Interactive 3D
Space Group Visualizer

www.spacegroup.info

AsCA’06 Satellite Conference on Theoretical Crystallography & Material Science,
19 November 2006, Tsukuba, Japan
(IUCr Commission on Mathematical and Theoretical Crystallography)

Eckhard Hitzler (Fukui/Japan)
Christian Perwass (Kiel/Germany)

vectors \rightarrow \text{geometric product} \rightarrow \text{pointgroup} \rightarrow \text{spacegroups} \rightarrow \text{CLUCalc} \rightarrow \text{SGV} = \text{crystal class}
Acknowledgements

- How great are your works, O LORD, how profound your thoughts! (NIV: Psalm 92v5)
- C. Perwass, University of Kiel
- Students: D. Ichikawa, M. Sakai, K. Yamamoto, University of Fukui, GA group
- Mois Aroyo, University of Bilbao
- Organizers of MathCryst Satellite Workshop
I do thank my family

E. Hitzer
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Introduction
- Crystal Classes -
Crystals and bulk material properties

This conference also: G. Ferrari, D. Pandey, etc.

- Fe: bcc (lose p.) $\rightarrow$ fcc (close packed)
  - austenite

- 32 crystal classes (=32 point groups)
  - No center of inversion (20 of 32) $\Leftrightarrow$ piezoelectricity
  - 10 polar point groups (C_1, C_s, C_k, C_{kv}, k=2,3,4,6) $\Leftrightarrow$ pyroelectricity
  - Perovskite structure (like CaTiO_3) $\rightarrow$ ferroelectricity, catalysts, superconductivity
<table>
<thead>
<tr>
<th>Crystal type</th>
<th>ITC No.</th>
<th>Geom. Name</th>
<th>Int. Name</th>
<th>Schoenflies</th>
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<tbody>
<tr>
<td>triclinic</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>$C_1^*$</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>22</td>
<td>$\bar{1}$</td>
<td>$C_i$</td>
</tr>
<tr>
<td>mono-</td>
<td>3</td>
<td>2</td>
<td>2</td>
<td>$C_2^*$</td>
</tr>
<tr>
<td>clinic</td>
<td>4</td>
<td>1</td>
<td>$m$</td>
<td>$C_s^*$</td>
</tr>
<tr>
<td></td>
<td>5</td>
<td>22</td>
<td>$2/m$</td>
<td>$C_{2h}$</td>
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<td>orthorhombic</td>
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<td>22</td>
<td>222</td>
<td>$D_2$</td>
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<tr>
<td></td>
<td>7</td>
<td>2</td>
<td>$mmm$</td>
<td>$C_{2v}^*$</td>
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<td></td>
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<td>22</td>
<td>$mmm$</td>
<td>$D_{2h}$</td>
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<td>4</td>
<td>$C_4^*$</td>
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<td></td>
<td>11</td>
<td>42</td>
<td>$4/m$</td>
<td>$C_{4h}$</td>
</tr>
<tr>
<td></td>
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<td>42</td>
<td>422</td>
<td>$D_4$</td>
</tr>
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<td></td>
<td>13</td>
<td>4</td>
<td>$4mm$</td>
<td>$C_{4v}$</td>
</tr>
<tr>
<td></td>
<td>14</td>
<td>42</td>
<td>$42m$</td>
<td>$D_{2d}$</td>
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<td></td>
<td>15</td>
<td>42</td>
<td>$4/mmm$</td>
<td>$D_{4h}^*$</td>
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<tr>
<td>cubic</td>
<td>28</td>
<td>33</td>
<td>23</td>
<td>$T$</td>
</tr>
<tr>
<td></td>
<td>29</td>
<td>43</td>
<td>$m\bar{3}$</td>
<td>$T_h$</td>
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<tr>
<td></td>
<td>30</td>
<td>$\bar{4}3$</td>
<td>$432$</td>
<td>$O$</td>
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<td></td>
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<td>33</td>
<td>$\bar{4}3m$</td>
<td>$T_d$</td>
</tr>
<tr>
<td></td>
<td>32</td>
<td>43</td>
<td>$m\bar{3}m$</td>
<td>$O_h$</td>
</tr>
</tbody>
</table>

* polar (pyroelectric)
Geometric Approach to Symmetry
- Reflections & Rotations -
Geometric Product
W.K. Clifford 1878

- Vectors $a, b$:
  \[ ab = |a||b|(\cos \alpha + i \sin \alpha) \]
  \[ i = e_1 e_2 \ldots \text{ unit area element of } a, b \text{ plane} \]
- Inner part: symmetric, scalar
  \[ a \cdot b = (ab + ba)/2 = |a||b| \cos \alpha \]
- Outer part: anti-symmetric \(\bigwedge, \bigvee\) bivector
  \[ a \bigwedge b = (ab - ba)/2 = |a||b| i \sin \alpha \]
Reflection at plane

reverse component perp. to plane

\[ x' = -a^{-1}x \cdot a \]

\[ a^{-1} = a/a^2 \]
Reflection Formula

- Parallel vectors **commute**
  \[ ax_{\parallel} = x_{\parallel} a \]

- Perpendicular vectors **anticommutate**
  \[ ax_{\perp} = -x_{\perp} a \]

- Reflection
  \[ x' = -x_{\parallel} + x_{\perp} = -a^{-1}a x_{\parallel} + a^{-1}a x_{\perp} \]
  \[ = -a^{-1}(x_{\parallel} + x_{\perp})a = -a^{-1}xa \]
2 Reflections $\rightarrow$ 1 Rotation

Angles:
$\alpha_{x,x''} = 2 \alpha_{a,b}$

$x' = a^{-1} x a$

$x'' = b^{-1} a^{-1} x a b = (ab)^{-1} x a b$
**Rotary-Reflection**

\[ x' = - (abc)^{-1} x abc \]

**Inversion** \(i\)

\[ a \perp b \perp c \perp a, \text{ e.g. } e_1, e_2, e_3 \]

\[ x' = - (abc)^{-1} x abc = - i^{-1} x i = - x \]

**Rotary-Inversion ...**
Reflection Sequences

Result

Sequences of reflections generate

(1) Simple reflections \( x' = -a^{-1}x a \)
(2) Rotations
(3) Rotary-Reflections, Inversions
(4) Rotary-Inversions

-all transformations of

2D and 3D crystal cell point groups

E. Cartan 1920ies, Coxeter 1934, Coxeter & Moser 1957
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2D Point Groups
2D Point Groups

regular polygons (n=2,3,4,6)

2 vectors from each reg. polygon

select

Image: SnowCrystals.com
2D Point Groups

regular polygons (n=2,3,4,6)

2 vectors from each reg. polygon generate its 2D point groups

select
2D Point Group Generation

• n=1: identity \( I \)

• n=2: reflections \( a, b \), 180° rot. \( R=ab \), \( I \)

• n=3: reflections \( a, b, bR \)
  120° rot. \( R=ab, R^2, R^3 = -1 \)

• n=4: ref. \( a, b, aR^2, bR^2 \)
  90° rot. \( R=ab, R^2, R^3, R^4 = -1 \)

• n=6: ref. \( a, b, aR^2, bR^2, aR^4, bR^4 \)
  60° rot. \( R=ab, R^2, R^3, R^4, R^5, R^6 = -1 \)

Representations: Tables 1, 2 of ICNAAM 2005 proc., pp. 939, 940
32
3D Point groups
- Crystal classes -
Seven types of space lattices with:

- Triclinic
- Monoclinic
- Orthorhombic
- Tetragonal
- Trigonal
- Hexagonal
- Cubic

3 vectors from each cell generate all 32 point groups!

Select elementary cells.
3 vectors $a$, $b$, $c$ selected from each crystal cell:
### Hestenes and Holt’s Geometric Notation

Similar to Table 2 of Coxeter & Moser, 4th ed. 1980

<table>
<thead>
<tr>
<th>Point Group Symbol</th>
<th>Generators</th>
</tr>
</thead>
<tbody>
<tr>
<td>( p = 1 )</td>
<td>( a )</td>
</tr>
<tr>
<td>( p \square 1 )</td>
<td>( a, b )</td>
</tr>
<tr>
<td>( \overline{p} )</td>
<td>( ab )</td>
</tr>
<tr>
<td>( pq )</td>
<td>( a, b, c )</td>
</tr>
<tr>
<td>( \overline{p}q )</td>
<td>( ab, c )</td>
</tr>
<tr>
<td>( pq )</td>
<td>( a, bc )</td>
</tr>
<tr>
<td>( \overline{pq} )</td>
<td>( ab, bc )</td>
</tr>
<tr>
<td>( \overline{pq} )</td>
<td>( abc )</td>
</tr>
</tbody>
</table>

\[(ab)^p = (bc)^q = (ac)^2 = -1;\]

\[p, q \square \{1, 2, 3, 4, 6\}\]

+ Bravais letter + glide & screw indexes \(\rightarrow\) GA space group symbols
Holohedric Point Groups
- highest order -

triclinic | monoclinic | orthorhombic | tetragonal | trigonal | hexagonal | cubic
Monoclinic Point Group $C_{2h}^{22}$

- identity
  
- 1 reflection $c$
- 1 rotation (180º)
  
\[ R = a \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} b = ic \]
- inversion $i = cR$ 

Total: 4 symmetry transformations

Subgroups:

\[ 1 = \{ c, 1 \}, \quad 2 = \{ ic, 1 \} \]
Hexagonal Point Group \(D_{6h}^{62}\)

- 6 reflections
  - \(a, b, aR^2, bR^2, aR^4, bR^4\)
- 6 rots. (60°, 120°, 180°, 240°, 300°, 360°)
  - \(R=ab, R^2, R^3, R^4, R^5, 1\)
- 6 rotary-reflections
  - \(c, cR, cR^2, cR^3 = i, cR^4, cR^5\)
- six 180° rotations
  - \(ac, bc, acR^2, bcR^2, acR^4, bcR^4\)

Total: 24 symmetry transformations
Interactive Visualization
- 32 point groups -
3D Interactive Point Group Visualization

free download from www.spacegroup.info

Generate all 32 point groups by clicking successive reflections!
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2D Spacegroups
- Wallpaper groups -
What is a Spacegroup?

Reflections (Rotations, …)

\[ a, b, c \]

and Translations

\[ T(ka), T(lb), T(mc), \quad k, l, m \in \mathbb{Q} \]

fractions
**Conformal Model** of Euclidean space (double projective) in $Cl(4,1)$


For including translations

$\bar{n}^2 = 0$

$\bar{n}$

$\{e_1, e_2, e_3\} \boxtimes \bar{n}, n$

origin

infinity

$n^2 = 0$

$n$

$X^2 = 0$

$X \cdot Y = - (x - y)^2 / 2$

$x^2 = x + 1/2 x^2 n + \bar{n}$

$\bar{n}^2 = 0$

$\bar{n}$

$5D$

$X = X^0 + \frac{1}{2} x^2 n + \bar{n}$

$R^3$

19 Nov. 2006
Conformal 5D model of Euclidean space in $Cl(4,1)$

Vectors represent points $X, P, Q$ and (mid) planes $m, r$

$m r$ ... generates general rotations & translations

Conformal group $C(3) \cong$ Orthogonal group $O(4,1)$

Eucl. group $E(3) \equiv$ subgroup of $O(4,1)$ leaving infinity $n$ invariant.

Use of versor (vector product) representation.
2D Spacegroups - Notation

- Translator (by vector $t$) $X \rightarrow T^{-1} X T$

  $$T(t) = \exp(tn/2) = 1 + tn/2$$

- Center of 2 fold rotation

- Axis of reflection with generating vectors $a, b$

- Glide reflection, $aT(b/2), a \parallel b$

- Bravais: principle, centered, hexagonally centered

- Locating symmetries: $T(-t)$ generator $T(t)$
Rectangular 2D lattice

2D space group

No. 9

Geometric

c2 cmm

Centers of Rotation

ab \ T([a+b]/2)

located at*

(a+b)/4+(ka+lb)/2,

k,l ⨁ ⨁

* with extra \( T(ka+lb) \)

Glide reflections:

\[ b \ T([a+b]/2) = \ T(-b/4) \quad \overline{b} \ T(a/2) \quad \ T(b/4) \]

located at*

b/4+lb/2, \ l ⨁ ⨁
230
3D Spacegroups
- Crystallographic Symmetry -
Example:
Monoclinic 3D Space Groups
### Example: 13 Monoclinic Space Groups

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>P2</td>
<td>P2</td>
<td>P2</td>
<td>ic = a ∧ b</td>
</tr>
<tr>
<td>4</td>
<td>P2₁</td>
<td>P2₁</td>
<td>P2₁</td>
<td>icT(½c)</td>
</tr>
<tr>
<td>5</td>
<td>C2</td>
<td>A2</td>
<td>A2</td>
<td>ic, T(½(b + c))</td>
</tr>
<tr>
<td>6</td>
<td>Pm</td>
<td>P1</td>
<td>P1</td>
<td>c</td>
</tr>
<tr>
<td>7</td>
<td>Pc</td>
<td>Pa₁</td>
<td>Pa₁</td>
<td>cT(½a)</td>
</tr>
<tr>
<td>8</td>
<td>Cm</td>
<td>A1</td>
<td>A1</td>
<td>c, T(½(b + c))</td>
</tr>
<tr>
<td>9</td>
<td>Cc</td>
<td>Aa₁</td>
<td>Aa₁</td>
<td>cT(½a), T(½(b + c))</td>
</tr>
<tr>
<td>10</td>
<td>P2/m</td>
<td>P22</td>
<td>P22</td>
<td>c, ic</td>
</tr>
<tr>
<td>11</td>
<td>P2₁/m</td>
<td>P22₁</td>
<td>P22₁</td>
<td>c, icT(½c)</td>
</tr>
<tr>
<td>12</td>
<td>C2/m</td>
<td>A22</td>
<td>A22</td>
<td>c, ic, T(½(b + c))</td>
</tr>
<tr>
<td>13</td>
<td>P2/c</td>
<td>Pa22</td>
<td>Pa22</td>
<td>cT(½a), ic</td>
</tr>
<tr>
<td>14</td>
<td>P2₁/c</td>
<td>Pa22₁</td>
<td>Pa22₁</td>
<td>cT(½a), icT(½c)</td>
</tr>
<tr>
<td>15</td>
<td>C2/c</td>
<td>Aa22</td>
<td>Aa22</td>
<td>cT(½a), ic, T(½(b + c))</td>
</tr>
</tbody>
</table>

Multivector generators, except T(a), T(b), T(c).

Monoclinic Space Group P2₁/m [P2̅2₁]  

**Kinoite**  
**Ca₂Cu₂Si₃O₈(OH)₄**  

**Axial Ratios:**  
\[ a : b : c = 0.5422 : 1 : 0.4386 \]  

**Cell Dimensions:**  
\[ a = 6.99, \, b = 12.89, \, c = 5.654, \, Z = 2; \]  
\[ \text{angle beta} = 96.08° \]  

P2\overline{2}_1\ symmetries from generator [products:

- Multiplying \( i c T(c/2), c T(c/2) \) and \( T(a), T(b), T(c) \)
  - Screw: \( T(c) \approx [icT(c/2)]^2 \)
  - Mirror: \( c T(c/2) T(kc) = T^{-1} \left( \frac{1}{4} c + \frac{1}{2} kc \right) c T \left( \frac{1}{4} c + \frac{1}{2} kc \right), k \in \mathbb{Z} \)
  - Family of inversions at \( (ka+lb+mc)/2 \)
    \( ic T(c/2) c T(c/2) \approx i, iT(ka+lb+mc) = T^{-1/2}(ka+lb+mc) iT^{1/2}(ka+lb+mc), k, l, m \in \mathbb{Z} \)
  - Family of screws at \( (ka+lb)/2 \)
    \( ic T(c/2) T(ka+lb) = T^{-1} (ka+lb) ic T(c/2) T^2 (ka+lb), k, l \in \mathbb{Z} \)
symmetries from generator products

$P\bar{2}1$

screw axis

reflection plane

inversion center

general element

$i = a \sqcap b c$

c$T(c/2)$

$\alpha \sqcap bT(c/2)$

http://webmineral.com/data/Kinoite.shtml

element:

Kinoite
Interactive Visualization
- software -
Interactive Software Implementation

- (Clifford) Geometric Algebra with
- Visual software CLUCalc (OpenGL graphics)
  - www.clucalc.info with
- Script 1: **Point Group Visualizer** free
- Script 2: **Space Group Visualizer** free demo
- Info and (sample) download at
  - www.spacegroup.info
The Space Group Visualizer
- 230 space groups -
Degree of Implementation of SG Visualizer (by 16 Nov. 2006)

- Triclinic: all
- Monoclinic: all
- Orthorhombic: all
- Tetragonal: 1 of 68
- Trigonal: all
- Hexagonal: all
- Cubic: 1 of 36
Space Group Visualizer Screen Shot

Select Space Group here

Symmetry Menu

Visualization Window

Drag border to see all tools

Info Window

Tool Window
Selecting crystal class and space group

<table>
<thead>
<tr>
<th>Step 1</th>
<th>Step 2</th>
<th>Step 3</th>
<th>Selection done</th>
</tr>
</thead>
<tbody>
<tr>
<td>Currently selected:</td>
<td>Currently selected:</td>
<td>Currently selected:</td>
<td>Currently selected:</td>
</tr>
<tr>
<td>- Nothing</td>
<td>- (list) Monoclinic</td>
<td>- (list) Monoclinic</td>
<td>- (list) Monoclinic</td>
</tr>
<tr>
<td>Select crystal system:</td>
<td>Select point group:</td>
<td>Select space group:</td>
<td>Selection complete</td>
</tr>
<tr>
<td>- Monoclinic</td>
<td>- No Int. Geo.</td>
<td>- No Int. Geo.</td>
<td></td>
</tr>
<tr>
<td>- Orthorhombic</td>
<td>3 2 2</td>
<td>10 P2/m P22</td>
<td></td>
</tr>
<tr>
<td>- Trigonal</td>
<td>4 m 1</td>
<td>11 P2_1/m P22_1</td>
<td></td>
</tr>
<tr>
<td>- Hexagonal</td>
<td>5 2/m 22</td>
<td>12 C2/m C22</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>13 P2/c P_c22</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>14 P2_1/c P_c22_1</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>15 C2/c C_c22</td>
<td></td>
</tr>
</tbody>
</table>

Help
Tools:
- Use tools 'Element offset' to move the asymmetric elements away from a centered position.
Current SGV Functionality (version 1.1)

- 3 Vector Basis
- General positions (Loci)
- General positions 3D offsets (x,y,z)
- Unit Cell Lattice
- 3D Cell Count (X,Y,Z)
- Change of free parameters (lengths a,b,c and angles)
- View Angle
- Fog Density

- Cell Type (ITC, GA, ...)
- B/W color scheme backgrd.
- Standard/central lighting

- Symmetries by category
  - Inversions
  - Reflections
  - Glide reflections
  - Rotations
  - Screws

- Symmetry selection by
  - Orientation, Location, Generator, ...

Demo, Design
Open SGV Design Questions

- 3D graphics symmetry symbols ↔ printed IT symbols?
- Standalone ↔ Plugin?
- Offspin: VRML?
- Visible menu ↔ context menu?
- Positioning of glide vectors when glide planes intersect?
- What other functions of interest?
Conclusions
Conclusions

- **Geometric Algebra** with Conformal Model of $\mathbb{R}^3$ represents 2D, 3D Pointgroups and Spacegroups
- Generation only by **physical vectors** of cell (lattice)
- **Interactive software** Space Group Visualizer

Future

- **Full** 3D space groups (230) visualization by 2007.
- **Applications** of Geometric Algebra (multivector Four. T., structure solution, molecules, real time cavities, …)
- **Paradigm** for practical combination of geometry & algebra
More Information

- internet, literature -
More Information

- Geometric Calculus Fukui
  http://sinai.mech.fukui-u.ac.jp/gcj/gcjportal.html

- Cognitive Systems Group (Kiel)
  http://www.ks.informatik.uni-kiel.de/

- Visualization software

D. Hestenes, J. Holt, recent *JMP* preprint.

J.D.M. Gutierrez, *Operaciones de simitria mediante algebra geometrica aplicadas a grupos cristalograficos*, Tesis, UNAM, Mexico 1996.

Literature – E. Hitzer / C. Perwass

Geometric Algebra background


Point Group Visualizer (theory and use)


Space Group Visualizer (theory and use)


Online available from: http://sinai.mech.fukui-u.ac.jp/gcj/pubs.html
Literature on Conformal Model


Halite
NaCl

Soli Deo Gloria

Image: minerali.it

end - fin