New views of crystal symmetry guided by profound admiration of the extraordinary works of Grassmann and Clifford

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Abstract. This paper shows how beginning with Justus Grassmann’s work, Hermann Grassmann was influenced in his mathematical thinking by crystallography. H. Grassmann’s Ausdehnungslehre in turn had a decisive influence on W.K. Clifford in the genesis of geometric algebras. Geometric algebras have been expanded to conformal geometric algebras, which provide an ideal framework for modern computer graphics. Within this framework, a new visualization of three-dimensional crystallographic space groups has been created. The complex beauty of this new visualization is shown by a range of images of a diamond cell. Mathematical details are given in an appendix.

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1. Introduction

Already Hermann Grassmann’s father Justus (1829, 1830) published two works on the geometrical description of crystals, influenced by the earlier works of C.S. Weiss (1780-1856) on three main crystal forces governing crystal formation. In his 1840 essay on the derivation of crystal shapes from the general law of crystal formation, Hermann established the notion of a three-dimensional vectorial system of forces with rational coefficients, that represent the interior crystal structure, regulate its formation, its shape and physical behavior. In the Ausdehnungslehre 1844 (§171), he finally writes: I shall conclude this presentation...
by one of the most beautiful applications which can be made of the science treated, i.e. the application to crystal figures [Scholz 1996]. The geometry of crystals thus certainly influenced the Ausdehnungslehre.

Grassmann’s work in turn influenced W.K. Clifford [Clifford 1878] in England: I propose to communicate in a brief form some applications of Grassmann’s theory . . . I may, perhaps, therefore be permitted to express my profound admiration of that extraordinary work, and my conviction that its principles will exercise a vast influence upon the future of mathematical science. Conformal Clifford (geometric) algebra has in turn led at the beginning of the 20th century to a new fully geometric description of crystal symmetry in terms of so-called versors [Hestenes & Holt 2007]. Versors are simply (Clifford) geometric products of five-dimensional vectors conformally representing general planes in three-dimensional (3D) Euclidean space (by their 3D normal vector and the directed distance from the origin). Each plane’s vector geometrically represents a reflection at the plane, the geometric products of several plane vectors represents the combination of reflections at the respective planes (Cartan-Dieudonné).

As expected three crystal specific 3D vectors are enough to construct all symmetry versors of any type of crystal. With the geometric algebra capable graphics software CLUCalc [Perwass 2001] this concept can be implemented in every detail, such that the abstract beauty of the enormously rich symmetry of crystals can be fully visualized by state-of-the-art 3D computer graphics: The Space Group Visualizer (SGV), a tailor-made CLUCalc Script [Hitzer & Perwass 2006, Perwass & Hitzer 2009, Perwass & Hitzer 2005b, Hitzer & Perwass 2004, Perwass & Hitzer 2005b, Hitzer & Perwass 2005a]. To be precise, the SGV is thus capable of showing every plane of reflection and glide-reflection symmetry, all axis of rotations, screw-rotations and rotary inversions, and every center of inversion. It further allows to dynamically visualize the action of any symmetry operation on a general element (representing atoms, molecules or ions).

We thus have, 165 years after the Ausdehnungslehre of 1844, an explicit form of the beauty, which Grassmann may have had in mind, when he wrote eloquently: one of the most beautiful applications.

The next section uses the symmetries of diamond in order to demonstrate how the SGV visualizes space group symmetry. For mathematically interested readers the appendix introduces the Clifford geometric algebra description of crystallographic space groups.

2. Computer visualization of crystal symmetry

Geometrically a diamond cell lattice (type: face centered cubic = fcc) is highly symmetric. That means there is an enormous variety of possible geometric transformations, that leave the lattice as a whole invariant, including all lengths and angles. These symmetry operations include single cell transformations that leave a cell vertex point invariant: planes of reflections (through the vertex), rotations
Figure 1. Left: Diamond cell in Space Group Visualizer. Right: 24 general elements in 3D showing diamond point symmetry of one vertex.

(with axis through the vertex, and inversions \((x \mapsto -x\), centered at the vertex), and rotoinversions (inversions followed by a rotation). The 24 symmetry transformations of a diamond vertex point group create 24 symmetric copies of a general asymmetric element placed next to the invariant point, see Fig. 1 (left), or enlarged in Fig. 1 (right). In pure diamond one carbon atom is located at the center of this cluster (plus one at \(1/4\) distance away along a cubic space diagonal).

The inclusion of integer lattice translations (from fcc vertex to fcc vertex) can lead to new planes of reflection, see Fig. 2 (left). The combination of a plane of reflection with a lattice translation not perpendicular to the plane leads to a combined glide reflection, see Fig. 2 (right), where (red) vectors indicate the parallel glide motion. The perpendicular translation component displaces the reflection plane in normal direction, and the parallel translation component creates a glide motion parallel to the plane. Pairs of characteristic diamond glides are shown in Fig. 3 (left).

A sequence of two reflections at two planes results in a rotation, see Fig. 3 (right). This rotation has the intersection line of the two planes as its axis and twice the (dihedral) angle between the two planes is the resulting rotation angle. All the rotation axis seen in Fig. 3 (right) are lines of intersection of reflection planes of Fig. 2 (left). A lattice translation perpendicular to the rotation axis after a rotation, effectively creates another rotation also already contained in Fig. 3 (right). But if we perform a translation not normal to the rotation axis, with a translation component parallel to the rotation axis, we get a new transformation, a so-called screw. So a screw is a rotation followed by a translation along the screw axis, resulting in a directed helical motion around the screw axis, see Fig. 4 (left).
Combining an inversion with a subsequent lattice translation yields a new center of inversion, see Fig. 4 (right). The combination of an inversion with a rotation leads to a rotoinversion. Characteristic for the diamond lattice are the $90^\circ$
Figure 4. Left: All screw symmetry axis of diamond. Right: All centers of inversion symmetry of diamond.

Figure 5. Left: All centers of inversion symmetry of diamond. Right: Diamond cell in Space Group Visualizer.

rotoinversions depicted in Fig. 5 (left). The total graphical depiction of these symmetries in Fig. 5 (right) gives an idea of the intricate complexity of the symmetries.
possessed by the diamond lattice. The International Tables of Crystallography, Vol. A [Hahn 2005], abbreviated ITA, depict the symmetries of diamond by showing a quarter of an orthographic 2D projection of a side of a cubic cell. The SGV allows to open an extra window with the ITA online and navigate synchronously in both, see Fig. 6 (left).

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Appendix A. Clifford geometric algebra description of space groups

A.1. Cartan-Dieudonné and geometric algebra

Clifford's associative geometric product $[\text{Clifford 1878}]$ of two vectors simply adds the (symmetric) inner product to the (anti-symmetric) outer product of Grassmann

$$ab = a \cdot b + a \wedge b.$$  \hfill (A1)

The mathematical meaning of the left and right side of (A1) is clear from applying the geometric product to the $n$ orthonormal basis vectors $\{e_1, \ldots, e_n\}$ of the underlying vector space $\mathbb{R}^{p,q}$, $n = p + q$. We thus have

$$e_k e_k = e_k \cdot e_k = +1, \quad e_k \wedge e_k = 0, \quad 1 \leq k \leq p,$$

$$e_k e_k = e_k \cdot e_k = -1, \quad e_k \wedge e_k = 0, \quad p + 1 \leq k \leq n,$$

$$e_k e_l = -e_l e_k = e_k \wedge e_l, \quad e_k \cdot e_l = 0, \quad l \neq k, \quad 1 \leq k, l \leq n.$$  \hfill (A3)

Under this product parallel vectors commute and perpendicular vectors anticommute

$$ax = x | a, \quad ax = -x \perp a.$$  \hfill (A5)

This allows to write the reflection of a vector $x$ at a hyperplane through the origin with normal $a$ as (see left side of Fig. 7)

$$x' = -a^{-1} xa, \quad a^{-1} = \frac{a}{a^2}.$$  \hfill (A6)
The composition of two reflections at hyperplanes, whose normal vectors \( \mathbf{a}, \mathbf{b} \) subtend the angle \( \alpha/2 \), yields a rotation around the intersection of the two hyperplanes (see center of Fig. 7) by \( \alpha \):

\[
\mathbf{x}'' = (\mathbf{ab})^{-1} \mathbf{x} \mathbf{ab}, \quad (\mathbf{ab})^{-1} = \mathbf{b}^{-1} \mathbf{a}^{-1}.
\]  

(A7)

Continuing with a third reflection at a hyperplane with normal \( \mathbf{c} \) according to the Cartan–Dieudonné theorem yields rotary reflections (equivalent to rotary inversions with angle \( \alpha - \pi \)) and inversions

\[
\mathbf{x}' = - (\mathbf{abc})^{-1} \mathbf{x} \mathbf{abc}, \quad \mathbf{x}'' = - i^{-1} \mathbf{x} i, \quad i \doteq \mathbf{a} \wedge \mathbf{b} \wedge \mathbf{c},
\]  

(A8)

where \( \doteq \) means equality up to non-zero scalar factors (which cancel out in (A9)).

In general the geometric product of \( k \) normal vectors (the versor \( \mathbf{S} \)) corresponds to the composition of reflections to all symmetry transformations [Hestenes & Holt 2007] of two-dimensional (2D) and 3D crystal cell point groups (also called crystal classes)

\[
\mathbf{x}' = (-1)^k \mathbf{S}^{-1} \mathbf{x} \mathbf{S}.
\]  

(A9)

A.2. Two dimensional point groups

2D point groups [Hestenes & Holt 2007] are generated by multiplying vectors selected [Hitzer & Perwass 2004, Hitzer & Perwass 2005a, Perwass & Hitzer 2005b] as in Fig. 8. The index \( p \) denotes these groups as in Table 1. For example the trigonal (square) point group (the symmetry group of the reg. triangle (square), leaving the center point invariant) is given by multiplying its two generating vectors \( \mathbf{a}, \mathbf{b} \)

\[
3 = \{ \mathbf{a}, \mathbf{b}, R = \mathbf{ab}, R^2, R^3 = -1, aR^2 \}.
\]  

(A10)

\[
4 = \{ \mathbf{a}, \mathbf{b}, R = \mathbf{ab}, R^2, R^3, R^4 = -1, aR^2, bR^2 \}.
\]  

(A11)
Figure 8. Regular polygons \((p = 1, 2, 3, 4, 6)\) and point group generating vectors \(\mathbf{a}, \mathbf{b}\) subtending angles \(\pi/p\) shifted to center.

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

| Crystal        | Oblique | Rectangular | Trigonal | Square | Hexagonal |
|----------------|---------|-------------|----------|--------|-----------|
| geometric      | 1       | 2           | 1        | 2      | 3         |
| international  | 1       | 2           | m        | mm     | 3m        |

In \((A10)\) and \((A11)\) the vectors \(\mathbf{a}, \mathbf{b}\) represent reflections \((A6)\) at lines normal to \(\mathbf{a}, \mathbf{b}\) and passing through the center of the reg. triangle (square) of Fig. 8. The rotor \(R = \mathbf{ab}\) represents as in \((A7)\) a double reflection at the two lines passing through the center and normal to \(\mathbf{a}\) and \(\mathbf{b}\), respectively. Because \(\angle(\mathbf{a}, \mathbf{b}) = 60^\circ\) \((45^\circ)\), the resulting rotation is by \(2 \times 60^\circ = 120^\circ\) \((2 \times 45^\circ = 90^\circ)\) around the center. The cyclic rotation subgroups are denoted in Table 1 with bars, e.g.

\[
\bar{3} = \{R = \mathbf{ab}, R^3 = -1 \doteq 1\}, \quad \bar{4} = \{R = \mathbf{ab}, R^2, R^4 = -1 \doteq 1\}, \quad (A12)
\]

containing the three (four) symmetry rotations of the reg. triangle (square) of Fig. 8 around its invariant center by \(120^\circ\), and the multiples \(240^\circ\) and \(360^\circ\) \((90^\circ, 180^\circ, 270^\circ\) and \(360^\circ\)). The vectors \(\mathbf{a}R^2\) in \((A10)\), \(\mathbf{b}R^2\) in \((A11)\) are the normal directions of the remaining one (two) lines (passing through the center) of reflection symmetry.

A.3. Three dimensional point groups

The selection of three characteristic vectors \(\mathbf{a}, \mathbf{b}, \mathbf{c}\) (see Fig. 6 (right) for diamond) from each crystal cell is sufficient [Hestenes & Holt 2007, Hitzer & Perwass 2004, Hitzer & Perwass 2005a, Perwass & Hitzer 2005b] for generating all 3D point groups.

For the purpose of point groups keeping a single cell as a whole invariant, the vectors \(\mathbf{a}, \mathbf{b}, \mathbf{c}\) have always to be attached to the invariant cell center. These three vectors are normals of characteristic planes passing through the cell center. The plane reflections which the vectors represent and their combinations as in \((A6)\) to \((A9)\) constitute all point symmetries of the 3D crystal cells. The point symmetry transformations are applied to every vertex of a cell and keep the cell as a whole invariant, transforming each vertex into another vertex.

Using \(\angle(\mathbf{a}, \mathbf{b})\) and \(\angle(\mathbf{b}, \mathbf{c})\) (right side of Fig. 7) we can denote all 32 3D point groups as in Table 2 \((pq = 43\) for diamond\). Again the overbar notation,
Table 2. Geometric 3D point group symbols \cite{Hestenes2007} and generators with \( \mathbf{a}, \mathbf{b}, \mathbf{c} \): \( \angle(\mathbf{a}, \mathbf{b}) = \pi/p, \angle(\mathbf{b}, \mathbf{c}) = \pi/q, \angle(\mathbf{a}, \mathbf{c}) = \pi/2 \), \( p, q \in \{1, 2, 3, 4, 6\} \).

| Symbol | \( p = 1 \) | \( p \) | \( \tilde{p} \) | \( \tilde{p}q \) | \( \tilde{p}\bar{q} \) | \( \tilde{p}\bar{q} \) | \( \tilde{q} \) | \( \tilde{q} \) |
|--------|-------------|-------|-------------|-------------|-------------|-------------|-------------|-------------|
| Generators | \( \mathbf{a} \) | \( \mathbf{a}, \mathbf{b} \) | 1 | \( \mathbf{a}, \mathbf{b}, \mathbf{c} \) | \( \mathbf{a}, \mathbf{b}, \mathbf{c} \) | \( \mathbf{a}, \mathbf{b} \) | \( \mathbf{a}, \mathbf{b} \) | \( \mathbf{a}, \mathbf{b}, \mathbf{c} \) |

e.g. \( \tilde{p} \), means that the two vectors concerned are only to be used in their fixed rotor combination, e.g. \( \mathbf{a}, \mathbf{b} \). If the closed overbar extends over both indexes \( pq \) all three vectors are only to be used in the fixed rotoinversion (alias rotary reflection) combination \( \mathbf{a}, \mathbf{b}, \mathbf{c} \) of \( (\mathbf{A8}) \).

Note that the notation of Table 2 is fully isomorphic to the notation used in Table 2 of \cite{Coxeter1980}, with \( p, q \) in the very same roles.

A.4. Space groups

The smooth composition with translations is best done in the conformal model \cite{Lie1872,Ahlfors1986,Li2008} of Euclidean space (in the GA of \( \mathbb{R}^{4,1} \)), which adds two null-vector dimensions for the origin \( \mathbf{e}_0 \) and infinity \( \mathbf{e}_\infty \).

\[
X = \mathbf{x} + \frac{1}{2} \mathbf{x}^2 \mathbf{e}_\infty + \mathbf{e}_0, \quad \mathbf{e}_0^2 = \mathbf{e}_\infty^2 = X^2 = 0, \quad X \cdot \mathbf{e}_\infty = -1. \tag{A13}
\]

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

\[
X \cdot A = -\frac{1}{2} (\mathbf{x} - \mathbf{a})^2 \Rightarrow X \cdot (A - B) = 0, \quad m = A - B \propto \mathbf{n} - d \mathbf{e}_\infty, \tag{A14}
\]

where \( \mathbf{n} \) 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 \( t/2 \) we get the translation operator (by \( t \))

\[
X' = m' m X m m' = T_t^{-1} X T_t, \quad T_t = 1 + \frac{1}{2} t \mathbf{e}_\infty. \tag{A15}
\]

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 \( \mathbf{e}_\infty \) invariant. Now general translations and rotations are represented by geometric products of invertible vectors (called Clifford monomials, Lipschitz elements, or \textit{versors}).

Applying these techniques one can compactly tabulate geometric space group symbols and generators \cite{Hestenes2007}. Diamond has space group \( F\overline{4}3 \) with generators \( \{ \mathbf{a}T_{c/4}, \mathbf{b}, \mathbf{c}, \mathbf{T}_a, \mathbf{T}_b/2, \mathbf{T}_c/2 \} \) (SGV correction to \cite{Hestenes2007}).
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I wish to thank God for his wonderful creation with the words of H. Grassmann: Ich glaube also den in der Bibel geoffenbarten Wahrheiten nicht darum, weil sie in der Bibel stehen, sondern weil ich ihre seligmachende Kraft, ihre ewige, göttliche Wahrheit in meinem Bewußtsein erfahren habe. [Grassmann 1878] (English: I therefore believe the truths revealed in the Bible, not because they are written in the Bible, but because I have experienced in my own conscience their power of blessing, their eternal, divine truth.) I thank my family for their loving support, O. Giering, D. Hestenes, C. Perwass, M. Aroyo, D. Litvin, and H.-J. Petsche.

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