



Contribution ID : 69

Type : **Poster**

COMPUTATIONAL CRYSTALLOGRAPHY: PROGRAMS FOR ANALYZING BIDIMENSIONAL DIFFRACTION PATTERNS

Thursday, 13 August 2015 17:30 (1:00)

Abstract content

Bi-dimensional diffraction is a promising technique for structural analysis and so it shows its recent use growth. The obtained data is analyzed through computational tools like the program ANAELU (ANALytical Emulator Laue Utility) to assist with the interpretation of X-ray diffraction patterns produced by textured samples. This program includes: structure representation, experimental bi-dimensional diffractogram analysis and diffraction patterns simulation. The project for the ANAELU program improvement includes: background modelling, experiment-model comparison and parameters manipulation; all the previous in order to upgrade it towards a Rietveld type quantitative bi-dimensional analysis. To deliver a better experience for the user, the new ANAELU has a complete new GUI (graphic user interface) programmed in wxPython, which is friendlier and more intuitive than before. This GUI born from the previous experience, making it more compatible with the current and future platforms, like Windows and the UNIX-like family. The present project is feasible through the use of mixed programming among compiled (FORTRAN 95/2003) and interpreted (wxPython) languages. Improvements in this matter have been achieved; regarding calculations, we can ensure greater portability, long term support and enhanced execution velocity (from 7 hours to 25 minutes in a specific example) with the use of the CrysFML library which allows us to take advantage of a highly efficient calculation process. Up to now the new GUI is able to read and compare two diffraction patterns, one calculated (like said before) and one experimental. The two images are linked to each other to improve the experience, allowing easier and faster comparison. The GUI also has the most common menus to open and save the files in several formats.

Summary

Primary author(s) : Mrs. BURCIAGA-VALENCIA, Diana (estudiante doctorado)

Co-author(s) : Mr. VILLALOBOS PORTILLO, Edgar Eduardo (Centro de Investigacion de Materiales Avanzados S.C (CIMAV)); Dr. FUENTES-COBAS, Luis E. (Centro de Investigación en Materiales Avanzados); Dr. FUENTES-MONTERO, Luis (Diamond Light Source)

Presenter(s) : Mrs. BURCIAGA-VALENCIA, Diana (estudiante doctorado)

Session Classification : Posters II