

Journal of

**Applied
Crystallography**

ISSN 0021-8898

Editor: **Gernot Kosterz**

***WinXMorph*: a computer program to draw crystal morphology, growth sectors and cross sections with export files in VRML V2.0 utf8-virtual reality format**

Werner Kaminsky

Copyright © International Union of Crystallography

Author(s) of this paper may load this reprint on their own web site provided that this cover page is retained. Republication of this article or its storage in electronic databases or the like is not permitted without prior permission in writing from the IUCr.

WinXMorph: a computer program to draw crystal morphology, growth sectors and cross sections with export files in VRML V2.0 utf8-virtual reality format

Werner Kaminsky

Department of Chemistry, University of Washington, Seattle, Washington, USA. Correspondence e-mail: wernerka@u.washington.edu

A Microsoft Windows application for PC-users, *WinXMorph*, is introduced with which near reality crystal morphologies are made and exported as virtual reality files in the VRML V2.0 format.

© 2005 International Union of Crystallography
Printed in Great Britain – all rights reserved

1. Background

Crystal morphologies, often called the shape or habit of a crystal, represent the idealized combination of crystal faces. A century ago it would have been unthinkable to present a scientific result on a crystal without showing a crystal shape that represents the type and size of morphic faces the crystal developed through its growth. Examples *par excellence* are the Volumes by Groth (1921). In these and other publications of the same time, crystal shapes were constructed from a stereographic projection of the material (in German, *Kopfbildprojektion*). This time-consuming process was replaced by computer generated images (Dowty, 1980). Today, some software packages are available for personal computers that allow the generation of morphologies, including shading of the faces with respect to their angle relative to a virtual light source (Weber, 2005; Dowty, 2005; Favreau, 2005). However, virtual reality, *i.e.* crystal model files that are encoded by the VRML V2.0 utf8 standard, are supported only by the commercial program *JCrystal* by Steffen Weber (2005). The possibility of generating near reality pictures of crystals, idealized or close to a real sample, is one of the special features of the program introduced here.

2. Description

The program takes as input the Miller indices and central distances. These can be edited freely and the input is automatically corrected, for example (063) is reduced to (021), or a face can be included to the set of faces only once. The program provides the 32 point symmetries and PG $\bar{5}32$ of the icosahedral system and allows as input non-integer numbers with which incommensurate crystal shapes can be realized. However, each face can be edited individually with respect to color, texture, central distance, indices and growth sector color, if desired.

The program exports VRML files that can be inserted as illustrations on the internet or a bitmap copy of the current image is saved as *.bmp on the hard drive.

As an example, we see in Fig. 1 the image simulating K_2SO_4 that was grown in a solution containing the dye Trypan blue, which colored only the {111} faces [for a discussion of dyed crystals see Kahr & Gurney (2001)].

Fig. 2 shows a cross section through the example in Fig. 1, cutting through one-fifth of the normal vector of the (010) face. Images like these are edited within a few minutes and rendered in real time, allowing smooth rotation of the models either by hand or animation.

A special feature is texture of the faces, illustrated in the pyrite crystal and rose-quartz examples in Figs. 3 and 4.

Non-integer indices were used to generate the brilliant-cut diamond model in Fig. 5. Grouping a model with itself at different displacements/scales/orientations is shown in Fig. 6, representing an ensemble of quartz crystals that can be rotated and viewed from any angle.

The program allows the combination of VRML files of a structure created from a shelx.res file (Oellien, 2005), a tensor-VRML created with *WinTensor* (Kaminsky, 2005), and a crystal shape from *WinXMorph*, correctly aligned to one another and rotated simultaneously. Fig. 7 gives an example on structure, optical rotation and morphology in mannitol, $C_6H_{14}O_6$.

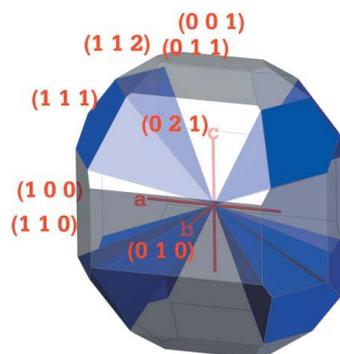


Figure 1
 K_2SO_4 dyed with Trypan blue (*WinXMorph* image).

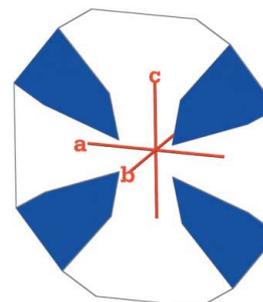


Figure 2
A cross section through Fig. 1.

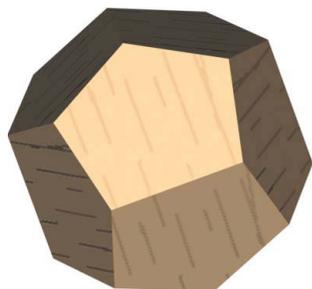


Figure 3
A *WinXMorph* image of pyrite {210}, showing texture.



Figure 4
A *WinXMorph* image of rose-quartz, showing texture.



Figure 5
Multiple refraction colors simulation on a brilliant cut diamond.

3. Software environment

WinXMorph runs under Windows 95/98/NT/2000/XP operating systems. The user interface and underlying code were written in Borland Delphi Pascal 6 (Delphi, 2005).

4. Documentation

The help documentation was developed with Doc-to-Help (Doc-to-Help, 2005) and incorporates a student friendly introduction into the world of crystal shapes by J. Michael Howard and Darcy Howard (Howard & Howard, 2005). A step-by-step introduction into the program with many illustrations will teach any user quickly to create appealing crystal shapes in minutes.

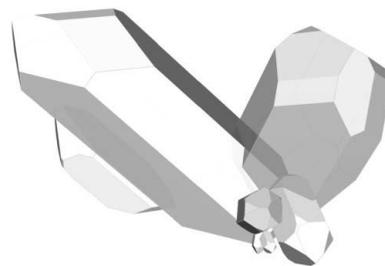


Figure 6
Combining a model with itself can be used to create realistic hand pieces.

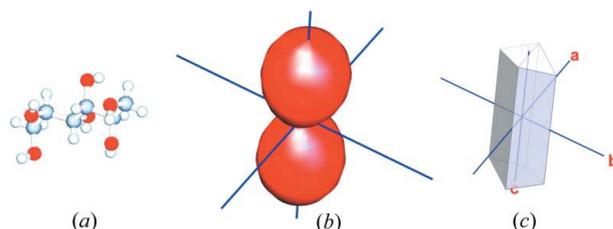


Figure 7
Molecule, optical rotation representation surface, and morphology of mannitol.

Included is a tutorial about the generation and mathematical algorithms of crystal shapes and a demonstration of how to incorporate VRML files into Microsoft PowerPoint presentations to allow interactive manipulation of crystals morphologies in class.

5. Availability

WinXMorph is available free of charge for teachers, students and members of educational institutions from http://depts.washington.edu/ventures/UW_Technology/Express_Licenses/winxmorph.php. Users need to accept the educational license agreement of the University of Washington to obtain a password (online, no charges) that releases restrictions of the demo version. Tax-deductible donations to support the program are welcomed.

References

- Delphi (2005). Borland Software Corporation, <http://www.borland.com/>.
- Doc-To-Help (2005). Component one, <http://www.componentone.com/>.
- Dowty, E. (1980). *Am. Mineral.* **65**, 465–471.
- Dowty, E. (2005). *SHAPE*, <http://www.shapesoftware.com/>.
- Favreau, G. (2005). *FACES*, http://un2sg4.unige.ch/athena/html/sc_prg.html.
- Groth, P. (1921). *Chemische Kristallographie*. Munich: Oldenburg.
- Howard, J. M. & Howard, D. (2005). *Introduction to Crystallography and Mineral Crystal Systems*, <http://www.rockhounds.com/rockshop/xtal/>.
- Kahr, B. & Gurney, R. W. (2001). *Dyeing Cryst. Chem. Rev.* **101**, 893–951.
- Kaminsky, W. (2005). *WinTensor*, <http://cad4.cpac.washington.edu/wintensor/home/wintensor.htm>.
- Oellien, F. (2005). *VRMLFileCreator*, <http://131.188.127.153/services/vrmlcreator/index.html>.
- Weber, S. (2005). *JCrystal*, <http://www.jcrystal.com/>.