Development of a graphical interface for the Rietveld refinement program DBWS

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1. The crystallographic problem and method of solution

The DBWS program, the latest version of which is 9807a (Young et al., 1999), an upgraded version of DBWS-9411, described by Young et al. (1995), is written in Fortran and can carry out Rietveld refinements using digitized data (from a neutron or X-ray diffractometer) stored in a text file. It also requires an Input Control File (ICF), constructed by the user, which stores information about the material and program execution. The ICF is a text file that contains crystallographic information about the material and program settings in lines and columns. Given the size of the input file needed by DBWS, compiling it can be confusing, difficult and time consuming (an ICF for quartz plus alumina, which has only two phases, uses an ICF with more than 60 lines). Most users edit new ICFs by opening previously used files in a non-formatted text editor (such as Microsoft Notepad or DOS Edit) and then substituting the old values for new ones. Editing these files manually can be confusing because the user needs to know the placement of each parameter in the ICF; furthermore, small errors in non-formatted text editor lines. Most users edit new ICFs by opening previously used files in a non-formatted text editor (such as Microsoft Notepad or DOS Edit) and then substituting the old values for new ones. Editing these files manually can be confusing because the user needs to know the placement of each parameter in the ICF; furthermore, small errors in the format of the ICF may cause problems when the program runs. After the program has run, a text file containing the refined data is returned, along with, optionally, a binary file that is used to plot the diffraction pattern using a graphics program such as DMPlot (Marciniak, 1997).

To solve the aforementioned problems, a graphical interface for DBWS (which works with versions 9411 and 9807 and runs under Windows 95/98/NT) has been developed. Known as DBWS Tools, the program makes DBWS much easier to use and manages each step of the process, from the creation of the ICF to the plotting of the diffraction pattern using the external program DMPlot. In this way, the user need not consult the program manual every time a new sample is analysed (because the meaning of each data field is shown on screen) and the entire process is much faster and user-friendly.

2. DBWS Tools

DBWS Tools was compiled using Borland C++ Builder and runs under Windows 95/98/NT (as a Windows-based program, it cannot run under DOS). It compiles ICFs and manages DBWS and DMPlot execution. The first and most important function of the program is the ICF editor. It collects data entered by the user in a series of fields arranged in windows, with descriptions of each option so that the User's Guide is not needed for the task. The input files generated by DBWS Tools are identical to those shown in the DBWS User's Guide (versions 9411 and 9807). The interface arranges data correctly, no matter what order the user enters them. ‘Default’ buttons are included in the windows so that the user can bypass the typing of the most common values. The program also runs DBWS in a DOS window using the files indicated by the user. Optionally, the diffraction pattern can be plotted using DMPlot, which is a shareware program that uses plot files produced by DBWS and has a wide range of options when working with these files. DBWS Tools can deal with the complete process of compiling an ICF, running DBWS and running DMPlot for a graphical analysis.

3. Availability

The program and its future updates can be downloaded from http://www.fisica.ufc.br/raiosx/DBWS.htm. There are still more options to be added to the DBWS Tools program. Future versions may open and edit previously generated ICFs and use .INI files to store the user preferences, so that the same parameters can automatically be used for multiple refinements. We recommend that users constantly check the web site for updates.

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References