Journal of
**Applied
Crystallography**
ISSN 0021-8898
Editor: **Anke R. Kaysser-Pyzalla**

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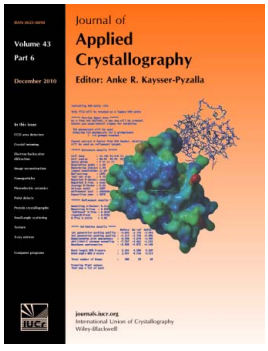
J. Appl. Cryst. (2010). **43**, 1532–1534



Journal of
Applied
Crystallography

ISSN 0021-8898

Received 21 July 2010
Accepted 14 October 2010

Jpowder: a Java-based program for the display and examination of powder diffraction data

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The ability to display and inspect powder diffraction data quickly and efficiently is a central part of the data analysis process. Whilst many computer programs are capable of displaying powder data, their focus is typically on advanced operations such as structure solution or Rietveld refinement. This article describes a lightweight software package, *Jpowder*, whose focus is fast and convenient visualization and comparison of powder data sets in a variety of formats from computers with network access. *Jpowder* is written in Java and uses its associated Web Start technology to allow 'single-click deployment' from a web page, http://www.jpowder.org. *Jpowder* is open source, free and available for use by anyone.

1. Introduction

There is no shortage of computer programs that are capable of displaying powder diffraction data, often as the logical outcome of an analysis step such as a Rietveld refinement. Such programs include, for example, *TOPAS* (Coelho, 2003), *FOX* (Favre-Nicolin & Černý, 2002), *HighScore* (2010), *Endeavour* (Putz *et al.*, 1999), *DASH* (David *et al.*, 2006), *FullProf_Suite* (Rodriguez-Carvajal, 1993), *GSAS* (Larson & Von Dreele, 1994), *EXPO2009* (Altomare *et al.*, 2009), *JANA2006* (Petricek *et al.*, 2006), *EVA* (2010), *PowderX* (Dong, 1999) and *Powder3D* (2008). However, such software packages are designed mainly for analysis of diffraction data (*e.g.* Rietveld refinement, structure solution, quantitative phase analysis, indexing *etc.*). Here, a simple, lightweight, easy-to-access program (*Jpowder*) for straightforward visualization and comparison of powder diffraction data sets is presented.

Jpowder uses both the Java Web Start and Java applet technologies. Java Web Start provides the power to launch fully featured Java applications with a single click and without the need to go through complicated operating system installation procedures. It increases performance by caching application resources and provides automatic update management by checking for application updates on each application launch. If new versions of any Java archive (JAR) files that constitute the application are available from the site from which they were originally accessed, Java Web Start downloads them before running the application. Furthermore, the nature of the Java Web Start model can enable applications to be installed by the end-user in a 'locked-down' environment, such as a student teaching laboratory in a university department.

Using the same codebase, a limited range of *Jpowder* functionality has been exposed in the form of a Java applet – a self-contained Java component that is embedded within a standard HTML web page. This provides an even more convenient mechanism to present data in an interactive style on the web.

The Java programming language has been used by many scientists to develop applications that offer excellent performance and portability, and some notable Java-based programs in the field of crystallography and molecular display include *Jmol* (2008), *MAUD* (Lutterotti & Bortolotti, 2003), *JCrystal* (2010) and *Kiosk* (2010). The *Jmol* applet has been widely adopted for the interactive display of molecules on the web. The applet version of *Jpowder* aims to do the same for powder diffraction data.

2. *Jpowder* overview

Jpowder is optimized for visual inspection of powder data. Data files can be dragged into *Jpowder* from the desktop or by using the *Jpowder* Explorer window (Fig. 1). When the Explorer window is

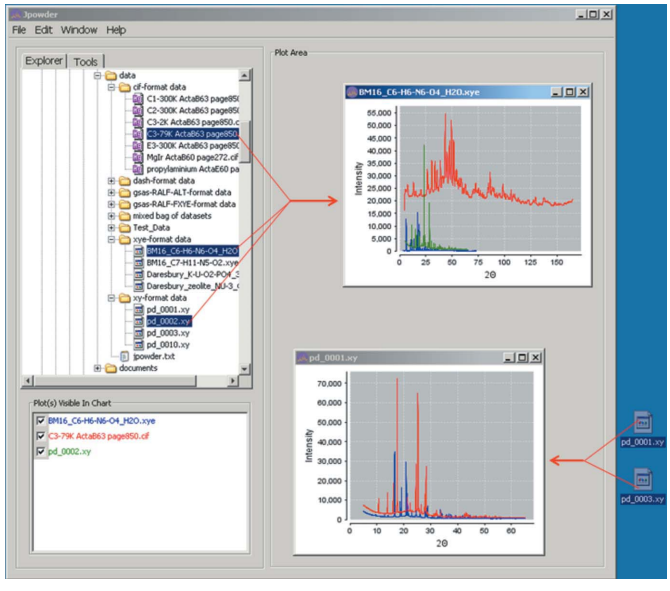

Figure 1
Two ways of displaying powder data in *Jpowder*: on the left using the *Jpowder* Explorer panel and on the right by dragging in files from the desktop.

Table 1
A list of available keyboard shortcuts in *Jpowder*.

Keys	Action
Ctrl + O	Open File chooser window
Ctrl + P	Print
Ctrl + Alt + P	Print for publication
Ctrl + Alt + A	Close all windows within the main plot area
Ctrl + Z	Undo closed window
Ctrl + Y	Redo closed command
Ctrl + C	Copy currently selected window to clipboard
Ctrl + E	Open the properties window
Ctrl + F2	Open online documentation and support
Ctrl + A	Open 'About' window
Ctrl + left click	Move the plots

used, multiple files from multiple folders can be selected simultaneously. The data are visualized as plots in charts, also referred to as plot windows. Plots may be manipulated using the mouse or a number of shortcut keys. In addition, various tools are available to aid plot comparison, for example, by moving, rescaling and changing the appearance of plots. Charts can be exported in various ways, including using the 'PDF for publication' option. *Jpowder* also includes tools for basic data analysis tasks, including, for example, selecting peaks to a peak list, which can subsequently be exported to an indexing program such as *DICVOL* (Boultif & Louër, 2004), and a tool for switching x axes between 2θ and d spacing to aid comparison of data sets collected at different wavelengths. Charts can be saved to disk in '*Jpowder*-applet format' (a serialized object), which can subsequently be loaded into the applet version of *Jpowder*. This feature can be used to publish powder data not only as static images but also as interactive applets that offer the same manipulation options as a *Jpowder* chart; see, for example, http://www.jpowder.org/JpowderApplet.html.

3. Program description

3.1. Supported file formats

The following file formats are supported for this version of *Jpowder*:

(*a*) XY format (.xy). Two-column ASCII format, where the data in the first column are assumed to be the diffraction angle in 2θ and those in the second column are X-ray or neutron counts.

(*b*) XYE format (.xye). As for XY format, but with an additional column listing the estimated standard deviations for the counts. This format also supports the use of a single real number, specifying a wavelength, as the first line of the file.

(*c*) CIF format. The crystallographic information file format is described in detail at http://www.iucr.org/resources/cif.

(*d*) ISIS *GSAS* format. At the STFC ISIS Facility (Rutherford Appleton Laboratory, Oxford, UK), *GSAS* is frequently used to refine structures against time-of-flight neutron powder data. The current version of *Jpowder* requires such data to be in what the *GSAS* manual refers to as 'RALF/FXYE format'. When reading such a time-of-flight .gss file, the x values are assumed to be given in units of microseconds.

Jpowder will attempt to read files with extensions .gss and .cif as ISIS *GSAS* format and CIF format files, respectively. For files with any other extension, *Jpowder* will attempt to read the file in XY or XYE format. All data are assumed to be constant-wavelength data with the exception of data using the ISIS *GSAS* format. The *Jpowder* code is open source and structured in such a way that it is straightforward for anyone used to Java programming to extend the list of supported file types.

3.2. Plotting data

Jpowder supports three methods for opening files: (1) by the standard 'File' menu approach, which permits the selection of one or more files from a single folder; (2) by dragging-and-dropping one or more files from a single folder (including the desktop) onto the Plot Area of *Jpowder*; (3) by dragging-and-dropping one or more selected files from one or more folders using the *Jpowder* Explorer window. Note that when multiple files are opened simultaneously, they do so in a single *Jpowder* chart. Furthermore, when a file is dropped onto an existing chart, an additional plot is created within that chart.

3.3. Visually exploring a chart

When multiple plots are displayed in a single chart, the 'Plot(s) Visible In Chart' panel is used to select which plots are visible at any given time. The mouse can be used to adjust the displayed region as follows: left click, hold down, and drag to the right and down to zoom in on a region (a semi-transparent rectangle highlights the area to be zoomed); left click, hold down and drag to the left to restore the default view; left click, hold down and drag whilst holding down the Ctrl key to move the plots. A list of shortcut keys is presented in Table 1.

3.4. Preparing a figure for publication in a scientific journal

A chart may be saved as a PDF file or an image (PNG) file or copied to the clipboard. In addition, a chart can be saved as a 'PDF for Publication' file, where the background colour is temporarily changed to white while the chart is saved to the selected format. Changing of the background colour can also be done manually using the 'Properties' window, which can be accessed either from the main 'Edit' menu or by right-clicking over the chart.

3.5. Preparing an interactive figure for web publication

A chart may also be saved as a '*Jpowder*-applet format' file. This file can be subsequently imported into an applet version of *Jpowder* in order to display the data on a web page in a form that has the same 'look-and-feel' and functionality as a *Jpowder* chart. Full details of

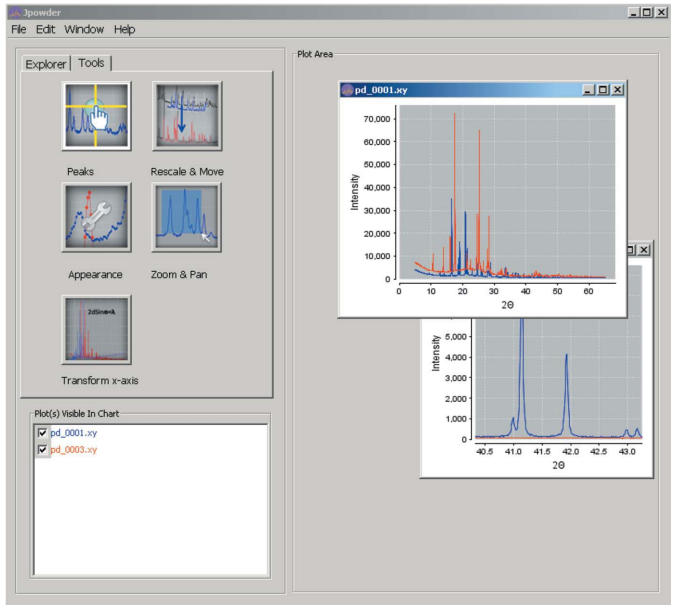

Figure 2
The *Jpowder* Tools panel.

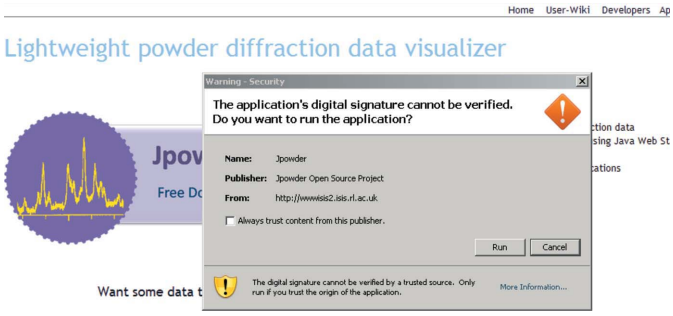

Figure 3
Jpowder certificate warning.

how to use this feature are given at http://www.jpowder.org/JpowderApplet.html.

3.6. *Jpowder* Tools

Upon clicking the Tools tab of *Jpowder*, the user is presented with several options (see Fig. 2) for interacting with, or changing the display of, plots in *Jpowder*, and these are summarized below.

3.6.1. Peak selection. This allows a user to select the location of peaks. These are stored in a peak list which can be copied to the clipboard and subsequently utilized in indexing programs such as *DICVOL*.

3.6.2. Rescale and move. The y data of a plot can be scaled by simple multiplication and division operations, or adjusted by the addition or subtraction of a constant value. These simple operations are provided to help users compare plots collected under different conditions more easily.

3.6.3. Appearance. This tool is complementary to the chart properties window and is used to change the appearance of plots in a chart. For example, it allows users to change features such as marker type, plot colour and axis tick spacing.

3.6.4. Zoom and pan. This tool currently only provides a description of the default zoom and pan functionality of *Jpowder* and is serving as a placeholder for the addition of more functionality.

3.6.5. *x*-axis transform. This tool uses supplied wavelength information to convert 2θ into d spacings and *vice versa*. It assumes that the data were collected at constant wavelength and therefore currently does not support time-of-flight data.

4. Software and hardware environment

Jpowder will run on any PC that supports a Java Runtime Environment (JRE). Specifically, version 1.6 or higher is required for the version of *JPowder* described in this paper; however, if a JRE version older than 1.6 (*i.e.* older than 11 December 2006) is installed on the local machine, the user is directed to the JRE update web page.

By default, Java Web Start applications run in a restricted environment, known as a sandbox – meaning they cannot access local files or the network. *Jpowder* provides functionality that goes beyond that allowed in the sandbox by signing the application's JAR files; this means that the user will need to accept a digitally signed certificate upon first installation, as depicted in Fig. 3. This model enables Java Web Start applications to be installed by the end-user in an environment without administrative permissions, such as a university department where students have roaming accounts.

Jpowder versions can be updated for all users worldwide simply by providing an updated JAR file on the web server. On each user's computer, Java Web Start checks the web server for updates when the application runs. Resources are cached locally, for improved performance, but this also confers the advantage that they can function independently during any network/internet outages.

The code is licensed under the GNU General Public License version 3.

5. Documentation and availability

Jpowder is downloadable from http://www.jpowder.org and the user wiki is available at http://www.jpowder.org/wiki. The source code is available to download from http://code.google.com/p/jpowder and bugs can be reported *via* http://code.google.com/p/jpowder/issues. The *Jpowder* discussion group at http://groups.google.com/group/jpowder provides a forum for the discussion of *Jpowder*-related issues, such as feature requests.

KP gratefully acknowledges the support of the Department of Computer Science at Kasem Bandit University. AJM is grateful to STFC, who provided the funding for MA. The authors are very grateful to Srikanth Nagella, Harriott Nowell and Norman Shankland for useful discussions, suggestions and extensive program testing. *Jpowder* uses the open source libraries JFreeChart (http://www.jfree.org/jfreechart), JXLayer (http://jxlayer.dev.java.net) and iText (http://itextpdf.com/terms-of-use/index.php), and we would like to thank the developers of these excellent libraries for making their software available.

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