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Interactive PDF files with embedded 3D designs as support material to study the 32 crystallographic point groups

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ABSTRACT

Crystallography and X-ray diffraction techniques are essential topics in geosciences and other solid-state sciences. Their fundamentals, which include point symmetry groups, are taught in the corresponding university courses. In-depth meaningful learning of symmetry concepts is difficult and requires capacity for abstraction and spatial vision. Traditionally, wooden crystallographic models are used as support material. In this paper, we describe a new interactive tool, freely available, inspired in such models. Thirty-two PDF files containing embedded 3D models have been created. Each file illustrates a point symmetry group and can be used to teach/learn essential symmetry concepts and the International Hermann–Mauguin notation of point symmetry groups. Most interactive computer-aided tools devoted to symmetry deal with molecular symmetry and disregard crystal symmetry so we have developed a tool that fills the existing gap.

1. Introduction

X-ray diffraction techniques are widely used to identify minerals and ascertain their crystal structures (Louër, 1999). Effective application of these techniques as analytical and characterization tools in geology and materials science requires a basic understanding of crystallography. Crystallography and X-ray techniques are present in geology graduate programs (Hluchy, 1999) as an independent topic or as a significant part of mineralogy courses. Moreover, many physics, chemistry (Fanwick, 2007; Pett, 2010) and materials science graduate programs also include introductory notes on crystallography (Borchardt-Ott, 2012).

In crystallography, one must understand the concept of symmetry first. Crystal symmetry includes several conceptual and geometrical notions that require capacity for abstraction and spatial vision. Additionally, crystallographic symbols and notations are very compact. As a result of this complexity, crystallography and specifically symmetry are considered too difficult by many students and in some measure these difficulties are also present among researchers and technologists of the above mentioned fields.

The symmetry of crystalline solids comprises point symmetry and space symmetry (Borchardt-Ott, 2012). The first is often referred as the symmetry that concerns finite figures, like well developed crystals (Fig. 1a) and the latter concerns infinite ordered media like the internal triply periodic structure of crystals (Fig. 1b). At both levels, symmetry is always described as a set of so-called symmetry elements. These sets of elements have the properties of a mathematical group and consequently are named groups. There are only 32 possible combinations or sets of point symmetry elements, whereas the number of possible combinations of space symmetry elements is 230. The increase from 32 Point Symmetry Groups to 230 Space Symmetry Groups arises from adding translational symmetry to point symmetry, which results in a wider variety of symmetry elements. Point and space symmetry are fully interconnected in such a way that every space group belongs to a single point group from which it can be said to have originated. The international crystallographic notation (or Hermann–Mauguin notation) reflects this link between point and space symmetry groups (Burzlaff and Zimmermann, 2006).

From the above considerations it can be said that point symmetry constitutes the basis of the crystallographic symmetry, and thus its deep understanding allows the comprehension of the apparently more complex space symmetry.

Historically, support materials in introductory crystallography courses have been crystal models that reproduce idealized crystal forms of minerals. These models were first developed by pioneering figures of modern crystallography in the 18th century (Touret, 2004). Wooden crystallographic models were distributed on a large scale from the second half of the 19th century by the German

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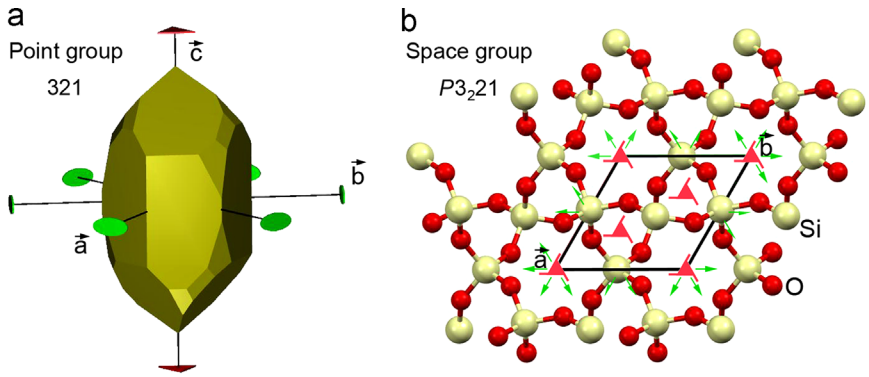

Fig. 1. Representations of the symmetry levels for α-quartz: (a) idealized crystal morphology with indication of the hexagonal axes ($\vec{a}$, $\vec{b}$, $\vec{c}$), the point symmetry elements and the Hermann–Mauguin notation of the corresponding point group (321); (b) internal crystal structure projected into the (001) plane with indication of the hexagonal axes, space symmetry elements and the Hermann–Mauguin notation of the corresponding space group ($P3_221$).

company Krantz (Burchard, 1994). These models are so useful that they are still being used today. In addition, the progressive introduction of computing-oriented environments and Internet as resources in geosciences (Butler, 1995) and chemistry has led to the development of several interactive virtual alternatives to the crystal models. Despite pioneering programs like Symmetry (Brady, 1978), the developed software relates mostly to molecular viewing and modeling (Goddard and Ferrin, 2007; Johnson et al., 2011), and only a few programs deal with periodicity and symmetry and generally these are not designed for teaching purposes (Khosrovani et al., 1999). Educational software for learning symmetry usually focus on molecular symmetry (e.g. Meyer and Sargent, 2007; Tuvi-Arad and Gorsky, 2007) and therefore they are not useful for teaching/learning crystallography. Few resources deal with crystal symmetry (e.g. Roullet et al., 1990; Johnston, 2012). There are commercial packages intended for viewing crystal morphology (Shape, 2011; KrystalShaper, 2013) though not designed for teaching purposes.

To our knowledge, the existing interactive virtual resources intended for teaching crystallographic point groups do not focus on complex and necessary aspects such as the crystallographic Hermann–Mauguin notation or the commonly used stereographic projection. This projection is a useful tool to describe angular relationships in three-dimensional space using two-dimensional plots (Liben and Titus, 2012) and it is the ideal tool to plot point symmetry groups. However, its use in the specialised textbooks often adds an extra complication for the students.

We have developed a modern and attractive tool to promote learning of crystal symmetry and to fill the aforementioned gaps. This tool combines 3D computer-aided design with the widespread Portable Document Format (PDF) from Adobe Systems. Interactive 3D polyhedra and their corresponding symmetry elements were designed as a representation of idealized crystals and their symmetry. Interactivity not only allows the user to explore the shape of polyhedra controlling their position, but also selectively enable/disable the graphic representation of their symmetry elements.

The developed virtual material consists of 32 interactive PDF files, one per point symmetry group, containing at least one polyhedron. The files are freely downloadable[1] and they are aimed at university students as well as researchers interested in Crystallography. Several features make these files an interesting and useful tool to learn point symmetry, such as the attractive graphic design, the usability and a diligent observance of the International Union of Crystallography (IUCr) criteria.

2. Creation of the interactive PDF files

The creation of the interactive PDF 3D files required the integration of design and programming using three different programs: SolidWorks 2011 (Onwubolu, 2011); Adobe Illustrator (Adobe Illustrator CS3, 2007) and Adobe Acrobat (Adobe Acrobat 9 Pro, 2010).

SolidWorks was used to design parametrically the 3D objects that will contain the files. These 3D objects are the polyhedra and their corresponding symmetry elements (axes and planes). Static graphical features such as the background, button icons and stereographic projections were drawn using Adobe Illustrator. We used Adobe Acrobat Pro to integrate dynamic and static contents and to define the functionality of all the buttons.

2.1. Mathematical generation of polyhedron vertices

The input parameters required to design the 3D polyhedra are the coordinates of their vertices (point cloud). For every polyhedron, the point cloud was obtained following a semiautomatic approach. A starting set of points (generator vertices) was selected manually and then, the rest of vertices were automatically generated by symmetry operators. Each polyhedron is designed to illustrate a given crystallographic point group, therefore its applied symmetry operations were selected according to the symmetry elements of the desired group. This approach, besides making simpler the point cloud generation process, ensures that the symmetry of the point cloud corresponds to the desired point group.

First, a given polyhedron must be selected (see Section 3.1). The generator vertices represent the asymmetric portion of the polyhedron to be designed; this asymmetric portion is analogous to the concept of asymmetric unit of a space group. The number of generated vertices from a given generator vertex will equal the multiplicity of the point group, provided that the generator vertex is not positioned on point-group symmetry elements. Again, an analogy with space symmetry concepts (special/general positions) can be made.

Every selected polyhedron belongs to a given crystal system and their generator vertices have been defined within the corresponding coordinate system. The crystallographic coordinate systems are characterized by a basis of three vectors ($\vec{a}$, $\vec{b}$, $\vec{c}$) which always respect the symmetry of their crystallographic system. Therefore, the relation between the three vectors depends on the restrictions imposed by the symmetry of each crystallographic

[1] Download the 32 interactive PDF files at http://departaments.uab.cat/geologia/PSG