

Using the American Mineralogist Crystal Structure Database in the Classroom

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ABSTRACT

The American Mineralogist Crystal Structure Database is a compilation of every crystal structure potentially of mineralogic or geologic interest. The database, seen as an outreach service, is funded and maintained by NSF, the Mineralogical Society of America and the Mineralogical Association of Canada. This database, when linked with visualization software, provides an invaluable resource for instructors, allowing direct access to crystal structures of almost any mineral, and many at various compositions, pressures or temperatures. Associated with the database is a freeware visualization program, XtalDraw with ancillary software modules, Xpow (for visualization of powder diffraction patterns) and SPEEDEN (for visualization of electron density maps). These software modules are user-friendly, allowing students, instructors, and researchers to easily access various crystal structures. Suggestions for using the database and software in an instructional setting are given; full lesson plans and instructional guides are being developed as Internet resources.

INTRODUCTION

One of the most difficult tasks an instructor faces is relating lecture information to real-world applications. In mineralogy and petrology, this is particularly evidenced when, as instructors, we try to convey the nature of crystalline materials and the inter-relationships between crystal structures and physical properties, ranging from hardness and cleavage to stable pressure-temperature regimes. An ideal pedagogical tool is a database of crystal structure information that is freely and easily accessible, combined with interactive software for visualizing and manipulating the structures so that the data can be viewed as crystal structure drawings, and not just as columns of numbers.

The American Mineralogist Crystal Structure Database is being developed to archive data for every crystal structure of interest to the mineralogical and geological communities (Downs and Hall-Wallace, 2003). It includes all crystal structures published in the American Mineralogist and The Canadian Mineralogist. Crystal structures from The European Journal of Mineralogy are currently being added to the database. The editors of Acta Crystallographica and Springer-Verlag have just formalized an agreement to include their mineralogical data and this will be added to the database soon. The database is funded by the National Science Foundation and is being maintained through the efforts of the Mineralogical Society of America and the Mineralogical Association of Canada. The information in this database is easily accessible through the Internet from the society web

pages or directly via <http://www.geo.arizona.edu/AMS/amcsd.php>. Structure data is easily downloaded from the database in both CIF and AMC formats; easily opened into most popular crystal visualization software programs.

In this paper, we provide some initial suggestions for using this information in the classroom. We view these ideas merely as ideas or starting points; individual experiences and instructional settings will undoubtedly suggest variations and/or additional uses.

THE DATABASE

Each crystal structure is archived in its own file, complete with a citation, cell parameters and symmetry, and a list of elements in the structure. This element list contains the atomic coordinates, site occupancies and, if published, thermal parameters for each element. Each dataset is analyzed for accuracy by checking that the cell parameters reproduce the cell volume, and the atomic coordinates reproduce the bond lengths and angles that are tabulated in the original publication. If there are inconsistencies, then they are corrected, and the corrected dataset is archived. This is an invaluable step, as it is estimated that approximately 50% of published data have errors of one sort or another (Downs and Hall-Wallace, 2003). An example of a dataset for phlogopite is given in Table 1. As of the beginning of the calendar year 2003, there are 3626 datasets in the database. The data that is archived not only represents structures for phases at ambient conditions, but it also includes data collected at various temperatures and pressures, if such information has been included in a published paper. The design and management of the database is described by Rajan et al. (2003) and Downs and Hall-Wallace (2003).

There are two primary means for accessing the data. One is to go directly to the web site through an interface following links off the Mineralogical Society of America website. From this interface you can find the crystal structure data by various means including selecting (1) a mineral name, (2) the author of the publication that contains crystal structure data, (3) chemistry of the phases of interest, (4) symmetry and cell parameters, or (5) a general search routine to find a given character string. These options can be combined through a logical AND/OR operator. A second way to access the data is through an Internet command such as

<http://www.geo.arizona.edu/AMS/result.php?mineral=heulandite>

where "heulandite" can be replaced with the name of any mineral. All five of the selection fields listed above can be queried in this manner. If a data file is found by this option, then the data is immediately and directly displayed and there is no need to surf the website.

THE ANCILLARY SOFTWARE

In addition to the data, free analysis software that is fully integrated with the database is also available (Downs and Hall-Wallace, 2003). The combination of this database with the ancillary software provides a valuable tool for instructors ranging from secondary education through graduate programs. The crystal structure database provides easy access to structure data in a tabular format. However, to make this source truly useful to educators, inexpensive, or better yet, free, visualization and analysis software is a necessity. There are several structure visualization programs available, and all have their strengths and weaknesses. For many, it is the cost-prohibitive nature of the software itself that puts it beyond the reach of educators and students. Individual licenses for other programs usually run between \$200 - \$400, with site licenses costing as much as \$1000 or more. XtalDraw and Xpow are freeware available following the "Extra" link off of the database website. Both software programs are easily installed on the user's Windows-based computer.

XtalDraw is a fully-functional crystal visualization program, on par with other software such as ATOMS[®] or CrystalMaker[®]. XtalDraw is a Windows-based computer program that generates crystal structures from either CIF or AMC (American Mineralogist Crystal Structure database) files. The program displays crystal structures in ball-and-stick, polyhedral, or thermal ellipsoidal renderings, which can be rotated, enlarged or shrunk. The sizes and colors of individual atoms can be altered, and they can be added or deleted from view. Combinations of ball-and-stick and polyhedra are possible, simply by selecting individual sites to alter. Bond lengths, angles, polyhedral volumes and other geometrical computations can be obtained. The image can also be saved as a bitmap. A particularly useful option in XtalDraw allows several bitmaps to be linked into a movie, which can either be looped or played forward and back (Downs and Heese, 2000). This enhances the ability to study structures and how they change with temperature, pressure, and chemistry, or even through a phase transition. Several examples are illustrated at the database website.

In principle, any property of a crystal can be determined from knowledge of its chemistry and crystal structure. A great deal of effort in modern science is devoted to unraveling the relationships between structure and properties. One relationship that is very well understood regards diffraction. The Windows-based software Xpow is an interactive program that computes and displays X-ray or neutron powder diffraction profiles (Downs et al, 1993) from the structure data available in the database. The software allows students or instructors to investigate the relationships between atomic structures and the related diffraction pattern from a variety of energy sources. This allows for the basics of diffraction to be studied at smaller institutions that lack the facilities for students to directly interact with diffraction equipment. At universities with diffraction equipment, it provides students an opportunity to develop some skill with interpreting diffraction data before they actually collect their own information. Given an assignment to collect their own data, students can also quickly compare their results to a gen-

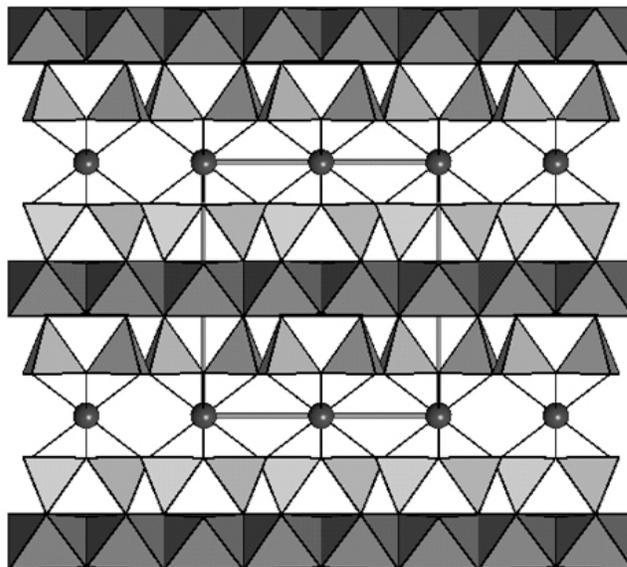


Figure 1. Structure drawing of biotite (viewed down the a -axis), generated using XtalDraw, to show the relationship between structure and cleavage. The unit cell is shown by the gray box.

erated pattern for a possible mineral species, and use the generated pattern to help index their pattern.

SUGGESTIONS FOR TEACHING APPLICATIONS

The most straightforward application of this database is the ability to generate crystal structure drawings for practically any mineral. The implications of this are huge! For instance, with the database and the software, secondary education teachers now have access to an unlimited number of crystal structure drawings. An example of how this might be used is to demonstrate how cleavage is related to atomic structure; an obvious example being the phyllosilicates. Figure 1 is a drawing of biotite, aligned with the a -axis perpendicular to the page. This image shows quite clearly the layered nature of the structure, and should immediately convey the relationship between atomic structure and cleavage, even to students unaccustomed to structure diagrams. After discussing this relationship, the instructor might assign the student pyroxenes and amphiboles to see if they can find the cleavage planes in those structures and determine their directions.

At university-levels, instructors can access this information to build whichever images they find applicable to the concept being taught. Often, as educators, we've been frustrated by not having a structure drawing that clearly indicates the difference between different structures. Figure 2 combines three structures generated in XtalDraw and depicts the unit cells of the three aluminosilicate polymorphs. Very little manipulation was needed in XtalDraw itself; essentially changing the Si to polyhedra and altering the size of some atoms so that the Al-sites stand out from the

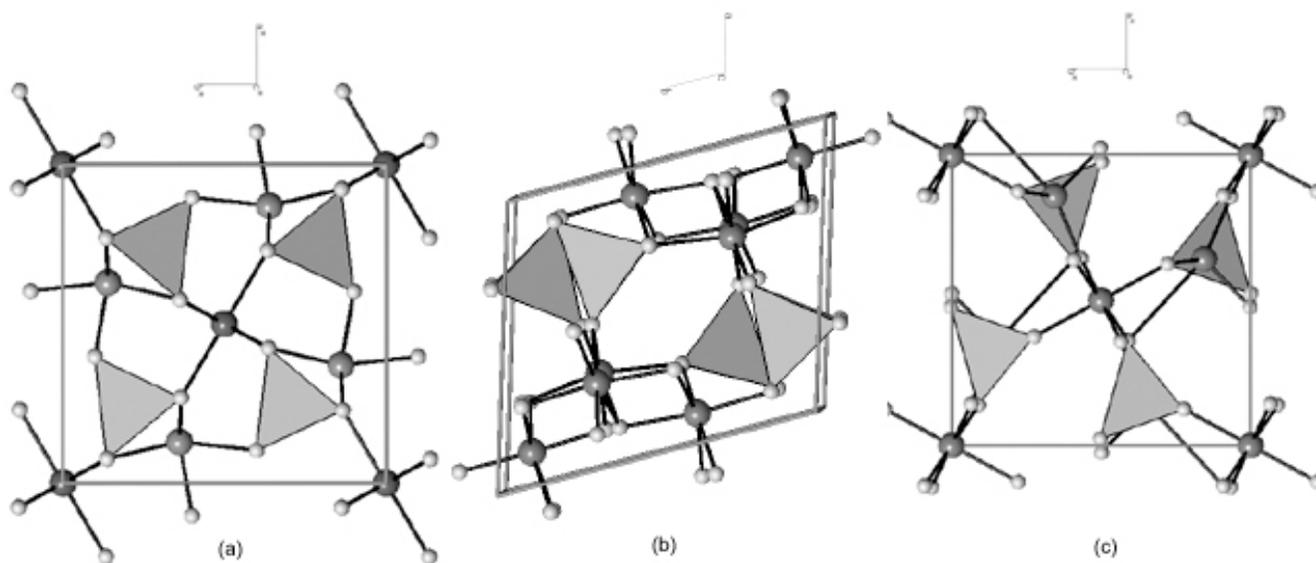


Figure 2. Structure drawing of the three aluminosilicate polymorphs which were generated using XtalDraw: (a) andalusite, (b) kyanite, and (c) sillimanite. Each crystal is viewed down the *c*-axis; the axial positions and unit cells are shown for each. Students can readily compare and contrast the structures of these three polymorphs. The drawings were manipulated to show Si as tetrahedral and to increase the size of the Al cation, making it stand out from the anions.

anions. The easy access of this information allows individual instructors to develop images of structures and views they find most relevant to the point they are trying to make. XtalDraw comes with a large set of crystal structure data, so users will have many of the structures they may want to generate already downloaded with the program.

Students themselves can easily access the software to manipulate atomic structures of different minerals to better understand how the atoms link to each other in order to form a crystal structure. XtalDraw automatically generates a drawing as soon as a file is opened, initially with the *c*-axis perpendicular to the screen (the International Tables for Crystallography default). Atoms are drawn in sizes that scale to Shannon and Prewitt (1969) radii and in colors suggested by Lipson and Cochran (1957). Manipulation of the structure is straightforward, and should be readily accessible to anyone with a basic understanding of Windows-based programs. With a brief introduction, students should be up to speed very quickly, generating structure drawings and bitmap (*.bmp) movies. Being able to directly "play" with a crystal structure allows instructors to better convey such concepts as unit cells, symmetry, and crystallographic axes, as well as closest-packing, for example. Additionally, students can directly generate polyhedra from "ball and stick" models with a single keystroke, allowing a fuller understanding of coordination polyhedra. When the additional data exists, thermal ellipsoids can also be generated for each atom, allowing for directionality of bonds to be explored, or the concept of probability distributions. Structures of minerals with complex anions can be developed to demonstrate the variety in strengths of bonds, building a better understanding of how these complex anions contribute to the properties of the mineral.

In addition to simple structure diagrams, the large amount of data available in the database allows for generation of structure diagrams that can be used to compare the structures of different variants of a mineral or mineral group. For example, end-members of a solid-solution such as forsterite-fayalite can be superimposed, allowing students to see how the structure changes between the Mg- and Fe-dominant olivines, and thus learn, for instance, how minerals can be used as geothermometers. Another example is the generation of a series of structures for crystals recorded at different temperatures and pressures, showing, for instance, how structures can expand at elevated temperatures. Finally, polymorphs can be explored, as well as the phase transitions between them (reconstructive or displacive).

SOFTWARE DEVELOPMENT AND REVISIONS

Additional software that can be used directly with the database is being created and revised. The NSF-funded revisions are designed to develop a more user-friendly visualization and analysis environment that is fully integrated with the crystal structure database, making the database more useful and accessible to a wider audience.

When completed, the revisions will allow students and scientists of all levels and disciplines more ease in exploring and analyzing crystal structure data. This software will include default settings that allow a range of users, from the high school student in chemistry to the professional mineralogist, to investigate fundamental properties of minerals. This includes such varied topics as crystal chemical parameters, diffraction patterns and electron densities (using SPEEDEN, a program that can produce a standardized electron density distribution for

Phlogopite
 Brigatti M F, Medici L, Poppi L, Vaccaro C
 The Canadian Mineralogist 39 (2001) 1333-1345
 Crystal chemistry of trioctahedral micas - 1M from the Alto Paranaiba
 Igneous Province, Southeastern Brazil
 Sample: Tpp16-6a

	5.330	9.239	10.305	90	99.89	90	C2/m							
atom	x	y	z	occ	Biso	B(1,1)	B(2,2)	B(3,3)	B(1,2)	B(1,3)	B(2,3)			
NaA	0	.5	0	.01	2.37	.0244	.0076	.0043	0	.0014	0			
KA	0	.5	0	.98	2.37	.0244	.0076	.0043	0	.0014	0			
MgM1	0	0	.5	.91	.54	.0029	.0009	.0025	0	.0010	0			
FeM1	0	0	.5	.07	.54	.0029	.0009	.0025	0	.0010	0			
TiM1	0	0	.5	.02	.54	.0029	.0009	.0025	0	.0010	0			
MgM2	0	.3322	.5	.91	.52	.0029	.0010	.0022	0	.0004	0			
FeM2	0	.3322	.5	.07	.52	.0029	.0010	.0022	0	.0004	0			
TiM2	0	.3322	.5	.02	.52	.0029	.0010	.0022	0	.0004	0			
SiT	.0760	.16674	.22814	.70	.54	.0032	.0014	.0020	.0002	.0005	.0000			
AlT	.0760	.16674	.22814	.26	.54	.0032	.0014	.0020	.0002	.0005	.0000			
FeT	.0760	.16674	.22814	.04	.54	.0032	.0014	.0020	.0002	.0005	.0000			
O1	.0143	0	.1698		1.55	.0160	.0046	.0031	0	.0009	0			
O2	.3280	.2277	.1706		1.51	.0124	.0057	.0030	-.0008	.0014	-.0005			
O3	.1299	.1674	.3910		.63	.0030	.0015	.0027	.0003	.0011	-.0001			
OH4	.1330	.5	.3976	.94	.55	.0037	.0010	.0022	0	.0004	0			
F4	.1330	.5	.3976	.06	.55	.0037	.0010	.0022	0	.0004	0			

Table 1. An example of one of the datasets that are archived in the American Mineralogist Crystal Structure Database.

a given crystal structure, which will also be integrated in the software package) (e.g. Downs and Halls-Wallace, 2002; Bartelmehs et al., 1993; Downs and Bartelmehs, 1996; Hazen and Downs, 1996; Downs, 1998; Hazen et al., 2000). Furthermore, the database can also display data in the CIF format. This is the standard data format for the International Union of Crystallography, and there are many free software packages available at their website (<http://www.iucr.org>) that read data in this format.

DISCUSSION

An ability to visualize and manipulate crystal structures is fundamental to understanding them, and utilization of crystal structure drawings should be standard in any instruction on minerals. The American Mineralogist Crystal Structure Database, in conjunction with the planned revisions to XtalDraw and its associated software will greatly improve the ease of use; opening the door to a much wider audience. The final stage in development to complete the outreach goals of the database is a set of instructional modules or guides. These guides are being developed to provide tutorials that explain how to use the software, as well as an exploration of the data and fundamental properties of crystals. Specific guides planned include step-by-step instructions, using the pyroxene group, to instruct in the basics of the XtalDraw module, including discussions on how to make animations, and the Xpow and SPEEDEN modules. Complete lesson plans will be developed for both the high-school and university classrooms; these lesson plans will be tested in the classroom as we teach our mineralogy classes prior to publication (Downs and Halls-Wallace, 2002).

The American Mineralogist Crystal Structure database provides a unique source of information for researchers and instructors alike. One of the goals of the

database is to provide an easy link between crystal structure data and a freely available, easy-to-use visualization program, allowing instructors and students to readily access the structures of various minerals. This can enhance the pedagogic goals of an instructor by giving the students the freedom to manipulate atomic structures, making them less abstract. Direct access to crystal structures and the tools to relate atoms, bonds, crystal chemical parameters, diffraction patterns, electron density, and unit cell variations will allow students to see the connections, deepening their understandings of what can be very esoteric concepts.

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