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Virtual models for crystallography teaching in Mineralogy: some suggestions

Carlos Alves [1,*], Carlos Figueiredo [2] and Jorge Sanjurjo-Sánchez [3]

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[1] LandS/Lab2PT-Landscapes, Heritage and Territory laboratory (FCT-UIDB/04509/2020) and Earth Sciences Department/School of Sciences, University of Minho, Braga, Portugal; casaix@dct.uminho.pt
[2] CERENA—Centro de Recursos Naturais e Ambiente, FCT-UIDB/04028/2020, DEcivil, Instituto Superior Técnico, University of Lisbon, Lisbon, Portugal; carlos.m.figueiredo@ist.utl.pt
[3] Instituto Universitario de Xeoloxía, Universidad de la Coruña, ESCI, Campus de Elviña, A Coruña, Spain; jorge.sanjurjo.sanchez@udc.es
* Correspondence: casaix@dct.uminho.pt; Earth Sciences Department/School of Sciences, University of Minho, Braga, Portugal.

Abstract: Crystallography concepts are usually among the most demanding subjects for Mineralogy students. Traditional onsite teaching of Mineralogy starts with physical models of crystal polyhedra and frequently also includes the observation of models of crystal structures. These teaching strategies could be difficult to implement under pandemic situations like the present one. But they have also other disadvantages under the usual access conditions as their use by the students is restricted by the number of students in relation to the number of models and by the availability of the models and teaching staff. Additionally, onsite teaching can pose challenges to both students and teachers with temporal or permanent disabilities. We consider here some possibilities of teaching with virtual models of crystal polyhedra, twinning and crystal structures, based on some of the available freeware options and considering the main concepts taught in the usual Mineralogy syllabus.

Keywords: polyhedra models; crystal structures models; distance teaching; COVID-19.

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1. Introduction

The current pandemic situation has caused disruptions in many activities around the world, including teaching. The promotion of physical distancing procedures become especially strenuous for subjects mostly based on laboratory work, since they have higher requirements in terms of spaces and materials.

Crystallography concepts are usually among the more demanding subjects for Mineralogy students. Traditional onsite teaching of Mineralogy starts with physical models of crystal polyhedra and twinning and frequently also includes the observation of models of crystal structures. These teaching strategies could be difficult to implement under pandemic situations like the present one. But they have also other disadvantages under the usual access conditions as their use by the students is restricted by the number of students in relation to the number of models and by the availability of the models and teaching staff. Additionally, onsite teaching can pose challenges to both students and teachers with temporal or permanent disabilities.

We consider in the present work some possibilities of using virtual models for teaching some crystallographic concepts usually deemed necessary for the study of mineral characteristics.

There have been several reviews of software dedicated to Mineralogy and a recent one dedicated to crystal shapes and structures is presented in Rakovan [1]. It is not our intention to present a software analysis or review, nor are we implying that the software programs mentioned in the following examples are the only option or even the best ones. The ones presented here are the ones that we know and that we have used. And all software referred to here is freeware; the interested reader can easily download the software (links for download are available in the references).

2. Materials and methods

All the presented work was prepared in a Windows-based computer and we present next an alphabetically ordered list with the software used and their reference for easier consultation by the reader:

+) KrystalShaper 1.4.0 [2];
+) PowderCell 2.4 [3];
+) VESTA 3.5.2 [4];
+) WinXMorph [5,6].

For any of the software examples considered in our analysis, the students can simply read files that are available in public repositories or that were prepared by the instructors or they can build the models from basic crystallographic principles which will be indicated in the next section where the examples are discussed.

We must also refer an important source of information for most of the work prepared in the context of this paper: The AMCSD (American Mineralogist Crystal Structure Database [7]).

There are also options allowing to see crystal models online such as, for example, http://webmineral.com/ and https://chemistry.beloit.edu/edetc/pmks/index.html but our discussion will be focused on examples were the user can create, keep and modify the files for the models.

We will analyze the use of these software examples in the teaching of crystallography concepts usually taught in Mineralogy undergraduate courses, considering namely models of internal crystal structures and models of crystal forms (including twinning).

3. Examples and discussion

3.1. Models of crystal structures

The AMCSD [7] has a series of files with information on structures of minerals that can be accessed online. These files that can be downloaded and open in software such as VESTA [4] that immediately prepares virtual 3D models of the structures. This software allows diverse types of representation such as ball-and-stick, sphere packing and coordination geometries (and it is very easy to indicate to the students a few commands for the visualization options).

The first author has verified that students can prepare suitable images from models in a matter of a few minutes, even when teaching through a chat. An example is presented in Figure 1a, showing an image of a model for the structure of sillimanite based on a file available in the AMCSD [8]. In this image, it is used a representation by coordination polyhedra showing, for example, isolated silicate tetrahedra and that aluminium has two different coordination geometries: octahedral (Al1) and tetrahedral (Al2). While the figure is a 2D object, VESTA produces 3D virtual objects that can be manipulated. While the software allows the instant creation of the model from the reading of the downloaded file, the user still has a lot of potential options that can be used to discuss different issues (labels and colours of atoms, presenting just some of the atoms or some of the coordination polyhedra, etc.).

It is also possible, and perhaps more interesting for teaching the concepts associated with mineral structures, to create models from scratch. We present in Figure 1b and 1c images from a model of the structure of graphite [9] prepared with PowderCell [3] which also produces 3D models. This example will be useful to relate the perfect and easy cleavage of graphite to its structural characteristics. The experience of the first author shows that first-year student can build these relatively simple models quickly (in a matter of some minutes). Afterwards, they can build models of more complex structures, which is, essentially, a matter of time given that it is necessary to introduce the positions of a bigger number of atoms.

It is also possible to present portions of a cell unit or with several cell units, as well as to show just some of the chemical elements.

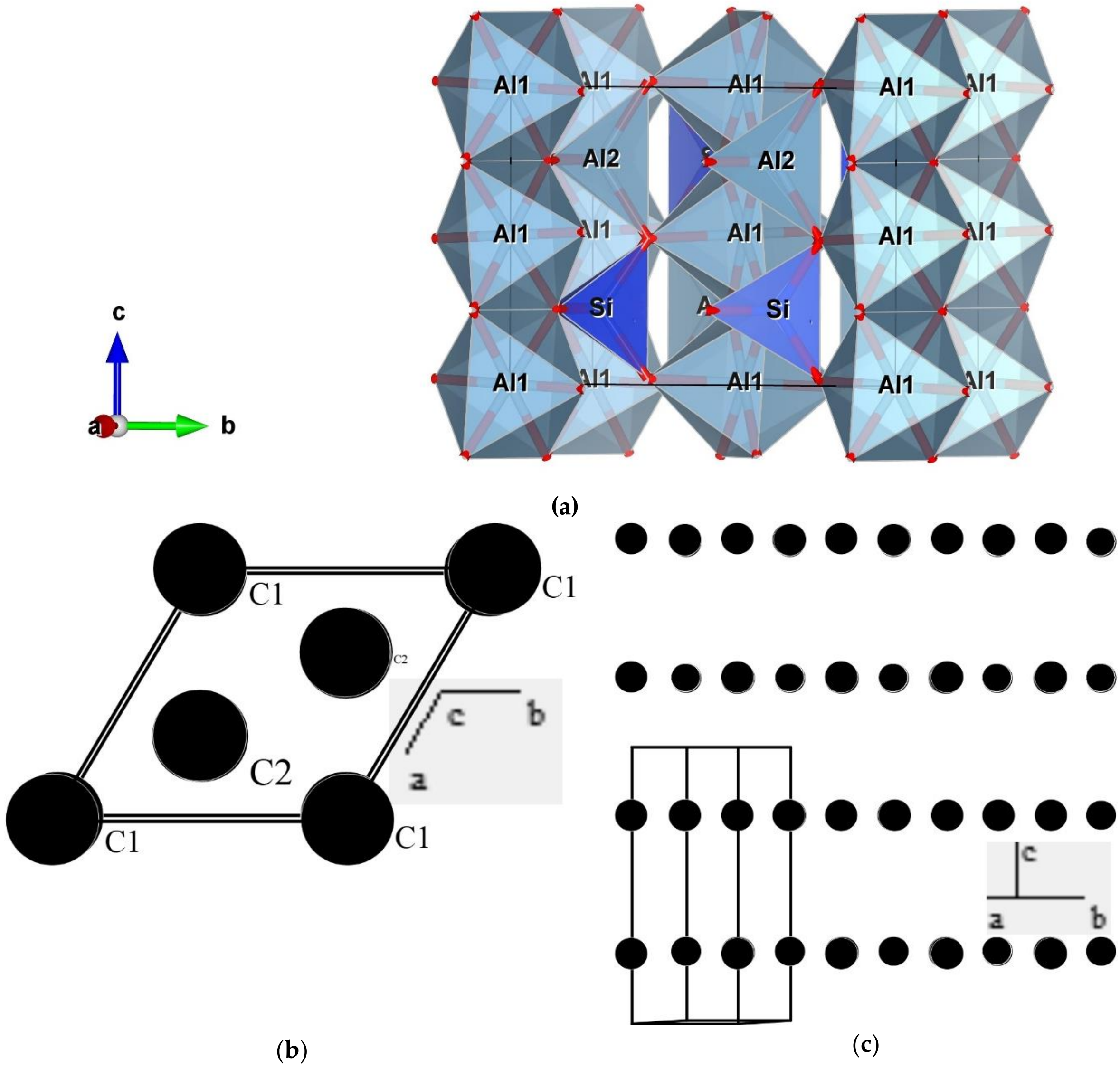

Figure 1. Images of models of crystal structures: (a) structure of sillimanite[8] obtained with VESTA[4] showing coordination polyhedra of Si (tetrahedral) and Al (octahedral), as well as the chains of Al coordination polyhedra and the isolated silicate polyhedra (typical of nesosilicates); (b) and (c) images of graphite structure[9] prepared with PowderCell[3] observed in a normal view to (001), showing the hexagonal cell and the two structural positions of carbon atoms (b) and with a view parallel to (001) showing the layered distribution of atoms that explain the easy pinacoidal (basal) cleavage of this mineral.

3.3. Models of external morphologies (crystal forms and twinning)

The study of crystal shapes in models where the faces have ideal proportions (frequently in materials such as wood) is a classic foundation stone of mineralogical teaching. This is useful both to better introduce students to certain concepts (reducing the variables that are studied in the beginning) and to promote a visual familiarization of the student with crystal shapes that in real mineral samples can occur distorted or truncated.

There are freeware software examples that can create virtual models of crystal forms, such as KrystalShaper[2], which only needs information on crystal class, the Miller symbol of the crystal form and, if necessary, the characteristics of the unit cell. The created model can be rotated freely as if it was a physical one. This works especially well for cubic crystals since all forms are closed (for the other crystal systems the models are created only when the crystal form or forms define a closed polyhedron).

There are options allowing to show the Miller symbols of the different faces and the normal to the faces (which will be helpful as a first step in the teaching of stereographic plotting).

Another useful feature of this software is the possibility to show students how the same Miller symbol could produce different crystal forms in different crystal classes, such as {111}, which, for example, produces an octahedron in class 432, a tetrahedron in class 23, a hexagonal bipyramid in 6/m, etc.

It is also possible in KrystalShaper to attribute different importance to the crystal forms, which could be used for a (limited) illustration of cleavage effects. In Figure 2 we present an example that attempts to expand the use of KrystalShaper to show the effects of cleavage considering a cubic crystal of fluorite with octahedral cleavage. For that, we consider the example of fluorite and the combination of cube and octahedron, used here to represent the {111} cleavage, with different proportions, from a cube with truncated corners (due to cleavage) to the final cleavage octahedron.

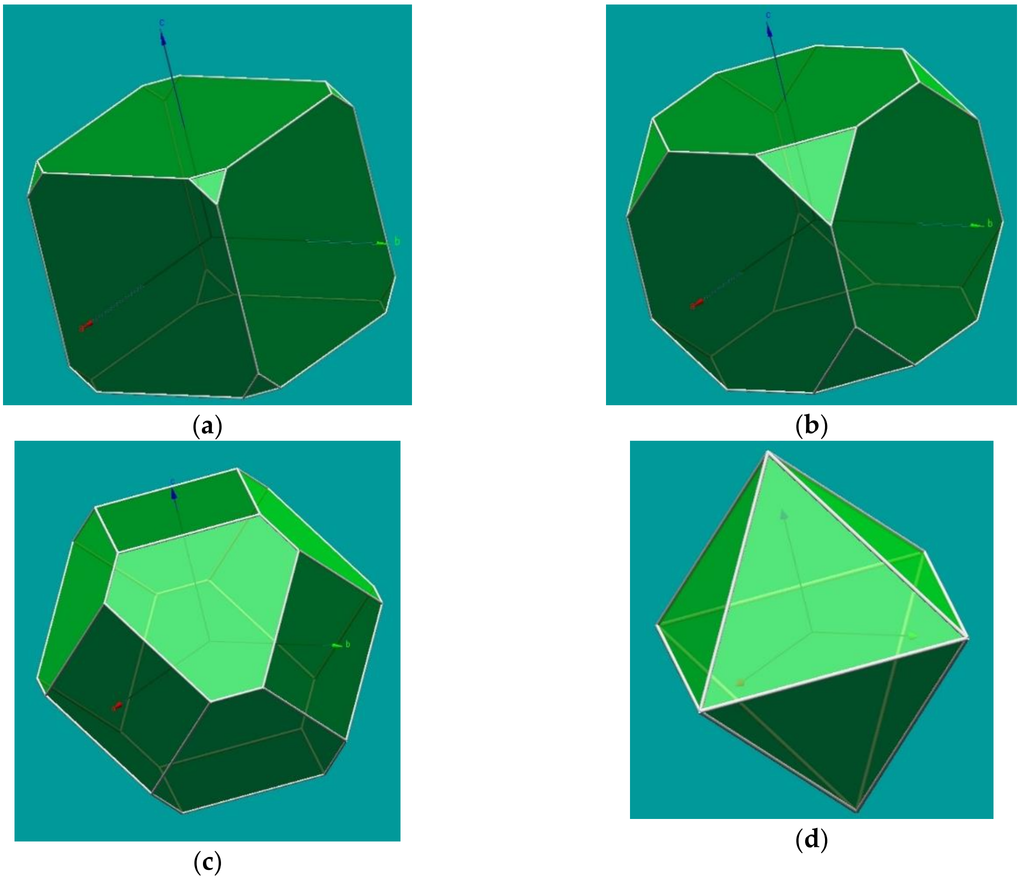

Figure 2. Images of a model of {100} and {111} in fluorite prepared with KrystalShaper[2], with different situations of the relative importance of these crystal forms, aiming to simulate the effect of the octahedral cleavage in fluorite, from little importance in (**a**), where octahedral cleavage cuts the corners of a cubic crystal, with b) and c) representing further effects of cleavage and, finally, d) corresponding to the cleavage polyhedron obtained for fluorite.

This software allows the user to attribute different colours to different crystal forms, something useful to show the concept of complementary forms and how they can create examples of pseudosymmetry, such as, for example, complementary rhombohedra of quartz creating a pseudo-hexagonal bipyramid. Another point concerns the relation of the considered crystal forms to the geometric characteristics of the unit cell and the Miller symbols, which can be useful for presenting other pseudosymmetry examples such as the pseudo-octahedral scheelite and pseudo-tetrahedral chalcopyrite.

KrystalShaper has the additional advantage of showing the stereographic projection of the crystal forms (with the option of presenting the Miller symbol of each pole). It is possible to show the change in the position of the stereographic poles with the rotation of the model (which, as mentioned above, could show the lines that are normal to the faces). These features can be used in the discussion of the symmetry elements of the model.

There are also software options for making models of crystal twinning. WinXmorph [5,6] is an easily accessible freeware that can be used for that end (this software can also prepare models of crystal forms from scratch and reading from available files). In Figure 3 is presented a model of fluorite twinning prepared with this software.

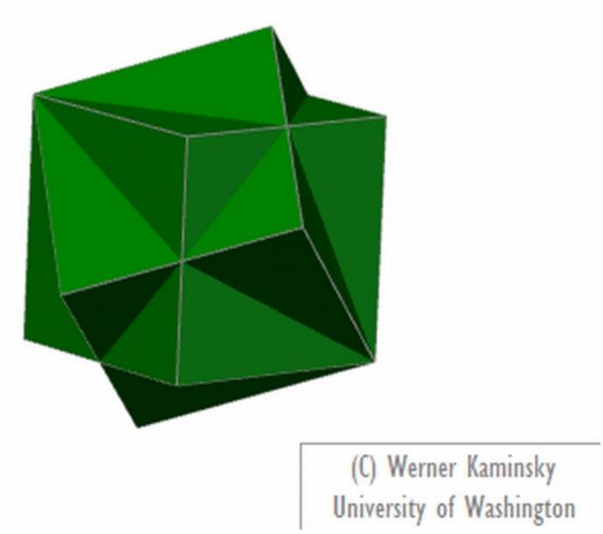

Figure 3. Image of a model of fluorite twinning prepared with WinXMorph[5,6].

4. Conclusion

While the software examples considered in this work were few, they all produce 3D objects that can be freely rotated and used as models and that show a high potential for teaching the main crystallographic concepts usually required in traditional Mineralogy lectures, both in terms of structures and crystal morphology (crystal forms and twinning).

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