

How can we enumerate all solutions in powder indexing? -- on the algorithm of Conograph

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Powder indexing (*i.e.*, cell determination of a crystal from its powder indexing diffraction pattern) is known as a comparatively difficult stage among various procedures required in *ab-initio* structure determination. Although there are already a lot of algorithms and softwares including classical Ito, Treor and Dicvol, they fail often in finding the true solution. Therefore, in powder indexing, it is supposed that crosscheck of solutions is necessary using several softwares. In order to change this tedious and error-prone situation in powder indexing, we developed a new algorithm and software Conograph. At present, the initial development of the graphical user interface of Conograph has been finished.

Although there might remain some bugs in the program of Conograph, the success rate of Conograph until now is already close to 100 per cent, and the failure occurs only when the quality of the diffraction pattern is so poor that the de Wolff figure of merit does not rank solutions appropriately. Our test data include all types of the Bravais lattices and diffraction patterns from characteristic X-rays, synchrotron, neutron spallation sources and reactor sources. We also tested Conograph with difficult cases including large unit cells. Even for two-phase data, it has always succeeded in finding the correct lattice constants of the main 1st phase.

Finally, we mention theoretical aspects of the new algorithm; as indicated in our title, in powder indexing, the number of solutions (*i.e.*, lattice constants) is not always unique (but proven to be finite theoretically) similarly with other stages in *ab-initio* crystal structure determination. However, even in cases that two different lattice constants have the completely same peak positions, Conograph is designed to detect both of them as solutions. That is, Conograph can pick up all the lattice constants having the best figures of merit at most in a few minutes. We shall present the algorithm and performance of Conograph.

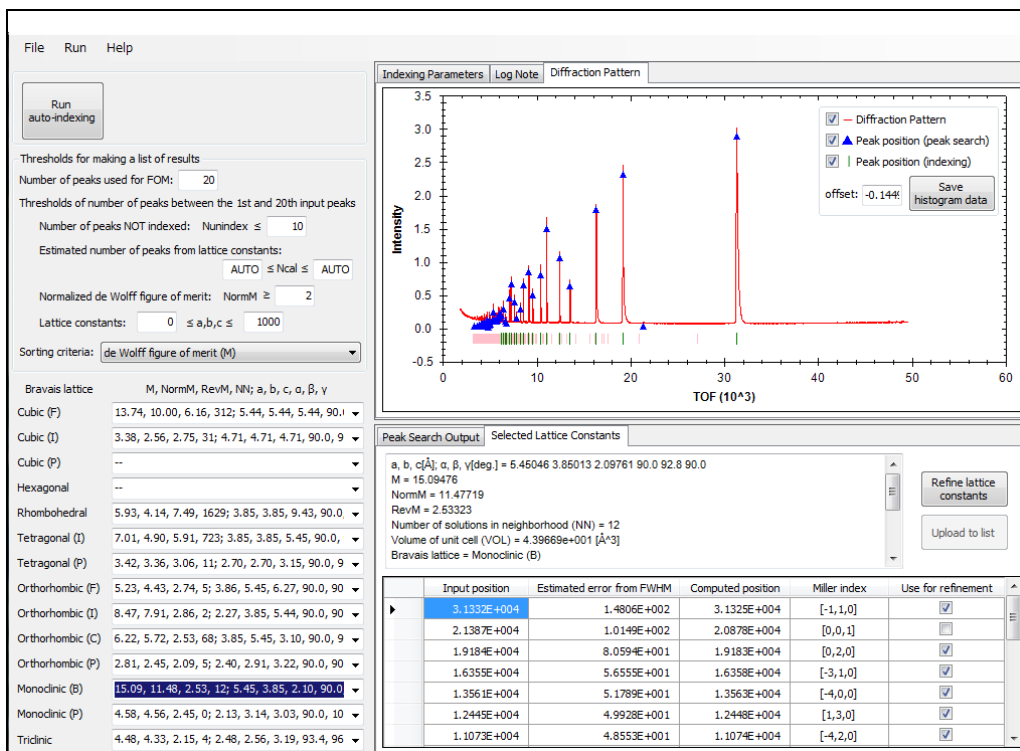


Fig. 1 Appearance of graphic user interface of Conograph