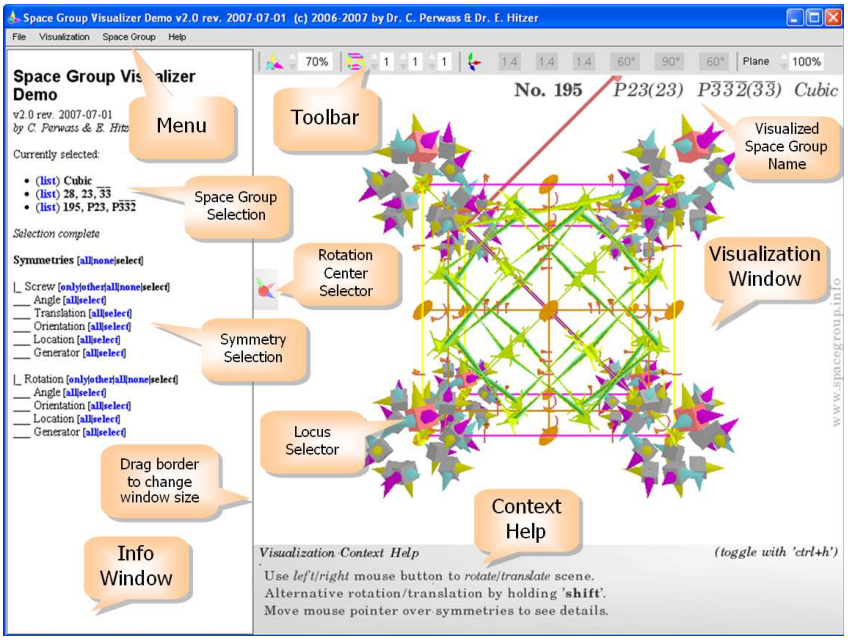

Fig. 3 GUI of the Space Group Visualizer.

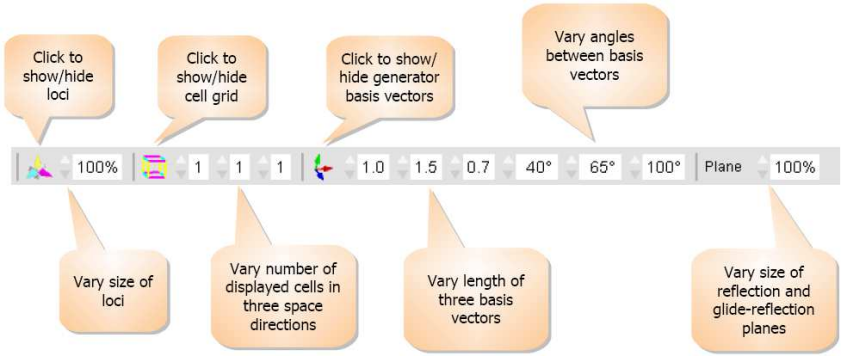

Fig. 4 Toolbar of the Space Group Visualizer.

Figure 6 illustrates the selection of symmetries from the complete list of *Symmetries* (left SGV GUI browser panel), which are present in the currently selected space group. Symmetries that are to be displayed can be selected according to their properties (angle, orientation, location, translation component). Several properties selected together will display only those symmetries that satisfy all properties. Another way is to open the generator product list of a certain type of symmetry and

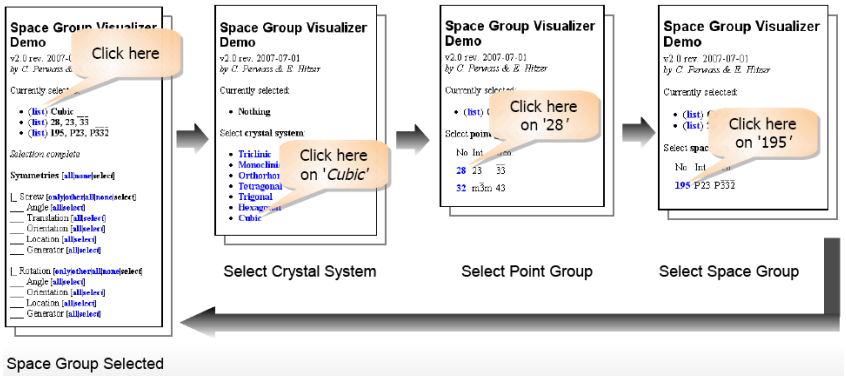

Fig. 5 Space group selection from the Space Group Visualizer browser panel.

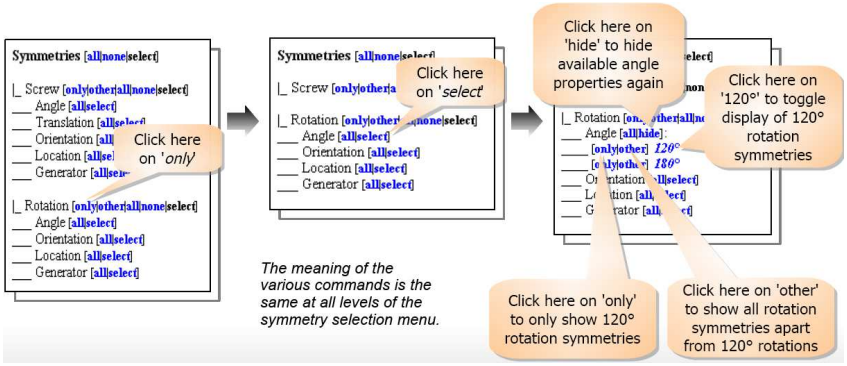

Fig. 6 Space group selection of individual symmetries or groups of symmetries to be displayed.

select individual geometric algebra generator products to be displayed (or to be removed from the display).

3.3 Mouse pointer interactivity

The mouse pointer allows a variety of visual interactions and animations, depending over which part of the visualization it is placed. Moving the mouse pointer over a symmetry element visualization both animates the symmetry and displays detailed information about this symmetry group element in the lower right corner. Animation means dynamic color and size changes; and the motion of general elements along a trajectory tracing the symmetry operation incrementally. Placement of the mouse pointer over a general element (locus) selector activates it (blinking). The mouse

pointer over the rotation center (of view) selector allows to change the rotation center of the mouse activated view rotation (described below).

The mouse pointer can be placed anywhere inside the visualization window. Holding down the left (right) mouse button and moving the mouse will rotate (translate) the visualization. Alternative rotation axes (translation directions) are activated by additionally holding the SHIFT key. With a 3D-mouse (3Dconnexion) one can rotate and translate the view along all axes simultaneously.

First placing the mouse pointer over a general element (locus) selector permits to translate and rotate it (together with all its symmetric partners). This provides an excellent way to grasp how one general element and the 3D symmetry represented in the space group determine the whole crystal structure.

A special feature of the SGV is the direct 3D graphics interaction. Simply placing the mouse pointer over a symmetry activates it and allows to:

- Select only the activated symmetry (left mouse button). All other symmetries disappear from the view.
- Holding the CTRL key at the same time (while pressing the left mouse button) shows all symmetries (and only these) of the same type.
- Clicking the right mouse button removes an activated symmetry from the view.
- Holding the CTRL key at the same time (while pressing the right mouse button) removes all symmetries of the same type.

3.4 Visualization options in detail

The visualization drop down menu allows to toggle (activate and deactivate) the following visual functions

- Full screen mode.
- Orthographic view. The orthographic view allows the most direct comparison with ITA orthographic projections [7].
- Animation of the origin locus when a symmetry is activated (animated).
- Rotation animation of the whole view when it is *pushed* with the (left) mouse button.
- Reset the crystal view to visualizer default values.
- Reset general element (loci) positions.

The special visualization lighting menu provides a relative position light source. It is positioned relative to the visualization coordinate frame and moves with the visualization. Deselecting this option fixes the light source relative to the observer. The light source can optionally be positioned at the center of the coordinate frame, which is relative (or absolute) depending on the (de)selection of the relative position option. The ambient light submenu allows to adjust the brightness of the ambient light, leading to more dramatic effects for darker settings.

The color scheme menu item allows to select the current color scheme. For example a scheme with black background is more suitable for use in presentations, while

a white background is better for publications, etc. It is possible via an XML file to individually define further color schemes. A color stereo option allows to specify cinema type stereo colors, which are best viewed with corresponding cinema color glasses in order to perform the full spatial 3D effect akin to virtual reality.

The cell type menu allows to select between different cell choices in the IT, Volume A [7], and (if different) a special geometric algebra type cell, which has the generating vectors $\boldsymbol{a},\boldsymbol{b},\boldsymbol{c}$ as cell axis attached to the cell origin. Details are given in [46].

3.5 Integration with the online International Tables of Crystallography

Through the window menu an additional window can be opened for displaying the pages of a space group from the online version of the International Tables of Crystallography, Volume A (ITA) [7]. For this the user must hold a valid user ID and password. When the online ITA can be accessed, the SGV and the online ITA window will always show the *same* space group. The user can synchronously navigate from space group to space group either in the SGV or in the online ITA window (cf. Fig. 7).

4 Subperiodic groups represented in Clifford geometric algebra

Now we begin to explain the details of the new geometric algebra based representation of so-called *subperiodic* space groups. These include the seven *frieze* groups (in 2D space, 1 DOF for translation), the 75 *rod* groups (in 3D space, 1 DOF for translation), and the 80 *layer* groups (in 3D space, 2 DOF for translations).

Compared to the geometric 2D and 3D space group symbols in [11] we have introduced dots: If one or two dots occur between the Bravais symbol ($\not$, p, c) and index 1, the vector b or c, respectively, is present in the generator list. If one or two dots appear between the Bravais symbol and the index 2 (without or with bar), then the vectors b,c or a,c, respectively, are present in the generator list.

In agreement [11] the indices a,b,c,n (and g for frieze groups) in first, second or third position after the Bravais symbol indicate that the reflections a,b,c (in this order) become glide reflections. An index n indicates diagonal glides. The dots also serve as symbolic a,b,c position indicators. For example rod group 5:$\not_c 1$ has glide reflection ${}_aT_c^{1/2}$, rod group 19:$\not_{\cdot c} 2$ has ${}_bT_c^{1/2}$, and layer group 39: $p_b 2_a 2_n$ has ${}_aT_b^{\frac{1}{2}}$, ${}_bT_a^{1/2}$ and ${}_cT_{a+b}{}^{1/2}$.

The notation $\overline{n}_p$ indicates a right handed screw rotation of $2\pi/n$ around the $\overline{n}$-axis, with pitch $T_t^{p/n}$ where t is the shortest lattice translation vector parallel to the

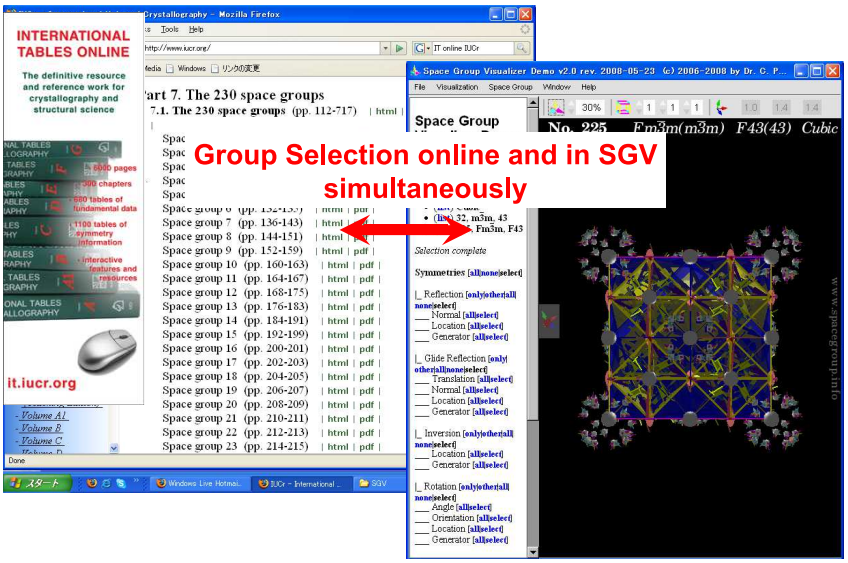

Fig. 7 Synchronous space group selection in the SGV window and the online ITA [7] space group window.

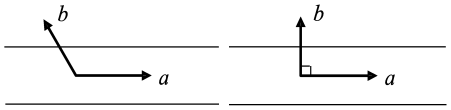

Fig. 8 Generating vectors a, b of oblique and rectangular cells for 2D frieze groups.

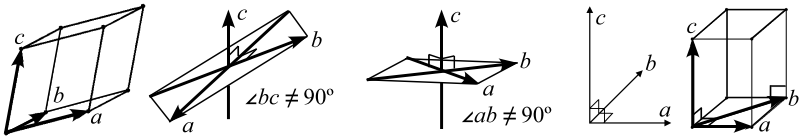

Fig. 9 From left to right: Triclinic, monoclinic inclined, monoclinic orthogonal, orthorhombic, and tetragonal cell vectors a, b, c for rod and layer groups.

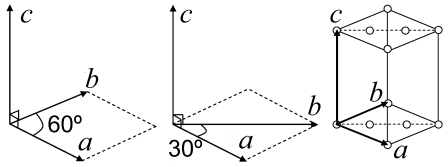

Fig. 10 Generating vectors a,b,c of trigonal (left), hexagonal (center) and hexagonally centered (right, Bravais symbol: H or h) cells for 3D rod and layer groups.

axis, in the screw direction. For example the layer group 21: $p\bar{2}\bar{2}_1\bar{2}_1$ has the screw generators $bcT_a^{1/2}$ and $acT_b^{1/2}$.

In the following we discuss specific issues for frieze groups, rod groups and layer groups. In the current publication we restrict ourselves to the new symbols for triclinic and monoclinic rod and layer groups. The full tables will be published elsewhere.

4.1 Frieze groups

Figure 8 shows the generating vectors a,b of oblique and rectangular cells for 2D frieze groups. The only translation direction is a. Table 5 lists the seven frieze groups with new geometric symbols and generators. The abbreviations SG# and SGN mean space group number and space group name (symbol), respectively.

4.2 Rod groups

Figure 9 shows the generating vectors a,b,c of triclinic, monoclinic, orthorhombic and tetragonal cells for 3D rod and layer groups. Figure 10 shows the same for trigonal and hexagonal cells. For rod groups the only translation direction is c. There is a total of 75 rod groups in all 3D crystal systems. Table 6 lists the triclinic and monoclinic rod groups with new geometric symbols and generators: Rod group number (col. 1), intern. rod group notation [42] (col. 2), related intern. 3D space group numbers [7] (col. 3), and notation [7] (col. 4), related geometric 3D space group notation [11] (col. 5), *geometric rod group notation* (col. 6), *geometric algebra generators* (col. 7).

Table 5 Table of frieze groups. Group number (col. 1), intern. frieze group notation [42] (col. 2), related intern. 3D space group numbers [7] (col. 3), and notation [7] (col. 4), geometric 3D space group notation [11] (col. 5), related intern. 2D space group numbers [7] (col. 6), and notation [7] (col. 7), related geometric 2D space group notation [11] (col. 8), *geometric frieze group notation* (col. 9), *geometric algebra frieze group versor generators* (col. 10). The pure translation generator T_a is omitted.

Frieze Group #	Intern. Notat.	3D SG#	Intern. 3D SGN	Geom. 3D SGN	2D SG#	Intern. 2D SGN	Geom. 2D SGN	Geom. Notat.	Frieze Group Generators
Oblique									
F_1	$\not{e}1$	1	$P1$	$P\bar{1}$	1	$p1$	$p\bar{1}$	$\not{e}\bar{1}$	
F_2	$\not{e}211$	3	$P2$	$P\bar{2}$	2	$p2$	$p\bar{2}$	$\not{e}\bar{2}$	$a \wedge b$
Rectangular									
F_3	$\not{e}1m1$	6	Pm	$P1$	3	$pm(p1m1)$	$p1$	$\not{e}1$	a
F_4	$\not{e}11m$	6	Pm	$P1$	3	$pm(p11m)$	$p1$	$\not{e}.1$	b
F_5	$\not{e}11g$	7	Pc	P_a1	4	$pg(p11g)$	p_g1	$\not{e}_{\cdot g}1$	$bT_a{}^{1/2}$
F_6	$\not{e}2mm$	25	$Pmm2$	$P2$	6	$p2mm$	$p2$	$\not{e}2$	a, b
F_7	$\not{e}2mg$	28	$Pma2$	$P2_a$	7	$p2mg$	$p2_g$	$\not{e}2_g$	$a, bT_a{}^{1/2}$

Table 6 Table of triclinic and monoclinic rod groups. The pure translator T_c is omitted.

Rod Group #	Intern. Notat.	3D Space Group #	Intern. 3D SGN	Geom. 3D SGN	Geom. Notat.	Rod Group Generators
Triclinic						
R_1	$\not{e}1$	1	$P1$	$P\bar{1}$	$\not{e}\bar{1}$	
R_2	$\not{e}2$	2	$P\bar{1}$	$P\bar{2}\bar{2}$	$\not{e}\bar{2}\bar{2}$	$a \wedge b \wedge c$
Monoclinic/inclined						
R_3	$\not{e}211$	3	$P112$	$P\bar{2}$	$\not{e}.\bar{2}$	$b \wedge c$
R_4	$\not{e}m11$	6	Pm	$P1$	$\not{e}1$	a
R_5	$\not{e}c11$	7	Pc	P_c1	$\not{e}_c1$	$aT_c{}^{1/2}$
R_6	$\not{e}2/m11$	10	$P2/m$	$P2\bar{2}$	$\not{e}2\bar{2}$	$a, b \wedge c$
R_7	$\not{e}2/c11$	13	$P2/c$	$P_a2\bar{2}$	$\not{e}_c2\bar{2}$	$aT_c{}^{1/2}, b \wedge c$
Monoclinic/orthogonal						
R_8	$\not{e}112$	3	$P112$	$P\bar{2}$	$\not{e}\bar{2}$	$a \wedge b$
R_9	$\not{e}112_1$	4	$P2_1$	$P\bar{2}_1$	$\not{e}\bar{2}_1$	$(a \wedge b)T_c{}^{1/2}$
R_{10}	$\not{e}11m$	6	Pm	$P1$	$\not{e}..1$	c
R_{11}	$\not{e}112/m$	10	$P2/m$	$P\bar{2}2$	$\not{e}\bar{2}2$	$a \wedge b, c$
R_{12}	$\not{e}112_1/m$	11	$P2_1/m$	$P\bar{2}_12$	$\not{e}\bar{2}_12$	$(a \wedge b)T_c{}^{1/2}, c$

4.3 Layer groups

For layer groups the two translation directions are a, b. There is a total of 80 layer groups. Tables 7, list the triclinic and monoclinic 3D layer groups with new geometric symbols and generators: Layer group number (col. 1), intern. layer group notation [42] (col. 2), related intern. 3D space group numbers [7] (col. 3), and notation [7] (col. 4), related geometric 3D space group notation [11] (col. 5), *geometric layer group notation* (col. 6), *geometric algebra generators* (col. 7). The layer groups are classified according to their 3D crystal system/2D Bravais system. The monoclinic/oblique(rectangular) system corresponds to the monoclinic/orthogonal(inclined) system of Fig. 9. Figure 10 shows the hexagonally centered cell with Bravais symbols H (space group) and h (layer group).

Table 7 Table of triclinic and monoclinic layer groups. The pure translators T_a, T_b are omitted.

Layer Group #	Intern. Notat.	3D Space Group #	Intern. 3D SGN	Geom. 3D SGN	Geom. Notat.	Layer Group Generators
Triclinic/oblique						
L_1	$p1$	1	$P1$	$P\bar{1}$	$p\bar{1}$	
L_2	$p\bar{1}$	2	$P\bar{1}$	$P\overline{2}\overline{2}$	$p\overline{2}\overline{2}$	$a \wedge b \wedge c$
Monoclinic/oblique						
L_3	$p112$	3	$P2$	$P\bar{2}$	$p\bar{2}$	$a \wedge b$
L_4	$p11m$	6	Pm	$P1$	$p..1$	c
L_5	$p11a$	7	Pc	P_a1	$p..{}_a1$	$cT_a{}^{\frac{1}{2}}$
L_6	$p112/m$	10	$P2/m$	$P\bar{2}2$	$p\bar{2}2$	$a \wedge b, c$
L_7	$p112/a$	13	$P2/c$	$P_a2\bar{2}$	$p\bar{2}2_a$	$a \wedge b, cT_a{}^{\frac{1}{2}}$
Monoclinic/rectangular						
L_8	$p211$	3	$P2$	$P\bar{2}$	$p.\bar{2}$	$b \wedge c$
L_9	$p2_111$	4	$P2_1$	$P\bar{2}_1$	$p.\bar{2}_1$	$(b \wedge c)T_a{}^{\frac{1}{2}}$
L_{10}	$c211$	5	$C2$	$A\bar{2}$	$c.\bar{2}$	$b \wedge c, T_{a+b}^{1/2}$
L_{11}	$pm11$	6	Pm	$P1$	$p1$	a
L_{12}	$pb11$	7	Pc	P_a1	p_b1	$aT_b{}^{\frac{1}{2}}$
L_{13}	$cm11$	8	Cm	$A1$	$c1$	$a, T_{a+b}^{1/2}$
L_{14}	$p2/m11$	10	$P2/m$	$P2\bar{2}$	$p2\bar{2}$	$a, b \wedge c$
L_{15}	$p2_1/m11$	11	$P2_1/m$	$P2\bar{2}_1$	$p2\bar{2}_1$	$a, (b \wedge c)T_a{}^{\frac{1}{2}}$
L_{16}	$p2/b11$	13	$P2/c$	$P_a2\bar{2}$	$p_b2\bar{2}$	$aT_b{}^{\frac{1}{2}}, b \wedge c$
L_{17}	$p2_1/b11$	14	$P2_1/c$	$P_a2\bar{2}_2$	$p_b2\bar{2}_1$	$aT_b{}^{\frac{1}{2}}, (b \wedge c)T_a{}^{\frac{1}{2}}$
L_{18}	$c2/m11$	12	$C2/m$	$A2\bar{2}$	$c2\bar{2}$	$a, b \wedge c, T_{a+b}^{1/2}$

5 Conclusion

We have briefly reviewed the geometric algebra representation of three dimensional Euclidean space $\mathbb{R}^3$ in the so-called conformal model in the GA of $\mathbb{R}^{4,1}$, and its use for the representation of 2D and 3D point groups and space groups. The key point is to only use physical crystal lattice vectors for the group generation. The second part introduced the interactive software visualization of 3D space group symmetries based on the established geometric algebra representation. This implementation uses the conformal model both for generating the graphics itself and for internally computing with space group transformations.

Future options are the visualization of *non-characteristic space group orbits* [43] and *magnetic space groups* [44]. The latter seems particularly attractive as it may nicely integrate the bivector representation of spin [9] in the real Dirac-Hestenes equation of relativistic quantum physics. Based on CLUCalc [34] a first rudimentary geometric algebra *protein visualizer* has been programmed recently for proteins of several thousand (up to 10 000) atoms. A possible future molecule (or ion group) toolbox may therefore be able to display complex biomolecule crystals as well.

We have further devised a new Clifford geometric algebra representation for the 162 subperiodic space groups using versors. In the future this may also be extended to *magnetic subperiodic space groups* [45]. We expect that the present work forms a suitable foundation for interactive visualization software of subperiodic space groups similar to the SGV visualization of the 3D space groups of section 3. Fig. 11 shows how the rod groups 13: $\not{p}\bar{2}\bar{2}\bar{2}$ and 14: $\not{p}\bar{2}_1\bar{2}\bar{2}$, and the layer group 11: $p1$ might be visualized in the future, based on [33, 35].

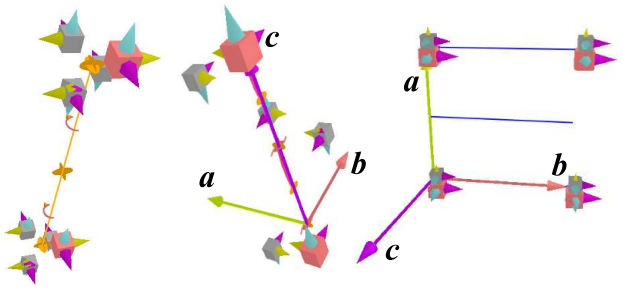

Fig. 11 How a future subperiodic space group viewer software might depict rod groups 13: $\not{p}\bar{2}\bar{2}\bar{2}$ and 14: $\not{p}\bar{2}_1\bar{2}\bar{2}$, and the layer group 11: $p1$, based on [33, 35].

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