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

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The NANOAIR project

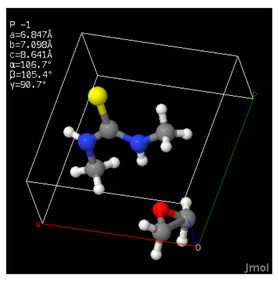
The air quality is one of the major concerns for health. There is a need for continuous monitoring of the particulates especially in the submicron range. An European project named Nanoair has been concluded successfully which aim was to develop a mobile instrument for qualitative and quantitative analysis of breathable particles using XRD and SAXS.

Nanoair was granted by FP7-RTD (Grant agreement N° 222333)

Goal of the project and general idea

Build a complete portable system that collect the dust, with automated analysis to obtain particle sizes (by SAXS), phase identification and quantification along with crystallites/microstrains (by XRD/Rietveld) and finally store all data and results online and the samples locally for reference. The idea is to use the Rietveld method also for the search-match step, as we are in any case limited to phases with known crystal structure usable in the Rietveld quantification. A Full Pattern Search-Match method has been developed and tested using the COD as an archive of crystal structures (www.crystallography.net).

WWW.CRYSTALLOGRAPHY.NET



Information card for 2105483

2105482 << **2105483** >> 2105484

Preview

Coordinates	2105483.cif
Structure factors	2105483.hkl
Original IUCr paper	HTML

Structure parameters

Formula	- C5 H12 N2 O S -
Calculated formula	- C5 H12 N2 O S -
Title of publication	Methylthioureas and their morpholine and dioxane adducts; hydrogen-bonding patterns
Authors of publication	Jones, Peter G.; Taouss, Christina; Teschmit, Nicole; Thomas, Lena
Journal of publication	Acta Crystallographica Section B
Year of publication	2013
Journal volume	69
Journal issue	4
Pages of publication	405 - 413
a	6.847 ± 0.0004 Å
b	7.0982 ± 0.0004 Å
c	8.6412 ± 0.0003 Å
α	106.676 ± 0.005°
β	105.448 ± 0.005°
γ	90.679 ± 0.004°
Cell volume	386 ± 0.04 Å^3
Cell temperature	100 ± 2 K

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Open-access collection of crystal structures of organic, inorganic, metal-organic compounds and minerals, excluding biopolymers

All data on this site have been placed in the public domain by the contributors.

COD Advisory Board thanks The Research Council of Lithuania for their financial support of the publication *"Crystallography Open Database (COD): an open-access collection of crystal structures and platform for world-wide collaboration"*, *Nucleic Acids Research*. (2012) PDF version

We thank Crystal Impact GbR for their financial support of the publication *"Crystallography Open Database - an open-access collection of crystal structures"*, *J. Appl. Crystallogr.* (2009) PDF version

Currently there are **241466** entries in the COD.
Latest deposited structure: 2105506 on **2013-11-06** at **12:23:17 UTC**

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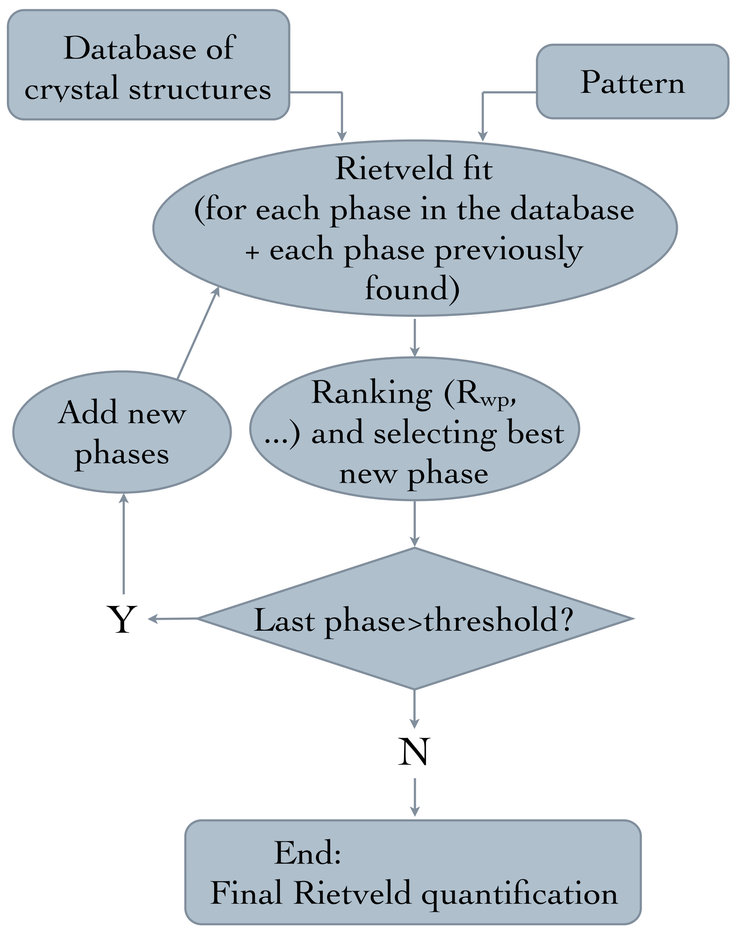
The FPSM (Full Pattern Search-Match method)

Developed inside the Nanoair project for the portable instrument

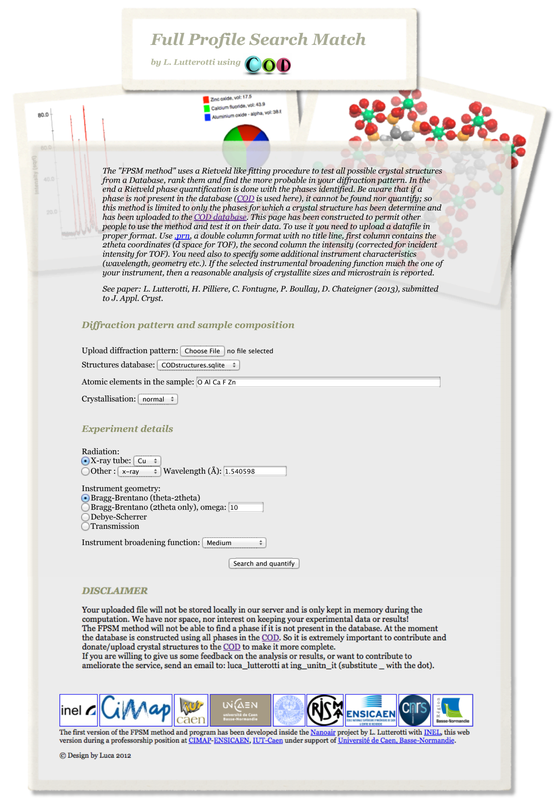


Pro:

- No user intervention, automatic analysis
- No peaks location/detection required (works with nano materials/particles)
- Full Rietveld quantitative analysis provided
- Works also for neutron and electron diffraction

Cons:

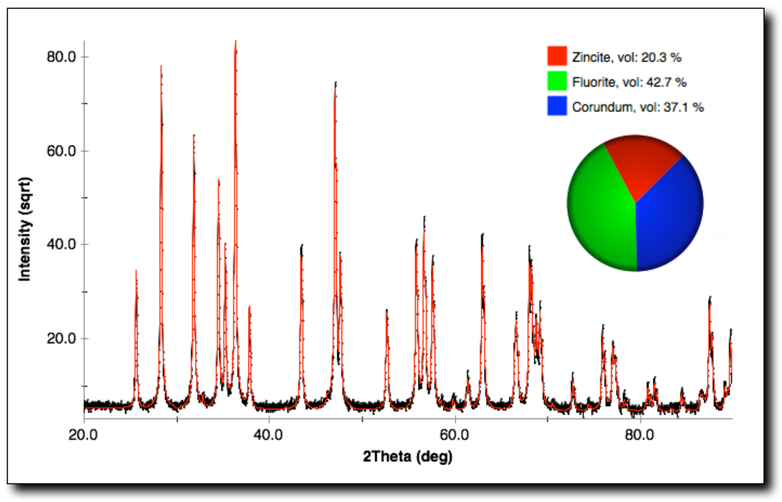
- Only phases with known crystal structure are ready to be used (unknown structures require a list of peaks and calibrated intensities, PONKS)
- Available databases are still incomplete
- If no elemental composition provided → requires > 20 minutes on 12 cores computer
- Good ranking algorithm required for very small phase amount



An open internet version has been setup at:
http://cod.iutcaen.unicaen.fr
http://nanoair.ing.unitn.it:8080/sfpm
search and quantification is limited by the time required (or better server response time) so it should be used restricting the composition as much as possible to speed up computation. A limited number of concurrent connections are supported also. INEL SAS can be inquired for the full version.

Testing FPSM using the COD

Sample cpd1h from quantitative analysis Round-Robin
http://www.iucr.org/resources/commissions/powder-diffraction/projects/qarr



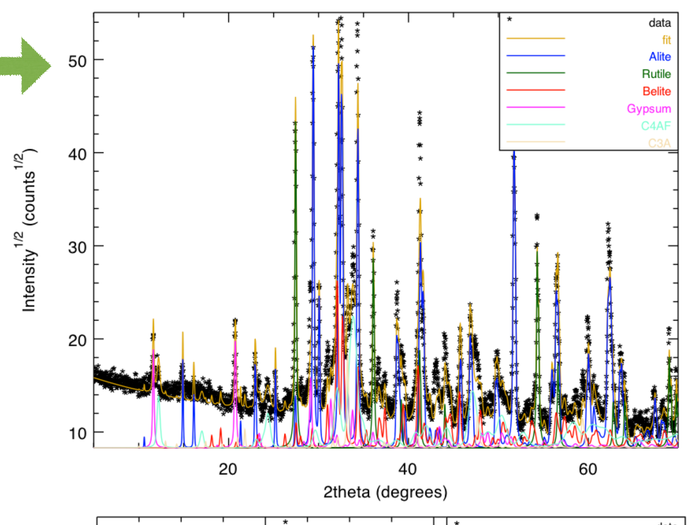
Phase (wt%)	FPSM	Round-Robin
ZnO	29	29.6
CaF	33.9	34.3
Al_2O_3	37.1	36.1

Total computation time (12 cores, 2.93GHz, COD, inorganic):

- No composition restriction: **565 secs**
- Only Al, Ca, F, Zn, O, Mg, Na, Si, Cl: **19 secs**

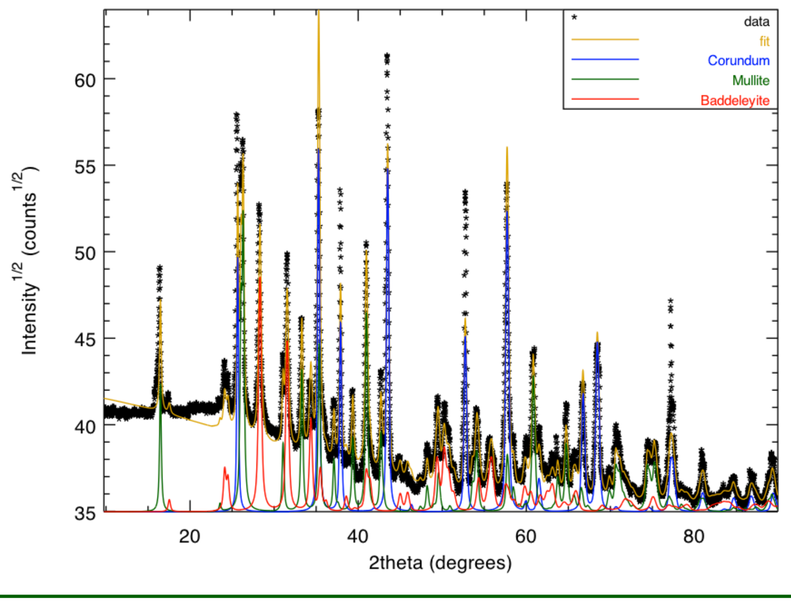
name	vol. (%)	wt. (%)	crystallites (Å)	microstrain
Alite	52.3359	50.1148	2722.86	0.000913623
Rutile	8.7909	11.3199	1382.41	4.9784e-05
Belite	14.6584	14.8578	1014.1	0.00145265
Gypsum	7.28186	5.03503	881.992	0.00175863
C4AF	14.4548	16.3939	485.795	0.00705494
C3A	2.47814	2.27862	1426.2	0.00125916

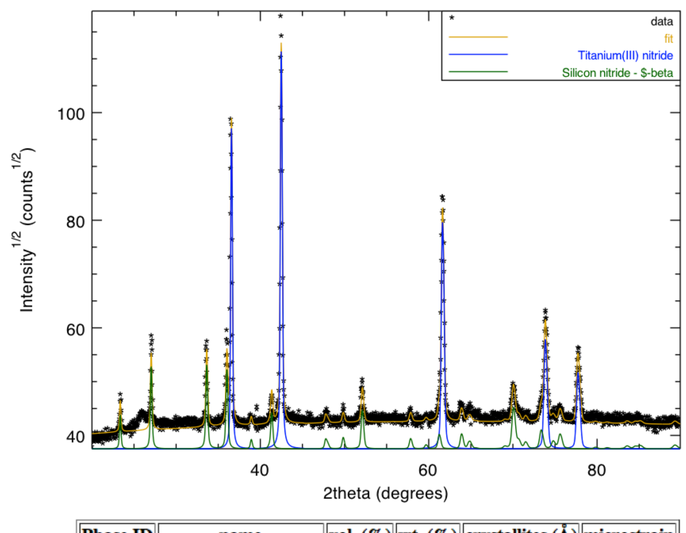
Some additional phases (cement phases) can been user added to the database if not present in the COD



Phase ID	name	vol. (%)	wt. (%)	crystallites (Å)	microstrain
9009672	Corundum	41.0726	45.1467	730.664	0.00137145
9005502	Mullite	53.5784	46.2318	515.483	0.000527227
9005833	Baddeleyite	5.34905	8.62151	371.805	0.00203445

Final Rietveld analysis, Rw: 0.0455532, GofF: 1.79502





Phase ID	name	vol. (%)	wt. (%)	crystallites (Å)	microstrain
1101045	Titanium(III) nitride	50.0729	62.8891	1682.09	0.00122093
1001246	Silicon nitride - $-beta	49.9271	37.1109	800.99	0.00129495

Final Rietveld analysis, Rw: 0.0601521, GofF: 2.66024