

INTERACTIVE VISUALISATION OF FULL GEOMETRIC DESCRIPTION OF CRYSTAL SPACE GROUPS

Christian Perwass¹ and Eckhard Hitzer²

¹Department of Computer Science, Christian-Albrechts-University Kiel, Kiel 24103, Germany

²Department of Applied Physics, University of Fukui, Fukui 910-8507, Japan

ABSTRACT

In this text we present a software tool that visualises the symmetry properties of the space groups of 3D Euclidean space, which play an important role in the investigation of crystalline materials. The main source that lists the properties of all space groups are the “*International Tables For Crystallography, Volume A*” [1], where the symmetries are shown in three orthographic projections. It is clearly much more intuitive to look at these symmetry properties in a 3D visualisation. The visualisation software presented here (for monoclinic crystals) allows the user to look at the space group symmetries from any view point and to modify lattice parameters in real time. The visualisation software is freely available from www.spacegroup.info.

1. INTRODUCTION

The main source describing the properties of the 230 space groups are the “*International Tables for Crystallography, Volume A*” [1] (ITC), where the symmetry properties are visualised as three orthographic projections along the lattice axes. The motivation to develop a visualisation tool for the space groups of 3D-Euclidean space is the simple fact that it is clearly much more intuitive to see the symmetries visualised in 3D and to be able to look at the crystal structure from any angle. This may not only help people who start learning about space group symmetries but also those who work with space groups on a daily basis.

There are quite a number of software programs available that visualise the crystal structures of 3D space groups, see e.g. [9, 10]. However, we not only visualise the positions of the atoms or molecules in a crystal, but also the symmetries themselves. Furthermore, the visualisation can be adopted interactively by the user.

Internally the space group symmetries are represented by operators of the Geometric Algebra [2]. To look at visualisations, users do not need to know anything about Geometric Algebra. However, this representation is not only advantageous for the internal calculations of the visualisation software but it is also useful for the representation of space group symmetries in general, due to its independence on a basis or a particular choice of origin.

The representation of group symmetries by geometric products of crystal vectors was first introduced by David Hestenes [2]. Eckhard Hitzer and Christian Perwass have since used this description to visualise point groups and 2D space groups (wallpaper groups) [3]. We will not give an introduction to Geometric Algebra here but would like to refer the interested reader to [1, 2, 3, 4, 5, 6].

The basic idea behind the structure of the space group visualisation software is that the space group symmetries are defined in XML files, which are then interpreted and visualised. The XML data structure used is described in the manual included with the *Space Group Visualiser* (SGV) software [8]. The advantages of using XML to define the space groups are:

- the space groups can be defined without detailed knowledge of the visualisation software,
- the XML data files are easily extendable without generating incompatibilities with older versions of the visualisation software,
- the XML files may also be used by other software.

The plan for the remainder of this text is as follows. Since the visualisation software is a script for the software program CLUCalc [7], we first describe CLUCalc itself. Then the usage of the space group visualisation script is described

and example visualisations are shown. We conclude the text with a summary of the software features.

2. THE CLUCALC SOFTWARE

The program CLUCalc [7] is an interactive visualisation tool, which is freely available. CLUCalc was initially developed to visualise Geometric Algebra. However, it has by now become a general visualisation tool, which is well suited to quickly develop interactive visualisations and tutorials. Some of the most important features of CLUCalc are:

- direct user interaction through mouse input, dialog elements and text links,
- easy plotting of parametric surfaces,
- automatic analysis and visualisation of Geometric Algebra entities,
- simple texture mapping of basic geometric entities and arbitrary surface plots,
- rendering and plotting or texture mapping of LaTeX code,
- reading, writing and manipulation of images in various formats,
- preparation of presentations with interactive 3D-graphics.

All features of CLUCalc are described in an online manual that can be found at [7]. We will now give two simple examples to demonstrate the power of CLUCalc.

The script language used by CLUCalc is similar to the C-programming language but has been geared towards the direct usage of mathematical symbols. In this way, mathematical expression can be written in the script language more or less as they are written on paper. The following script generates the image shown in figure 1.

```
imgTex = ReadImg("cog_siegel.png");
SetTexture(imgTex);
:White;
:Plot(VecE3(s, sin(s)*cos(t), -t),
      [s, -Pi, Pi, 10],
      [t, -Pi, Pi, 10]);
```

The following CLUScript visualises a plane passing through three points in projective space with texture mapping. The result can be seen in figure 2.

```
imgTex = ReadImg("cog_siegel.png");

:a = VecP3(1,0,0) :Red;
:b = VecP3(0,1,0) :Green;
:c = VecP3(0,0,1) :Blue;

SetTexture( imgTex );
:Yellow + Alpha;
:a^b^c; // The plane through a,b,c
```

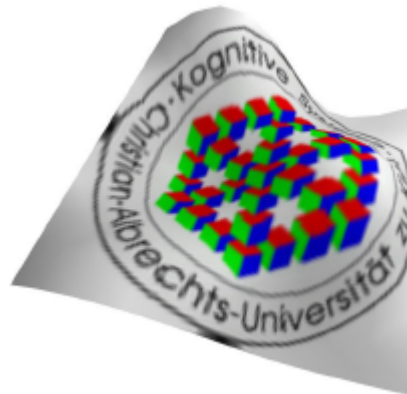


Fig.1 Result of first example script.

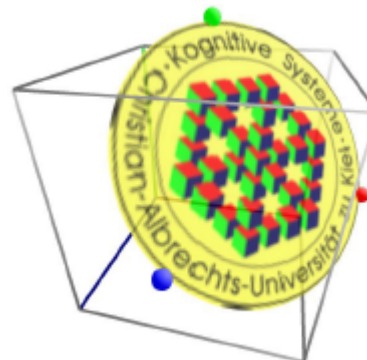


Fig.2 Result of second example script.

A large number of example scripts are included in the CLUCalc distribution. Presentations and tutorials using CLUCalc can also be found on [7].

3. SPACE GROUP VISUALISATION

The space group visualisation CLUScript that will be discussed in the following is called “Space Group Visualiser” (SGV). After starting the SGV you see a visualisation as shown in figure 3.

To the left is the “info window” in which you can choose the currently displayed space group by clicking on the blue ‘list’ links. The choice is

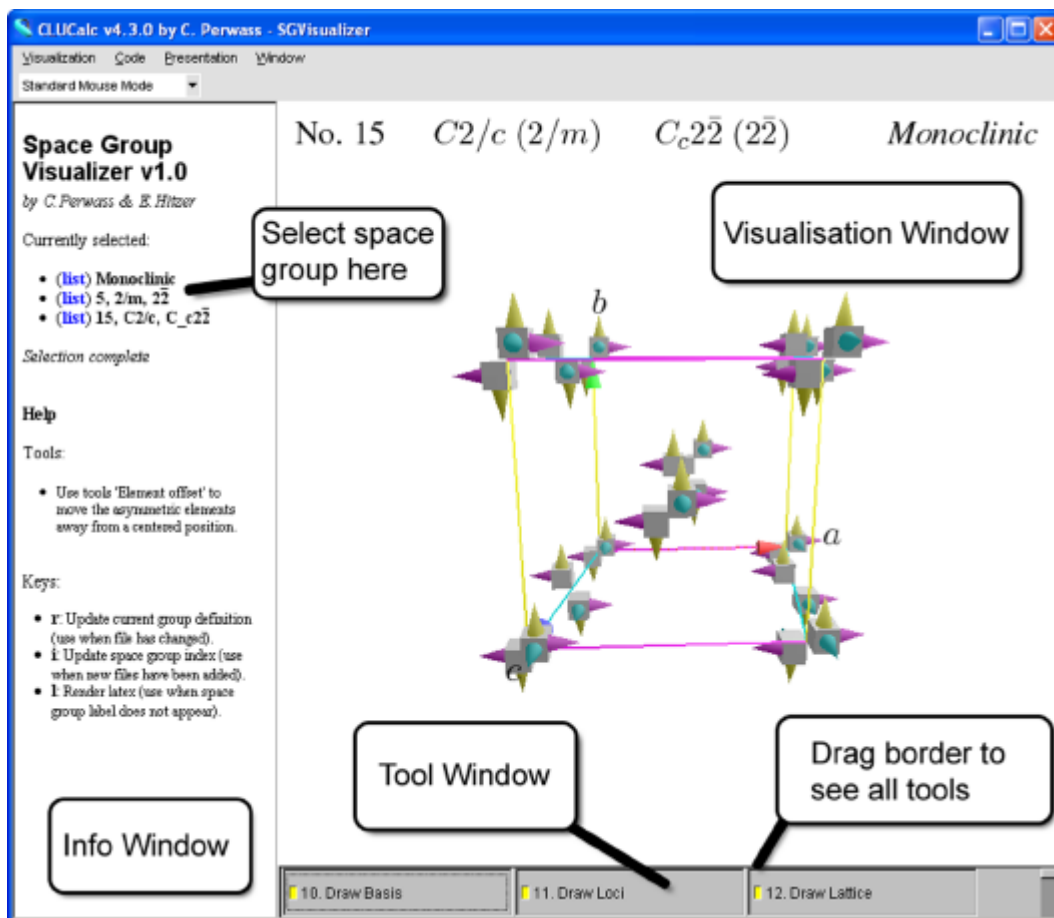


Fig.3 “Space Group Visualiser“ main window.

done by first selecting the crystal system (e.g. *monoclinic*) then the point group and finally the space group. The point group and space group are denoted in three different ways: their ITC number, the international symbol and the new geometric annotation. The size of the info window can be changed by dragging its right border with the mouse.

The “*tool window*” at the bottom contains a number of tools that allow you to modify the visualisation. You can drag the top border of the tool window in order to display all tools. Alternatively you can use the scroll bar to the right of the tool window to scroll through all tools.

Above the tool window is the actual “*visualisation window*”. You can rotate the visualisation by placing the mouse pointer into this window, holding down the left mouse button and moving the mouse. If you hold down the **SHIFT** button at the same time you can rotate

about two alternative axes. Also note that you can select **Local Rotation** in the **Visualisation** menu to rotate the visualisation in a different way.

If you hold down the right mouse button instead of the left, you can translate the visualisation. By holding the **SHIFT** button at the same time you can translate the visualisation up/down and left/right instead of away/towards and left/right.

3.1. Tools

The tools available in the SGV are shown in figure 4.

- **Draw Basis.** If this is selected the generator basis vectors are drawn and labelled. These vectors need not be identical with the lattice basis. They only form the vectors from which the symmetry generators are constructed.

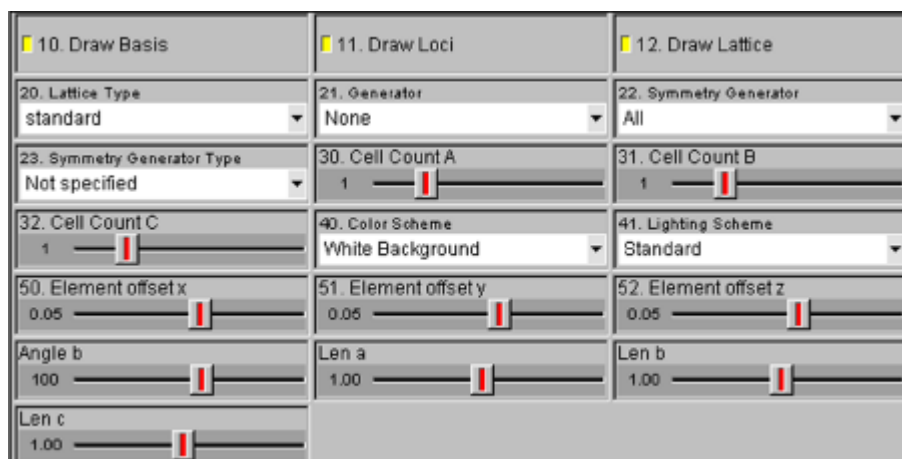


Fig.4 Available tools in *Space Group Visualiser*.

- **Draw Loci.** If this is selected, asymmetric elements are drawn at the loci (locations) generated through the space group symmetries. In real crystals there are molecules at these positions. An asymmetric element is necessary to show the relation to the initial element, which is located near the origin of the vectors **a**, **b** and **c**.
- **Draw Lattice.** If selected the lattice is drawn.
- **Lattice Type.** Whether different lattice types are available depends on the space group currently displayed. Select here the lattice that is to be display.
- **Generator.** Here a basis generator (symmetry) that is to be drawn can be selected. These generators basically form the group basis. That is, all products of these generate the whole space group.
- **Symmetry Generator.** Select here the symmetry that is to be visualised.
- **Symmetry Generator Type.** If the selection is 'All' in the **Symmetry Generator** tool, the type of symmetry that is to be visualised can be selected here. For example, you can select here '**Rotation**' to visualise only the rotation symmetries.
- **Cell Count.** The three cell count tools allow you to select how many crystal layers are drawn in the three lattice directions. This even allows you to draw the point group symmetries or the 2D-
space group symmetries.
- **Color Scheme.** Here a color scheme can be selected. For example, the **White Background** color scheme is useful to store visualisations for printing on paper.
- **Lighting Scheme.** Selecting '**standard**' here results in a well lit scene. The lighting scheme '**centered**' places a light in the center of the visualisation, which gives a good impression of the 3D structure.
- **Element Offset.** The three element offset sliders allow you to move the initial asymmetric element away from the origin. By default it is already placed away from the origin, so that all symmetry transformations can be seen clearly.
- **Angle.** The number of these types of sliders depends on the space group currently selected. For example, in the monoclinic crystal system, one angle in the crystal lattice can change without invalidating any symmetries. By changing this value you can see what this potential change looks like.
- **Len.** The number of these sliders depends again on the space group currently selected. They control the length of the lattice basis vectors. For example, in the monoclinic crystal system the lengths of all three basis vectors can be chosen arbitrarily, while in other systems certain lengths may be fixed.

3.2. Symmetry Visualisation

In this section it is shown how the various symmetries of space groups are visualised.

- **Rotational Symmetry**

This is visualised as a rotation axis together with an arc in the rotation plane indicating the rotation angle, as shown in figure 5. Note that a 180 degree rotation is equivalent to a reflection on the rotation axis line.

- **Screw Motion Symmetry**

A screw motion is a rotation together with a translation in the direction of the rotation axis. This is visualised as a rotation axis together with a twisted band spiralling along the direction of translation and indicating the rotation angle, as shown in figure 6.

- **Reflection Symmetry**

A reflection symmetry is visualised as the reflection plane, as shown in figure 7.

- **Glide Reflection Symmetry**

A glide reflection is a reflection in a plane together with a translation along a direction in the plane. This is drawn as a reflection plane together with an arrow indication for direction and length of the translation, as shown in figure 8.

- **Inversion Symmetry**

An inversion is a reflection in a point. This is drawn as a transparent sphere centred on the inversion point, as shown in figure 9.

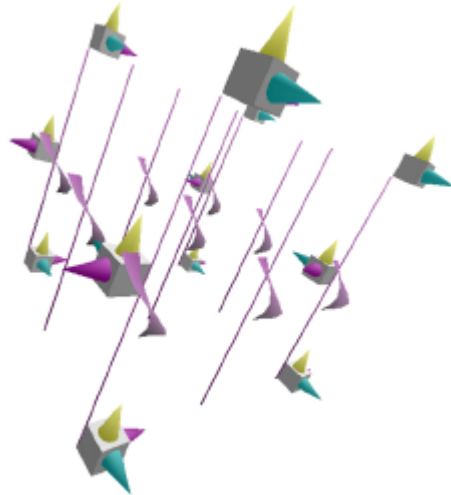


Fig.6 Visualisation of screw symmetry.

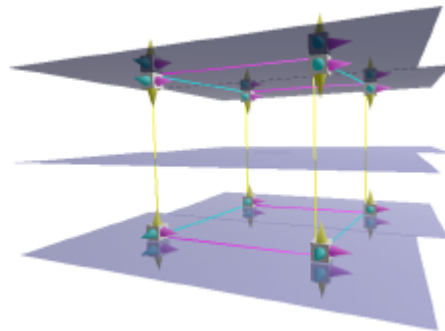


Fig.7 Visualisation of reflection symmetry.

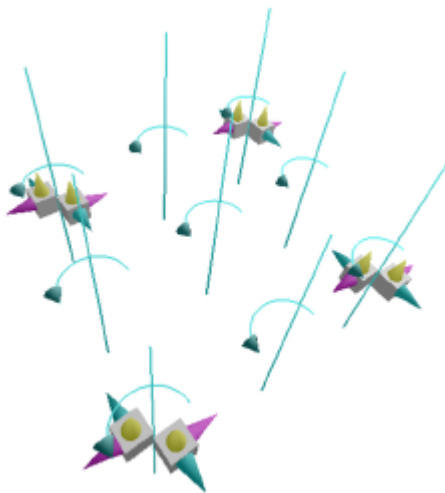


Fig.5 Visualisation of rotational symmetry

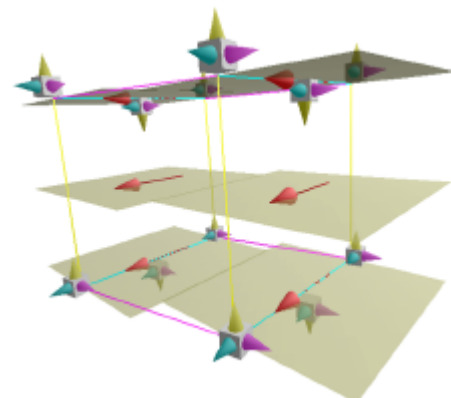


Fig.8 Visualisation of glide reflection.

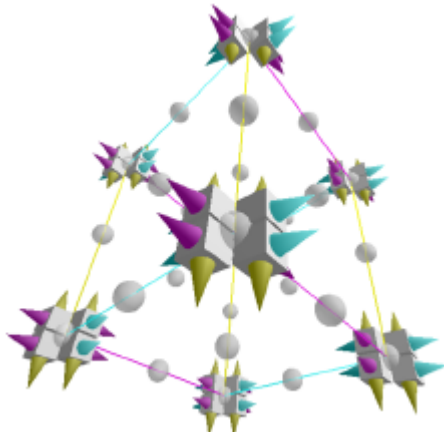


Fig.9 Visualisation of inversion symmetry.

4. CONCLUSIONS

In this text we have presented the software tool *Space Group Visualiser* for the 3D-visualisation of space group symmetries. This tool facilitates the understanding of the symmetry properties of 3D space groups, since it allows the user not only to view the symmetries from an arbitrary view point, but also lets the user visualise the symmetries selectively. That is, the user can choose exactly which part of the whole symmetry group to see. It is also possible to visualise a number of crystal cells or to reduce the visualisation to a plane or even a point. In this way, also the corresponding 2D-space groups (the wallpaper groups) and the corresponding point groups can be visualised.

So far, only the 13 monoclinic space groups have been defined. However, since the space group definitions are given in separate XML files, the remaining space groups can be added step by step in the future without the need to change the SGV script. The exact specification of the XML space group definition files is given in the manual that is included in the SGV distribution [8]. This should also allow the interested reader to enter the definition of space groups.

Future work on the SGV will mainly consist of preparing the XML space group definition files for the remaining space groups. Furthermore, additional methods of selecting particular symmetries and alternative visualisations will be investigated, whereby feedback from users will be very welcome and of high importance.

REFERENCES

1. T. Hahn (ed.): *Space-Group Symmetry*, volume A of *International Tables for Crystallography*, 5th ed., Springer.
2. D. Hestenes: *Point Groups and Space Groups in Geometric Algebra*, in *Applications of Geometric Algebra in Computer Science and Engineering*, Birkhäuser, Boston, 2002, pp. 3-34.
3. E. Hitzer and C. Perwass: *Crystal cells in geometric algebra*, in proceedings of International Symposium on Advanced Mechanical Engineering, Fukui, Japan, 2004, pp. 290-295.
4. D. Hestenes and G. Sobczyk: *Clifford Algebra to Geometric Calculus: A Unified Language for Mathematics and Physics*, Reidel, Dordrecht, 1984.
5. L. Dorst: *Honing Geometric Algebra for its use in the Computer Sciences*, in *Geometric Computing with Clifford Algebra*, G. Sommer (ed.), Springer, 2001, pp. 127-151.
6. C. Perwass and D. Hildenbrand: *Aspects of Geometric Algebra in Euclidean, Projective and Conformal Space*, technical report no. 0310, Dept. of Computer Science, CAU Kiel, 2003.
7. C. Perwass et al.: *CLUCalc – A Visual Calculator*, available from www.clucalc.info, 2005.
8. C. Perwass and E. Hitzer: *Space Group Visualiser*, available from www.spacegroup.info, 2005.
9. Naval research laboratory: *Crystal Lattice Structures*, available from cst-www.nrl.navy.mil/lattice/spcgrp/, 2005.
10. *JCrystal*, available from www.jcrystal.com, 2005.
11. E. Hitzer and C. Perwass: *Full Geometric Description of Crystal Space Groups by the Suitable Choice of only Three Vectors for Each Bravais Cell of Crystal Family*, in Proc. of ISAME, Busan, Korea, 2005.