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 Nanaire has been concluded successfully which aim was to develop a mobile instrument for qualitative and quantitative analysis of breathable particles using XRD and SAXS.

Nanaire was granted by FP7-RTD (Grant agreement N°222335)

Goal of the project and general idea

Build a complete portable system that collect the dust, with automated analysis to obtain particle sizes (by SANS), phase identification and quantification along with crystallite/ microstrain (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).

Instrument broadening function:

- Radial-Scherrer
- Debye-Scherrer (2θ only), omega:
- Bragg-Brentano (θ-2θ)
- Other:

Instrument geometry:

- Transmission
- Debye-Scherrer
- Bragg-Brentano (2θ only), omega:
- Bragg-Brentano (θ-2θ)
- Other:

Radiation:

- x-ray

Atomic elements in the sample:

- Medium

Structures database:

- CODstructures.sqlite

Upload diffraction pattern:

- Diffraction pattern and sample composition

Diffraction pattern and sample composition from a Database, rank them and find the more probable in your diffraction pattern. In the COD database.

Some additional phases (cement phases) can been user selected.

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

Full Profile Search Match search and quantification is limited by the time required (or better average 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 cpdRbn from quantitative analysis Round-Robin
http://scx0.guests.commissions/particle-diffraction/journals/gazet

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

Summary of the results:

- Phase (wt%)
- PFSM
- Round-Robin

<table>
<thead>
<tr>
<th>Phase</th>
<th>PFSM</th>
<th>Round-Robin</th>
</tr>
</thead>
<tbody>
<tr>
<td>ZnO</td>
<td>29.6</td>
<td>29.6</td>
</tr>
<tr>
<td>CaF</td>
<td>34.3</td>
<td>34.3</td>
</tr>
<tr>
<td>Al₂O₃</td>
<td>36.1</td>
<td>36.1</td>
</tr>
</tbody>
</table>

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