MPOD: a Matitial Property Open Database related to Structural information

D. Chateigner, G. Pepponi, S. Grazulius

INEL, Artenay France
IUT-Caen, Université de Caen Basse Normandie, France
FBK, Trento, Italy
IBL, Vilmius, Lithuania

ICOTOM 16, 2011, Bombay
Data are arriving in ever-increasing rates. Thus, automated software tools are needed to cope with the growing amount of data, to provide consistent, uniform and accurate information: > 155000 cif files

The following goals are set by COD team:

- build automated structure deposition tools;
- build a collaboration platform for structure validation and curation;
- ensure data quality – uniformity, integrity, and trustworthiness;
- make scientific data freely accessible to anyone.
Deposit your data to COD for publication!

http://www.crystallography.net/

Crystallography Open Database Validation and Deposition Interface

Select CIF file for check:
/home/saulius/ALL.CIF Browse...

Validate

About this Validation Interface

This interface allows you to upload, validate and edit CIF files before submitting them for deposition.

Steps

The process of files deposition, after you have uploaded your data is pretty simple. First step, after files have been uploaded, is validation. Our scripts performs some validation. Results are displayed to you next to your files.
COD - Automatic data deposition

Crystallography Open Database Validation and Deposition Interface

<table>
<thead>
<tr>
<th>File</th>
<th>Status</th>
<th>Actions</th>
</tr>
</thead>
<tbody>
<tr>
<td>ALL.CIF</td>
<td>valid</td>
<td>Edit, Deposit to COD</td>
</tr>
</tbody>
</table>

File [ALL.CIF] is correct

You can now check new CIF file.
Expanding the PCOD

2011 state: 898,707 SiO$_2$ entries were added from ZEFSAII zeolite predictions and the contributions from GRINSP increased to 163,520 (silicates, phosphates, sulfates of Al, Ti, V, Ga, Nb, Zr, or zeolites, fluorides, etc). The PCOD is the first database to attain and offer more than one million of CIF entries.

Software: a new GRINSP version is now available [3] for parallel computing (for instance using fully the 8 processors of an INTEL core i7).

Other data from other prediction computer programs (CASTEP, CERIUS2, CRYSTAL, G42, GULP, USPEX…) are expected, just send them, please.
All powder patterns (> 1 million) were calculated and gathered in the P2D2 (Predicted Powder Diffraction Database [4]), they can be used for search-match purposes with EVA (Bruker), Highscore (Panalytical) and more soon.
VIRTUAL MODELS in PCOD

Zeolites

B$_2$O$_3$ nanotubes

[Ca$_3$Al$_4$F$_{21}$]$^{3-}$

Titanosilicates
MPOD
Material Property Open Database
www.materialproperties.org

- Inspired by COD, MPOD
- Collect and make open mode published material properties data
- Keeping connection to the structural information
- New cif-compliant .MPOD files
- Search tool
- Online view of tensors
- Publication references
Coded Properties

- elastic stiffness and compliance
- internal friction
- resistivity
- dielectric permittivity and stiffness
- heat capacity
- thermal conductivity, diffusivity and expansion
- piezoelectricity, electrostriction, electromechanical coupling
- piezooptic, photoelastic
- superconducting critical fields, penetration and coherence lengths

Original published paper serves as reference
Experimental information is given
One mpod file for one publication and one phase.
Coding

- Uses a Starfile syntax: developed for the Crystallographic Information Files (CIF)
- Structural information in the CORE CIF dictionary
- New dictionary for properties in Dictionary Definition Language DDL1
- Some tricks were adopted to adapt vs Starfile syntax
- Units are univocally define in the dictionary itself
- Experimental conditions (temperature, pressure, …) are inserted
- All non-zero components explicitly written
- Diagonally symmetric components not repeated
**Input search parameters**

Phase Name: [aluminum]
Formula contains: 
COD code: 
Publication author: 

**Search results:**

**Found datafiles**

<table>
<thead>
<tr>
<th>code</th>
<th>filename</th>
<th>cod code</th>
<th>phase generic</th>
<th>phase name</th>
<th>chemical formula</th>
<th>publication</th>
</tr>
</thead>
<tbody>
<tr>
<td>1000002</td>
<td>1000002.mpod</td>
<td>9008460</td>
<td>None</td>
<td>aluminum</td>
<td>Al</td>
<td>2</td>
</tr>
<tr>
<td>1000003</td>
<td>1000003.mpod</td>
<td>9008460</td>
<td>None</td>
<td>aluminum</td>
<td>Al</td>
<td>3</td>
</tr>
<tr>
<td>1000093</td>
<td>1000093.mpod</td>
<td>9008460</td>
<td>None</td>
<td>Aluminum</td>
<td>Al N</td>
<td>53</td>
</tr>
<tr>
<td>1000094</td>
<td>1000094.mpod</td>
<td>9008860</td>
<td>None</td>
<td>Aluminum nitride</td>
<td>Al N</td>
<td>54</td>
</tr>
</tbody>
</table>
### Datafile info

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>code</td>
<td>1000069</td>
</tr>
<tr>
<td>filename</td>
<td>1000069.mpod</td>
</tr>
<tr>
<td>cod code</td>
<td>1010458</td>
</tr>
<tr>
<td>phase generic</td>
<td>KDP</td>
</tr>
<tr>
<td>phase name</td>
<td>Mn-doped potassium dihydrogen phosphate</td>
</tr>
<tr>
<td>chemical formula</td>
<td>La₃Ga₅SiO₁₄</td>
</tr>
<tr>
<td>publication</td>
<td>37</td>
</tr>
</tbody>
</table>

### Property values

#### General experimental conditions/parameters

- **measurement method**: RUS-Laser-Doppler
- **conditions temperature [K]**: 297

#### Properties' values

<table>
<thead>
<tr>
<th>elastic stiffness cij [GPa]</th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>189.5</td>
<td>105.3</td>
<td>97.16</td>
<td>14.25</td>
<td></td>
</tr>
<tr>
<td>-</td>
<td>189.5</td>
<td>97.16</td>
<td>-14.25</td>
<td></td>
</tr>
<tr>
<td>-</td>
<td>-</td>
<td>262.6</td>
<td></td>
<td></td>
</tr>
<tr>
<td>-</td>
<td>-</td>
<td>53.5</td>
<td></td>
<td></td>
</tr>
<tr>
<td>-</td>
<td>-</td>
<td></td>
<td>53.5</td>
<td>28.5</td>
</tr>
<tr>
<td>-</td>
<td>-</td>
<td></td>
<td></td>
<td>42.1</td>
</tr>
</tbody>
</table>

#### Other experimental conditions/parameters

- **measurement method [n.a.]**: XRD

#### Properties' values

<table>
<thead>
<tr>
<th>piezoelectric dij [m.V⁻¹]</th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>-</td>
<td>-</td>
<td>2.3(1)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>-</td>
<td>-</td>
<td></td>
<td>2.3(1)</td>
<td></td>
</tr>
<tr>
<td>-</td>
<td>-</td>
<td></td>
<td></td>
<td>47(2)</td>
</tr>
</tbody>
</table>
data_1000280
_cod_database_code               2101499
_structure_refined 'no'
_phase_name 'diamond'
_chemical_formula 'C'
_chemical_formula_sum 'C'
_symmetry_point_group_name_H-M 'm -3 m'
_cell_length_a  3.56658
_cell_length_b  3.56658
_cell_length_c  3.56658
_cell_angle_alpha  90
_cell_angle_beta   90
_cell_angle_gamma  90
loop_
_publ_author_name
'Ramachandran, G.N.'
_publ_section_title
;
  Photoelastic constants of diamond
;
_journal_name_full               'Proceedings of the Indian Academy of Sciences A'
_journal_volume                  25
_journal_issue                   ?
_journal_page_first              208
_journal_page_last               219
_journal_year                    1947
_phase_density                   ?
_prop_measurement_method 'Birefringence'
_prop_conditions_wavelength 0.5893
_prop_photoelastic_pij 'pij'
_prop_piezooptic_pijj 'piij'
loop_
_prop_data_label
_prop_data_tensorial_index
_prop_data_value
pij 11 0.12(5)
pij 12 -0.32(5)
pij 13 -0.32(5)
pij 21 -0.32(5)
pij 22 0.12(5)
pij 23 -0.32(5)
pij 31 -0.32(5)
pij 32 -0.32(5)
pij 33 0.12(5)
pij 44 0.11
pij 55 0.11
pij 66 0.11
### Publication details

<table>
<thead>
<tr>
<th>Title</th>
<th>Anisotropy of the superconducting state parameters and intrinsic pinning in low-level Pr-doped YBa2Cu3O7-d single crystals</th>
</tr>
</thead>
<tbody>
<tr>
<td>Journal</td>
<td>Superconductor Science and Technology</td>
</tr>
<tr>
<td>Year</td>
<td>2010</td>
</tr>
<tr>
<td>Volume</td>
<td>23</td>
</tr>
<tr>
<td>Issue</td>
<td>10</td>
</tr>
<tr>
<td>First Page</td>
<td>None</td>
</tr>
<tr>
<td>Last Page</td>
<td>None</td>
</tr>
<tr>
<td>Reference</td>
<td>065001</td>
</tr>
<tr>
<td>Pages Number</td>
<td>7</td>
</tr>
</tbody>
</table>

### Associated datafiles

<table>
<thead>
<tr>
<th>Code</th>
<th>Filename</th>
<th>Code Code</th>
<th>Phase Generic</th>
<th>Phase Name</th>
<th>Chemical Formula</th>
<th>Publication</th>
</tr>
</thead>
<tbody>
<tr>
<td>1000107</td>
<td>1000107.mpod</td>
<td>None</td>
<td>None</td>
<td>YBCO</td>
<td>Y Ba2 Cu3 O6.915</td>
<td>65</td>
</tr>
</tbody>
</table>
Property details

<table>
<thead>
<tr>
<th>tag</th>
<th>_prop_superconducting_critical_field2_Hc2i</th>
</tr>
</thead>
<tbody>
<tr>
<td>name</td>
<td>prop superconducting critical field2 Hc2i</td>
</tr>
<tr>
<td>description</td>
<td>_superconducting_critical_field2_Hc2i</td>
</tr>
<tr>
<td>tensor dimensions</td>
<td>3</td>
</tr>
<tr>
<td>units</td>
<td>T</td>
</tr>
<tr>
<td>units detail</td>
<td>tesla</td>
</tr>
</tbody>
</table>

Associated datafiles

<table>
<thead>
<tr>
<th>code</th>
<th>filename</th>
<th>code</th>
<th>phase generic</th>
<th>phase name</th>
<th>chemical formula</th>
<th>publication</th>
</tr>
</thead>
<tbody>
<tr>
<td>1000097</td>
<td>1000097.mpod</td>
<td>9088326</td>
<td>None</td>
<td>LiFeAs</td>
<td>Li Fe As</td>
<td>56</td>
</tr>
<tr>
<td>1000102</td>
<td>1000102.mpod</td>
<td></td>
<td>?</td>
<td>iron arsenide</td>
<td>Ba Fe2 As1.3 P0.7</td>
<td>60</td>
</tr>
<tr>
<td>1000107</td>
<td>1000107.mpod</td>
<td></td>
<td>None</td>
<td>YBCO</td>
<td>Y Ba2 Cu3 06.915</td>
<td>65</td>
</tr>
<tr>
<td>1000108</td>
<td>1000108.mpod</td>
<td></td>
<td>None</td>
<td>YBCO</td>
<td>Y Ba2 Cu3 06.973</td>
<td>65</td>
</tr>
<tr>
<td>1000109</td>
<td>1000109.mpod</td>
<td></td>
<td>None</td>
<td>Pr-YBCO</td>
<td>Y0.992 Pr0.008 Ba2 Cu3 06.934</td>
<td>65</td>
</tr>
</tbody>
</table>
Acknowledgments

- Vilnius COD development group: Research Council of Lithuania, contract No. MIP-124/2010
- all CIF donators, listed on our Web page, numerous anonymous volunteers who help to collect data and keep COD running
- Commercial supporters for donation (hardware and financial support)
- Xmat project (“Combination of X-Ray diffraction and X-Ray Fluorescence techniques in material science”), supported by the Provincia Autonoma di Trento and the European Union in the framework of the Marie Curie COFUND program - Call for proposals 4 - researcher 2009 – Outgoing.