A NOVEL WAY TO REPRESENT THE 32 CRYSTALLOGRAPHIC POINT GROUPS

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ABSTRACT

This paper describes a novel way to represent the 32 crystallographic point groups for use in a classroom environment. The groups are rendered using a 3D ray-tracing package and a variety of movie and still image formats are made available in the public domain.

Keywords: point groups; freeware; animation; stereographic projection; ray-tracing

INTRODUCTION

Crystal structures are commonly described by stating the lattice parameters, the space group symbol or number, and the atom positions in the asymmetric unit (often by means of the Wyckoff symbols) [1]. This is standard practice, accepted across a wide range of scientific disciplines (physics, geology, materials science, to name just a few), and the International Tables for Crystallography (Volume A) provide all international conventions in the form of detailed space group tables [1].

When teaching a crystallography course to a group of students, in particular at the undergraduate level, it is often a daunting task to explain what space groups are and how they work. Let us consider the case of space group # 63: Cmcm. It is generally not too difficult to explain the meaning of the first letter of the space group symbol, the centering of the Bravais lattice. There are only six possible centering symbols (P, I, F, A, B, C), and one can readily draw a unit cell on the blackboard and illustrate the differences between these cases. That is the easy part. The difficulties begin when one attempts to explain the remainder of the space group symbol, the point group symbol.

The point group symbol is derived from the space group symbol by replacing all glide planes by regular mirror planes (in the example above this would result in the point group mmm), and all screw axes by regular rotation axes of the same order. An experienced crystallographer can then immediately name the crystal system to which the space group belongs (orthorhombic for the example above), but this is by no means obvious to the novice. An additional source of confusion lies in the fact that many of the point group symbols are commonly used in abbrevi-
ated form (mmm actually stands for \( \frac{2}{m} \frac{2}{m} \frac{2}{m} \)) and unless the student memorizes these abbreviations and the crystal systems to which they belong, there is little or no hope that he or she will be able to associate a point group with the appropriate crystal system.

A further difficulty lies in the representation of the actual point groups. Individual symmetry elements can readily be represented by simple drawings, and many textbooks offer very clear drawings of rotation axes, mirror planes and so on (e.g. [2, 3]). When these elements are then combined to generate the 32 crystallographic point groups, most texts rely on a representation in terms of stereographic projections. This is where the problems begin. The stereographic projection, introduced by William Hallowes Miller in 1839 [4], is an important tool for the representation of three-dimensional objects in a two-dimensional drawing. While it is an accepted research tool, as standard as, for instance, a parallel projection or a Mercator projection, the difficulty from the student’s perspective lies in the fact that many students have a hard time visualizing a three-dimensional object. When this object is then reduced to two dimensions it becomes even more difficult for them to reconstruct, in their mind, the original three-dimensional object. And now we are asking them to reconstruct from a stereographic projection an object – a point group – which is itself abstract and difficult to visualize. Should we be surprised, then, to find that students have a difficult time with stereographic projections of point groups? They are asked to visualize and understand a rather abstract 3D object, represented in a 2D projection, and to re-create in their mind the original 3D object.

Not everyone has the ability to perform mental operations, such as rotations, on 3D objects without actually touching them or observing them in 3D. And yet, the very definition of symmetry operations involves the concept of motion of an object: an object has a symmetry property when it can be brought into self-coincidence by an isometric motion (i.e., by a translation, rotation, mirror, or inversion operation). It is not a trivial matter to execute such motions by pure thought alone. Research into the way the brain interprets 3D visual cues indicates that there are two different levels at which this information can be processed. If 3D information is presented in 2D, then the brain has to perform a cognitive effort to convert the information to a 3D representation. Different people have different approaches to this conversion, and not everyone can easily perform this task. On the other hand, if the information is presented in true 3D form, then the brain, which is highly capable of 3D perception, does not need to use its cognitive centers to convert the information; all cognitive efforts can go towards interpreting and understanding the meaning of the 3D object itself, rather than its 3D structure.

We would substantially simplify the student’s task if we could eliminate one or more intermediate steps in the representation of point groups. Since a point group represents a 3D object, why not directly visualize the point group in 3D, using computer graphics and animation? Once the 3D representation is understood, the corresponding stereographic projection should pose no substantial problems; indeed, an understanding of the 3D nature of point groups may even help to understand the stereographic projection itself!

In this paper we present a novel way to represent a point group. The method uses a 3D ray-tracing package to create animations of a “world” which contains two types of objects:

1. symmetry elements, represented by their appropriate 3D symbols (i.e. a mirror plane is represented by a plane whose surface properties include the appropriate reflectivity),

2. a “general point”, to represent the equivalent positions of the point group.

The general point should itself have minimal symmetry; in particular, it should have a handedness so that the action of improper symmetry operators (in the nomenclature of [3]) is cor-
rectly represented. In the standard representation of point groups by means of stereographic projections one does not usually distinguish between points with opposite handedness. The only distinction taken into account is the location of the point above or below the stereographic projection plane (usually represented by a closed or open circle, respectively). The lack of handedness information on the standard projections of point groups is an important deficiency, since the true symmetry is not fully represented in the drawing; the student must infer the change of handedness from the presence of the symmetry elements.

The animations discussed in this paper use as general point either a sphere (for low resolution animations), or a right-handed helix, consisting of 20 small spheres. The nature of the ray-tracing process is such that if objects are assigned the proper surface properties, then a ray will bounce off of each of the surfaces according to the proper laws of physics, in this case Snell’s Law. The resulting renderings are realistic representations of all symmetry operators, as will be illustrated in the remainder of this paper.

The structure of the paper is then as follows: first we discuss the technical aspects of the definition of the “symmetry worlds” and the subsequent conversion of the individual animation frames into a movie. Then we discuss the various movies and stills, which can be downloaded from a dedicated website. We conclude this paper with a few suggestions for the classroom use of the animations and for additional animations which can be generated from the ray-tracing world definitions.

All software and animation files are available in the public domain and can be accessed through the author’s website [5]. The following file archives are available:

- The point group and Bravais lattice browser; both Macintosh (Quicktime) and Windows (AVI) versions are available;
- 32 high resolution (640×480 pixels) animated GIF-files using the helix as general point;
- 32 high resolution rendered drawings of the point groups (1200×1200 pixels, JPEG-format), again with the helix as general point;
- all input files for the raytracing computations, including a README file detailing the entire procedure.

All rendered images and animations were created using the public domain ray tracing package Rayshade (version 4.0) [6]. This program creates a rendered image based on the definition of a scene containing various objects (i.e., a “world”). The objects are constructed from primitive shapes, such as cylinders, spheres, and so on. An example input file for the pointgroup $\overline{2}$ is shown below. The file consists of a variable definition section, surface properties definitions, object definitions, and scene descriptions (viewing point, light sources, and so on). The entire scene is instantiated by the last command in the file.

```plaintext
/*********************/
/* define parameters */
/*********************/
define px 0.85
define py 0.15
define pz 0.40
define mpx (-px)
define mpy (-py)
define mpz (-pz)
define pp 0.005
define mp -0.005
/*********************/
/* define surface properties */
/*********************/
surface mirror
ambient 0.14 0.14 0.14 diffuse 0.01 0.01 0.01
specular .8 .8 .8 specpow 60
```

**TECHNICAL DESCRIPTION**

**Overview**

Several programs, sets of animations, and still images have been created for a variety of uses.

---

1Improper operators include mirrors and the inversion operator; they change the handedness of an object.
Figure 1: Screen dump of the graphical user interface for the point group and Bravais lattice browser.

reflect 1.

surface white
ambient 0.06 0.06 0.06 diffuse 0.50 0.50 0.50
specular 0.7 0.7 0.7 specpow 38
reflect 0.5

surface black
ambient 0.00 0.00 0.00 diffuse 0.0 0.0 0.0
specular 0.2 0.2 0.2 specpow 3
reflect 0.4

surface blumirror
ambient 0.00 0.00 0.32 diffuse 0.00 0.00 0.15
specular 0.9 0.9 0.9 specpow 60
reflect 1.0

surface ylwmirror
ambient 0.25 0.25 0.12 diffuse 0.25 0.25 0.12
specular 0.4 0.4 0.4 specpow 20
reflect 0.2

surface bluflat
ambient 0.04 0.06 0.22 diffuse 0.05 0.08 0.25
specular 0.4 0.4 0.4 specpow 20
reflect 0.2

/********************/
/* object definitions */
/********************/
/* locate a white plane 10 units below horizontal */
plane white 0 0 -10 0 0 1

name mirrormap
list
poly mirror 1 1 (pp) -1 -1 (pp) -1 -1 (pp) 1 1 (pp)
poly mirror 1 1 (mp) -1 -1 (mp) -1 -1 (mp) 1 1 (mp)
poly black 1 1 (pp) 1 1 (mp) 1 1 (mp) 1 1 (pp)
poly black -1 -1 (pp) -1 -1 (mp) -1 -1 (mp) -1 -1 (pp)

name disc_two
list
cylinder ylwflat 1 0 0 0 0 1
disc ylwflat 1 0 0 0 0 -1
disc ylwflat 1 0 0 0 0 1
end

name axis_two /* define two-fold rotation axis */
list
cylinder mirror 0.02 0 0 -1.2 0 0 1.2
disc ylwflat scale 0.15 0.07 1
translate 0 0 -1.210
disc ylwflat scale 0.15 0.07 1
translate 0 0 -1.210
end

name sympoint /* inversion symmetry element */
list
sphere ylwmirror 0.075 0 0 0
end

name blupoint /* general sphere */
list
sphere blumirror 0.075 0 0 0
end

name refaxis /* reference axis */
list
cylinder bluflat 0.01 0 0 -1.4 0 0 1.4
end

name point_group /* point group 2/m */
list
object axis_two
object mirrormap
object sympoint
object blupoint translate ( px) ( py) ( pz)
object blupoint translate ( mp) ( mp) ( mp)
object blupoint translate ( mp) ( mp) ( mp)
object blupoint translate ( px) ( py) ( pz)
object refaxis
Running this scene description file through Rayshade results in the image shown in Fig. 2a. When the viewing point is systematically changed along a predefined trajectory, or, equivalently, the entire object is rotated around one or more axes, one can easily obtain a sequence of images which can then be merged into a single movie (QuickTime, AVI, or animated GIF format). Generating a sequence of frames is simplified by the frames command of the Rayshade package. For more information we refer to the Rayshade documentation [6].

The general point in Fig. 2a is a single sphere; as discussed in the Introduction one should actually use an object which itself does not have a high order symmetry. A sphere is thus not the best general point. It has only been used to produce the low-resolution animations. For all high resolution animations and still images the general point was taken to be a right-handed helix consisting of 20 spheres. The general positions of all spheres in the helix were computed using the symmetry transformation matrices for each point group. We refer the reader to the International Tables for Crystallography, Volume A [1], for more details and for tables of symmetry matrices. The sphere coordinates for each helix are stored in *.pos files, one for each point group, and are included in the raytracing description files. The resulting rendered image for the point group $\mathbb{2}_m$ is shown in Fig. 2b.

One single Rayshade run then requires the following set of input files:

\[(\text{main file}) \ pg\_name.ray \text{ includes} \]

\[
\begin{align*}
\text{preface.ray (defines primitives and surfaces)} \\
\text{name.pos (atom positions for all helices)} \\
\text{tail.ray (defines rendering parameters)}
\end{align*}
\]
groups takes about 24 hours on a 600 MHz processor, and produces 757 Mb of RGB output. Various UNIX tools must then be used to convert this output into animated GIF, Quicktime, or AVI formatted movies. This can all be done with public domain and shareware software, and a detailed description of the procedure is available in a README file.

Figure 3: Rendered representations of all point groups, using a single sphere as general point.
The Point Group Browser

To facilitate the teaching of the crystallographic point groups we have developed an interactive module, which can be used by the teacher for classroom demonstrations and by the student for individual study. The program allows the user to select one of the 14 Bravais lattices or one of the 32 crystallographic point groups for display. A screen dump of the main user interface is shown in Fig. 1 (gray-scale version; all renderings are performed in full 24-bit color, and were converted to grayscale images for reproduction in this paper). By clicking on the crystal systems, the program will display the various centering options available for the selected crystal system. The user can then select a centering symbol to display a low resolution
rendered animation of a representative unit cell of the selected Bravais lattice. The international symbol for the Bravais lattice is displayed near the center of the screen. The animation loops once and can be restarted with the control buttons.

The 32 crystallographic point groups are ranked according to the crystal system to which they belong. The program uses the standard international (or Hermann-Mauguin) notation. The Schönflies notation is also displayed near the center of the display. When the user selects one of the point groups, the program displays a low resolution (240×180 pixels) rendered animation of the symmetry elements of the group, along with a set of equivalent point positions represented by blue spheres. The point group objects rotate around two axes simultaneously, so that the 3D nature of the object is emphasized. The first frame of each of the 32 movies is shown in Fig. 3.

Supported Platforms

The point group module is written in cT, a multi-platform programming language developed at the Center for Innovation in Learning (CIL) at CMU and distributed by Physics Academic Software [7]. The cT programming environment is available in forms executable on Macintosh, Windows and UNIX platforms. The current version of the point group browser was written using cT version 2.5, on the Macintosh platform, and then converted to the Windows 95 environment. For compatibility with standard graphics screens on both Macintosh and PC platforms, the program is designed to work on a display with 640×480 pixels with only 256 colors (8-bit), but it will also function on machines with a higher resolution screen and/or larger color palette. On the Macintosh, the animations are stored in compressed QuickTime format, while the Windows 95 version uses AVI format. A UNIX version will also be made available.

Program Availability

The point group module and associated still images and high resolution animated GIFs are made available in freeware form. Both Macintosh and Windows versions may be downloaded via the Internet from the author’s website [5]. Detailed instructions for installation and use of the program are included in the archived files. After installation, the complete set of files, including the cT-Executor, occupies 46.6 Mbytes of disk space on the Macintosh platform, and 123.4 MBytes on the Windows 95 platform (version 2.5 of the cT environment does not recognize compressed AVI format, hence the difference in required disk space).

The fileset consists of the binary file, the background image (PICT or BMP), the cT Executor, 14 Bravais lattice animations, 32 point group animations numbered according to the International Tables for Crystallography, Volume A [1], and a brief README file. To facilitate the teaching of point groups in an environment where computer projection is difficult or unavailable, a set of 32 still images (the first frame of each of the animations) is also included. These images are computed at high resolution (1200×1200 pixels) and stored in compressed, 24-bit JPEG format. They can be printed onto transparencies on a high quality color printer and used in a more conventional classroom setting. An example of a high resolution rendering of point group m\(\overline{3}m\) is shown in Fig. 4.

The last fileset available from the website contains animated GIF movies of the point groups, rendered at 640×480 pixels, using the helix as the special object. Animated GIF movies can be downloaded directly into a web browser, without the need for additional software. The 32 movies can be downloaded individually, for real-time display in a classroom setting, or as an archive.
LECTURE DEMONSTRATIONS AND OTHER SUGGESTED USES

The low-resolution points group movies have been used since 1995 in an undergraduate course on Structure of Materials in the Materials Science and Engineering department at Carnegie Mellon. The Quicktime movies have been used by about 100 sophomore students in a classroom setting; they have also been made available to the students over the campus network.

The 1200 × 1200 JPEG still images are provided to the teacher for use in a more traditional, i.e. computerless, classroom setting. The images can be printed onto transparencies on any good quality color printer, and can then be used with a standard overhead projector. In the author’s experience this is already a major improvement over the use of the standard stereographic projections; the still images convey the true 3D nature of point group symmetry, and from them one can easily derive the corresponding stereographic projections, as shown in Fig. 5.

Figure 4: High resolution rendered representation of the point group m̅3m for a right-handed helix as general point.
Ideally the teacher would have two surfaces available in the classroom: a traditional black-(or white-) board, and a computer projection screen. The point group module would be projected on this screen, and from the movies stereographic projections and other point group information (such as the order and the international symbol) could be derived on the other board. This method works well and all 32 point groups can be derived in this way in a regular lecture period (about 1 hour). Alternatively, one could provide the students with the point group module and have them explore the point groups outside of class, as preparation for the lecture. This has the advantage that every student can approach the module at his/her own pace, and the lecture would then serve to clarify remaining problems, if any. If the classroom computer is hooked up to the Internet, then the teacher can make use of the animated GIF movies, provided a fast network connection is available. If this is not the case, then the animated GIF file archive can be downloaded from the author’s website [5], and shown as local files through a browser. Both methods work fine, and have the advantage that the movies offer a higher resolution than the ones making up the point group module.

One may now ask the question: What about space groups? Can one use similar graphics tools to illustrate the structure of space groups? In principle the answer is of course positive, but there are several practical problems associated with renderings of space groups. First of all, space groups are groups of infinite order, so one would have to restrict the renderings to the fundamental unit cell, or perhaps a small number of unit cells (say $2 \times 2 \times 2$);

Second, one would have to create semi-transparent mirror planes, especially when mirror planes bound the unit cell faces (otherwise one could never see inside the cell). While this is certainly possible within the framework of the Rayshade program, the computational times involved become prohibitively long, even for a single image.

Finally, instead of rotating the entire space group, as is done for the point group objects, one would ideally give the observer control over eye point and view point locations. The Rayshade ray tracer is a batch program, normally running in background, so this is not the proper platform for real-time image renderings. Perhaps one could use VRML concepts and structures to permit the user to observe space group symmetry from an arbitrary direction, or, indeed, even move inside the fundamental unit cell and look around. This would require a substantial time and programming investment and is outside the scope of the author’s expertise.

**Conclusion**

A new representation of point groups has been created. Using ray-tracing techniques, rendered drawings and movies of the 32 crystallographic point groups have been created; they are available to the public from a dedicated website. Four years of teaching using this new representation have shown that students acquire a better understanding of the 3D nature of point groups. They also have a better understanding of the more standard stereographic projection representations of the point groups, since they can always compare the projection with the original 3D representation.

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References


List of Figures

1. Screen dump of the graphical user interface for the point group and Bravais lattice browser........................................ 5

2. Rendered representations of the point group $\frac{2}{m}$, for a) a sphere as general point, and b) a right-handed helix. ........................................ 6

3. Rendered representations of all point groups, using a single sphere as general point. ....................................... 7

3. Rendered representations of all point groups, using a single sphere as general point (continued). ...................................... 8

4. High resolution rendered representation of the point group $m\bar{3}m$ for a right-handed helix as general point. ........................................ 10

5. Illustration of the conversion of a rendered point group image to the corresponding stereographic projection. On the original point group drawing (a) a projection sphere is superimposed (b); the general points are connected with North or South pole, depending on their location the intersections of those connection lines with the equatorial plane mark the stereographic projections (c). The standard representation is then shown in (d). ........................................ 14
Figure 5: Illustration of the conversion of a rendered point group image to the corresponding stereographic projection. On the original point group drawing (a) a projection sphere is superimposed (b); the general points are connected with North or South pole, depending on their location the intersections of those connection lines with the equatorial plane mark the stereographic projections (c). The standard representation is then shown in (d).