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Observations on online educational materials for powder diffraction crystallography software

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This article presents a series of approaches used to educate potential users of crystallographic software for powder diffraction. The approach that has been most successful in the author's opinion is the web lecture, where an audio presentation is coupled to a video-like record of the contents of the presenter's computer screen.

1. Introduction

Crystallography has been dependent on the use of computers for quite a few decades, but some aspects of crystallography demand greater computer skills than others. I argue that determination of structural models from powder diffraction requires perhaps the largest time investment in learning software of any of the common crystallographic specializations. This is because some tasks, such as indexing of patterns or structure solution, are hit-or-miss processes, where the most skilled researchers utilize an arsenal of programs; moreover, even within a single program, different sets of optional settings may need to be tried before the task is properly completed. Additionally, while there are several widely used generalized structural refinement programs, including *FullProf* (Rodríguez-Carvajal, 1993), *GSAS* (Larson & Von Dreele, 2000) and *TOPAS* (Coelho, 2007), and many more that have specific specialized or historical applications, such as *MAUD* (Lutterotti *et al.*, 1999), *JANA* (Petricek *et al.*, 2006) and *Rietan* (Izumi & Ikeda, 2000), no single program implements all of the widely used refinement capabilities so it is common to use different programs for different projects.

It could be argued that learning to use software should be easy. In the ideal world, high-quality software will be constructed in a self-documenting fashion, where its use is obvious to the neophyte, and experts will find a greater range of options from browsing the built-in documentation as they gain experience. Such software would also be accompanied by comprehensive manuals that provide a mathematical explanation of what is 'under the bonnet' (Billinge & Cranswick, 2006), along with literature citations that lead an interested scientist through the research that led to the development of the method. However, most scientific software is under continual development and is maintained by researchers without programmatic software development support. A visit to the computer books section of a well stocked bookstore makes it clear that the professional software development industry for mainstream applications fails as a model for the development of easy-to-learn and well documented programs; still, crystallographic software tends to be even less exemplary in both areas.

This leaves a significant need for crystallographic software instruction at the introductory level. However, I feel the need is even greater for instruction on advanced features in these programs. The most specialized and unusual techniques are the most complex to learn and are usually only peripherally documented – often only in papers that describe how a technique was developed to solve a problem of pressing interest.

For well over a decade, I have been involved in educating scientists (not always crystallographers) at short courses and workshops, primarily in the use of the *GSAS* crystallographic analysis package and the *EXPGUI* graphical interface to that package (Toby, 2001). *GSAS* is a general package for fitting all types of crystallographic problems, from simple inorganics to proteins, and can be used with both X-ray and neutron data from both powder and single-crystal samples. Over this period I have been interested to find good mechanisms to present this material that make efficient use of my time. This article discusses some of my experiences and conclusions, particularly with respect to audio-visual instructional materials in comparison to more traditional approaches.

2. Motivation

The motivation for teaching powder diffraction crystallography is more than academic. It is a commonly used technique in many fields, including solid-state chemistry, condensed-matter physics, mineralogy, pharmaceutics and materials engineering. Increasingly, researchers with specialties in other areas will use crystallographic characterization as one aspect of their research study. For better or worse they wish to do this without mastering crystallography as a professional specialization.

While my recent employers are not educational institutions, it is very much in the interest of synchrotron and neutron user facilities to ensure that individuals who wish to perform structural studies utilizing the exquisite data that we provide will have the skills needed to perform the required analyses. Building it, and letting them come, is certainly not enough.

Historically, facility users travelled to perform experiments and spent days or weeks collecting and then analyzing data at

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these facilities with the help of the local staff. That is much less possible today. Experiments now are completed frequently in hours or days, and users may access the facilities remotely or through mail-in protocols. E-mail, phone calls and instant messaging allow for conversations between users and the beamline staff who would educate them. However, all these forums are very time consuming and the staff has very little time available, which must be divided between very large numbers of users.

During this same period, both software and its users have changed. Software has become more visually driven, in part through development of graphical user interfaces (GUIs), but also through codes that allow for the visual presentation and manipulation of data and results. It is intrinsically harder to document the actions of a program that interacts dynamically with the user, in contrast to an older style program, where input is prepared in a fixed manner and provided to the program before the program is run. Also, the learning style of graduate students and perhaps even young faculty has changed. The pressure for immediate productivity is higher. Students thrive on types of audio-visual media that have been made possible by personal computers and the internet.

3. Contrasting printed, web and audio-visual instructional materials

I have explored a number of approaches to teaching the use of crystallographic software, through instructing users on use of the *GSAS* package. The *GSAS* manual is unusually large in comparison to most crystallographic software packages. It is over 200 pages and is divided into three sections. The first part provides user training through four worked-through example refinements using the original text-based *EXPEDT* interface; this part fills approximately half of the manual. The second part of the manual (30%) presents the methodology used in the program, which is a fairly comprehensive description of the mathematics of Rietveld refinement. The final section describes some of the programming internals, which is usually not of interest to users. While I myself make fairly frequent use of the second section of the manual, based on the questions I see, my belief is that few novice users have read it.

As I wrote *EXPGUI*, I documented most aspects of how the GUI functions on web pages that are distributed with the program and can be accessed *via* the Help menu. As new features have been added, the documentation was expanded and has now reached ~25 000 words. Again, my experience is that only a fraction of users read much of this documentation. Fairly early in the development of *EXPGUI*, I also created additional sets of web pages that worked through two of the tutorial exercises in the *GSAS* manual that use the *EXPGUI* interface, rather than the original *EXPEDT* program. Since these examples paralleled the *GSAS* manual, my tutorials were given relatively little background explanation, as I felt the user could read the manual for such explanations. These tutorials were still quite time consuming to prepare, as graphics were created to show the computer screen at each stage of the process. My experience was that few people used the web site as I had intended, as an accompaniment to the manual, and used the two in parallel. The users who did work through a tutorial saw what buttons to press and where to supply input but did not understand what they were doing and why. Thus, the pedagogical value was poor.

To try to improve, I then created another web-based sample exercise with a more complete narrative discussion. This tutorial encompassed 12 web pages and 67 figures, the equivalent of a 32-page single-spaced document. The effort required for this exercise was comparable to the creation of a research paper or book chapter. Depressingly, however, web pages are never done – corrections and improvements are always needed. This tutorial was used more frequently, but even with this very significant time investment, it was less than optimal. Users were sometimes confused as to exactly what needed to be done at some stages, since they could not see all the dynamic aspects of the computer software: which buttons were pressed, what menus were opened and how other, perhaps idiosyncratic, controls work, such as plot magnification. In comparison, one-on-one instruction or demonstration to a live audience would provide this, since users could see the computer screen as the mouse moved and windows changed.

I prepared a much more satisfactory tutorial some years later by repeating this training exercise while using the *Camtasia* software product (TechSmith, 2006) to record both my verbal narrative and what was displayed on the computer screen. This provided a recorded lecture that has most of the advantages of a live software demonstration, but with the advantage that a viewer can rewind and repeat sections of the presentation as desired. Further, the time needed to prepare this was a tiny fraction of that needed for the web page tutorial.

Camtasia creates a computer-based presentation, which is similar to video, though potentially with a much large number of pixels. *Camtasia* is able to save these presentations in a wide number of formats. The Flash format (.swf) was selected from these because it creates relatively compact files and viewers are widely available. The ~40 min tutorial presentation resulted in a 26 Mb file, which is a manageable download for most regions of the world. The presentation was then posted on a web site, for which reason I refer to it as a web lecture. However, these presentations are small enough to distribute on CDROMs to parts of the world where web access is problematic.

Based on the positive feedback that I obtained on the first few presentations, a total of 32 web lectures, ranging in length from a few minutes to an hour and a half, were developed and have been placed on the Advanced Photon Source web site (Toby, 2007*a*,*b*). A few presentations were introductory, for example, presenting concepts in the Rietveld method or Newton–Raphson least squares. However, the bulk instructed on use of the software or introduced concepts in crystallography and then how that related to aspects of the software. A summary of the topics on the web site is given in Table 1 and the content of a typical page is shown as Fig. 1. The web-lecture format is also appropriate for more advanced material. Nearly half of the lectures are shorter presentations that

Table 1
A summary of the topics presented on the Advanced Photon Source's powder diffraction crystallography educational resources web site.

Presentation topic	Description
Introductory Topics	
An introduction to crystallography	A series of lectures by Professor Cora Lind from her course introducing concepts in crystallography, such as the lattice, symmetry, single-crystal and powder diffraction, crystal structure determination, and refinement
Getting started with Rietveld	A review of background concepts needed for powder diffraction crystallography and an introduction to how the Rietveld method works
Space groups: a primer on topics significant for powder diffraction	A discussion on space-group naming and subgroup transforms; also, how space groups are input to *GSAS*, and common errors
A casual introduction to least-squares fitting	A non-rigorous introduction to linear algebra, linear and nonlinear least-squares correlation, and uncertainty estimation
Software Tutorials	
An overview of *GSAS* and *EXPGUI*	An overview of the *GSAS* and *EXPGUI* packages' functionality and organization
GSAS/*EXPGUI* demonstration: constant wavelength neutron alumina example	A step-by-step demonstration of how to fit a structure to a neutron data set
GSAS parameters and controls: what to refine when	A discussion of the commonly used parameters for Rietveld analysis and guidelines on the order in which they should be introduced
Le Bail intensity extraction	An explanation of the uses for the Le Bail technique, how it works and tricks for *GSAS*
Judging quality: catching common refinement problems	Comments on how to review Rietveld fits for fitting problems
Combined Rietveld refinements: where 1 + 1 can be >2	How and why to use multiple data sets to fit a single structural model
Advanced Topics	
Advanced Rietveld techniques: tricks and tips with *EXPGUI*	A series of 20 shorter talks on 11 topics; many, but not all, show items of interest to more experienced users
ACNS Magnetic Structure Analysis Workshop	The notes from a workshop and a demonstration showing how to set up a magnetic refinement

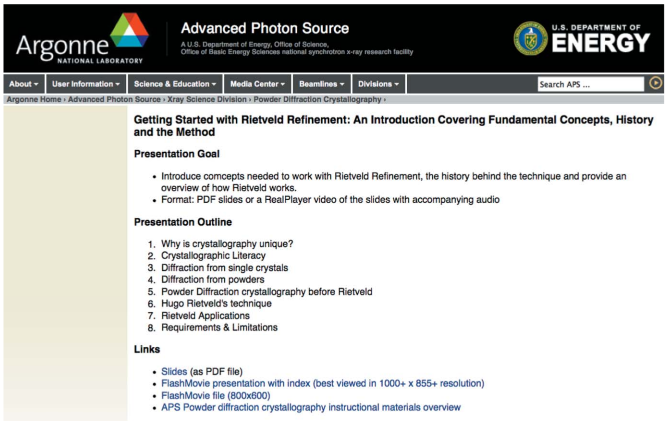
introduce more sophisticated aspects of the programs to users who have already mastered the basics of the software. Most of the lectures are computer demonstrations, displaying the computer screen as software is used, as shown in Fig. 2; others show *PowerPoint* slides. Notes with *PowerPoint* slides are also available for download. Most of the presentations are adapted from lectures prepared for workshops, but others were prepared specifically for web presentation. In all presentations the computer screen display is accompanied by audio dialog. In most cases the presentations were recorded specifically for use on the web, but in one case *Camtasia* was used to record the presentation as it was given as a lecture to a live audience. *Camtasia* can also capture a video stream, but this was not used, as inclusion of video of the speaker seemed to offer no added value. Its omission permitted presentation recording at times with rather relaxed attire.

One failing of this initial set of presentations was that the audience was expected to have a good background in crystallography. This is frequently not true. To address this shortcoming, the web site has been expanded with a series of 15 lectures from Professor Cora Lind's introductory crystallography course at the University of Toledo, which allows the web site to be used by a true novice. The Toledo lectures differ from the others in that they are video images taken in front of an audience rather than screen images. Copies of Cora's slides and lecture handouts are available for download.

There has been no formal evaluation of the impact of the series of web lectures, but there are some anecdotal measures of success: students, faculty and industrial scientists frequently thank me for the presentations. Another measure is the number of graduate students who try unsuccessfully to offload parts of their thesis projects by asking me to analyze their data. Perhaps a more important measure of utility is given by statistics on the viewing of the web pages. The top-level pages for each of the sets of web lectures were viewed in calendar 2009 a total of 21 000 times, with the most visited page, an introduction to the Rietveld method, obtaining more than 3000 visits and the least visited page (on combined refinements) having over 200 visits. Clearly there are people finding these presentations to be of value.

4. Are web lectures the best way to teach?

In my experience, regular interactions with a good teacher, accompanied by reading of a well crafted textbook, are the best mechanism to learn the core concepts in crystallography, so I would say 'no' to the heading question for the case of learning crystallography. Recorded lectures are a helpful adjunct to classroom instruction. However, since many universities do not have faculty teaching these methods, many potential students do not have access to crystallographic instruction; for these people web lectures may be the only 'course' available to them. Distance learning is a growing and



Getting Started with Rietveld Refinement: An Introduction Covering Fundamental Concepts, History and the Method

Presentation Goal

- Introduce comcepts needed to work with Rietveld Refinement, the history behind the technique and provide an overview of how Rietveld works.
- Format: PDF slides or a RealPlayer video of the slides with accompanying audio

Presentation Outline

1. Why is crystallography unique?
2. Crystallographic Literacy
3. Diffraction from single crystals
4. Diffraction from powders
5. Powder Diffraction crystallography before Rietveld
6. Hugo Rietveld's technique
7. Rietveld Applications
8. Requirements & Limitations

Links

- Slides (as PDF file)
- FlashMovie presentation with index (best viewed in 1000+ x 855+ resolution)
- FlashMovie file (800x600)
- APS Powder diffraction crystallography instructional materials overview

Figure 1
A typical web page for a presentation, showing the lecture goals and outline. Links are provided to the presentation slides as well as the video presentation.

effective component of higher education, but for web lectures to be most productive they are best preceded by assigned readings from text books and followed by discussion sessions with an instructor.

The area of interactive graphics could be much more advantageous in teaching crystallography than it is at present. There are many aspects of crystallography where understanding of spatial relationships is important. The Fourier transform is very much a spatial concept. For teaching concepts of diffraction, graphics are invaluable. The *DISCUS* program (Proffen & Neder, 1997; Neder & Proffen, 2008), which simulates diffraction in a graphically compelling manner, has been shown to be of great value for teaching concepts in diffraction (Proffen *et al.*, 2001).

Translational symmetry elements and diffraction geometry are also concepts that require mastering three-dimensional relationships and can be difficult for students to understand. The computer can be of great assistance here. My experience is that the best way to visualize objects in three dimensions (short of having a physical model in one's hand) is to view simulations that appear to rotate. The opportunity to view a simulated object from different directions allows the brain to perceive the internal three-dimensional relationships. My experience is that this works far better than viewing static stereoscopic images, where a slightly different view is supplied to each eye. True dynamic stereo imaging, where a different view of a simulated rotating object is supplied to each eye, provides even better visualization for people with average vision. While three-dimensional visualization equipment has been available for 20+ years for high-end computer workstations, it will probably not be routinely accessible for education unless three-dimensional television becomes popular in the consumer market. I am not aware of any pedagogical tools that use three-dimensionally rendered objects to teach concepts such as the Ewald sphere or glide planes, but this could greatly help students grasp these concepts. However, it is unclear what would be the best methodology to use. One possible mechanism for creation of such 'figures' would be using the VRML graphics description language, which is portable and is implemented as a plug-in for many web browsers, but its use is not common and it has been succeeded by X3D, which also does not seem to have wide acceptance. Better choices might be small application programs written in Flash, Java or OpenGL.

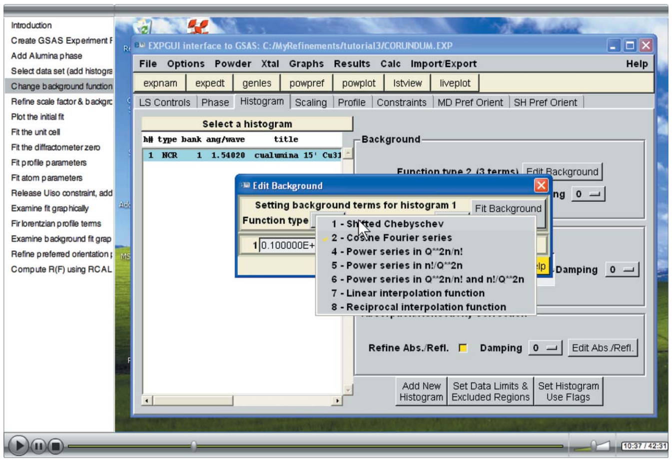


Figure 2

A video (Flash movie) presentation shown in the larger format. This format provides the playback controls at the bottom of the screen and a topic index to the left. The viewer can see the presenter's computer screen and hear the presenter's narration. Note that the actions performed in running the software can be followed from the position of the mouse cursor, seen here as a white arrow.

In contrast, for teaching software, web lectures seem an almost ideal method to present material. They save time for the instructor, while offering the student instruction on demand. They provide a level of detail in experience of how the software is operated that is not possible through static materials. However, for a more complete educational experience, they need to be expanded to include student exercises and discussion groups, which could also occur in an online setting. The web lectures on our web site could likely benefit from design of an overall curriculum in crystallographic education that links together the various examples and lessons into a coherent and logical program of study.

5. Access for the disabled

One aspect of this work that has not been given significant attention is access by the disabled. In the US, this covered under Section 508 of the Federal law, which mandates that government agencies provide the disabled with access to information that is comparable to the access available to the nondisabled. The use of audio materials certainly increases accessibility to the blind over more traditional printed materials. Captioning of the web presentations would be of significant benefit to the deaf. This has been prevented by the costs of transcribing the many hours of speech and the difficulties associated with synchronizing the text display with the presentation. Very recently, Google (2009) has developed automated speech recognition software that creates first-draft transcripts with dialog timing information. It can be expected that significant manual editing will be needed to correct the technical terminology used; nonetheless, this type of technology has the promise to considerably simplify the process of captioning video materials that would be of benefit to the hearing-challenged community, as well as to students who do not speak English well.

6. Conclusions

In this paper I have presented my beliefs on the advantages and disadvantages of different approaches to teaching core concepts in crystallography, as well as computer tools used for crystallographic analysis. Clearly there are people who find web-based tools to their liking, but it is unknown if this is for lack of access to other methods of learning. I would very much like to see a quantitative study of the efficacy of this teaching approach in comparison to more traditional instructional techniques. In the absence of formal studies, I remain convinced that web lectures, such as those described here that combine a screen view with a verbal presentation, provide the most optimal tool for teaching use of modern crystallographic software. I plan to use this format in the future to provide tutorial presentations for my future software development projects.

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