Full-Pattern Search-Match using the Crystallography Open Database: an internet tool

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The COD project (Crystallography Open Database, www.crystallography.net/) with more than 240000 cif structure files, opens the way to free search-match tools via internet [1,2]. COD structure files harvesting is now routinely operated and automated for a growing number of publishers' journals, like IUCr's.

A subversion has been relocated on a new server dedicated specifically to a newly developed Search-Match procedure, at cod.iutcaen.unicaen.fr [3], called Full-Pattern Search-Match (FPSM), dedicated to the powder diffractometry community. Indeed, COD is interesting not only as an archive of structures solved by powder diffraction methods, but also as a possibility to use it in existing and search-match procedure to come. The search-match softwares from the main diffractometer companies (Panalytical, Bruker, Rigaku, Crystal Impact) already implemented COD in their routines.

The FPSM internet tool is not a simple search engine allocating phases from peak maxima. It works on a full Rietveld analysis including the line profiles. It then allows quantitative phase analysis when several are detected in the user-uploaded diffraction pattern. This quantification is available from x-ray, neutron and electron powder patterns, with high or medium resolution instruments, obviously provided the structures are already in COD. Four different instrument geometries are accepted. The sole fact that it works on the full pattern prevents bad peak allocations when severe peak overlaps are present. It proved particularly suited for nanocrystalline powders, in which severe line broadening appears precluding phase identification from only peak maxima, and for strongly multiphasic samples for which even with well crystallized phases strong peak overlapping occurs. We successfully tested up to nine phases. A typical FPSM result (Figure 1) for a tri-phase sample, together with phase quantification and fit reliabilities, also includes isotropic crystallite sizes and microstrains determination, since the line broadening is treated and the instrument resolution estimated.

Phase ID	name	vol. (%)	wt. (%)	crystallites (Å)	microstrain
9004178	Zincite	20.5148	29.1683	1893.8	4.76139e-08
1000043	Fluorite	42.3438	33.7285	2154.45	0.00036731
9007498	Corundum	37.1414	37.1032	1941.94	0.000229095

Final Rietveld analysis, Rw: 0.154707, GofF: 1.90021

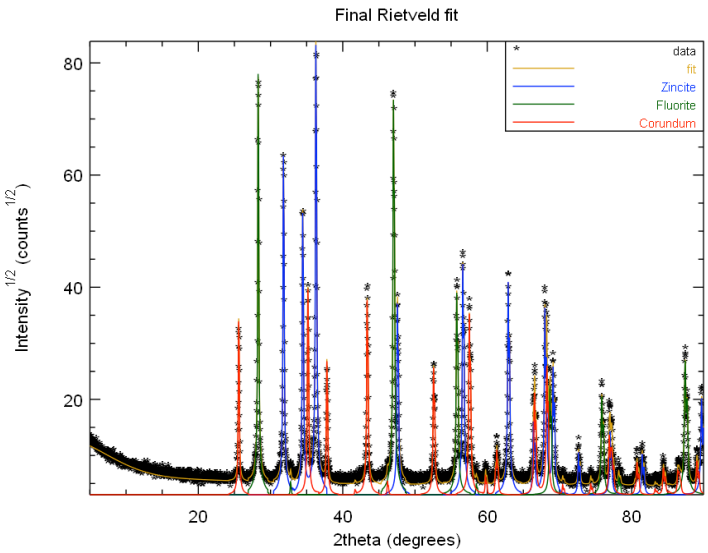

Fig. 1 Table showing the FPSM results for quantitative phase and line broadening analysis on a tri-phase sample, and plot of the fitted pattern with all phases.

In addition to COD, FPSM will be operated in the future on sister databases, PCOD, that contains structures predicted by the GRINSP program [4], and TCOD, which collects DFT(or other)-optimised structures.

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References

1. Gražulis, S.; Chateigner, D.; Downs, R. T.; Yokochi, A. F. T.; Quirós, M.; Lutterotti, L.; Manakova, E.; Butkus, J.; Moeck, P. & Le Bail, A. (**2009**). *Crystallography Open Database -- an open-access collection of crystal structures*, Journal of Applied Crystallography 42 : 726-729.

2. Gražulis, S.; Daškevič, A.; Merkys, A.; Chateigner, D.; Lutterotti, L.; Quirós, M.; Serebryanaya, N. R.; Moeck, P.; Downs, R. T. & Le Bail, A. (**2012**). *Crystallography Open Database (COD): an open-access collection of crystal structures and platform for world-wide collaboration*, Nucleic Acids Research 40 : D420-D427.

3. L. Lutterotti, H. Pilliere, C. Fontugne, P. Boullay, D. Chateigner (**2013**), in preparation
4. Le Bail, A. (**2005**). *Inorganic structure prediction with it GRINSP*, Journal of Applied Crystallography 38 : 389-395.