

Preliminary report Moeck, September 12, 2008

Work accomplished

Our project is going very well and does serve the needs of the international community of materials science educators and active research scientists. This is, for example, demonstrated by the more than 15,800 hits to the websites of our interactive crystallography databases since January 1st 2008, see Fig. 1 below. The development of the Lattice-fringe Fingerprinting search and match routine makes good progress, Fig. 2.

List of expenditures made to date and positions filled

\$7,100 salary for undergraduates: Jan “Irigi” Oslina and Jan Zahornadský, both for 2 month over this summer,

Timeline for the completion of grant-funded activities

Based on our current results, it is safe to conclude that all tasks of the grant funded activity will be completed within the time frame of this project. The results of this project will be presented at the symposium “Electron Crystallography for Materials Research” of the forthcoming Spring 2009 Meeting of the Materials Research Society, http://www.mrs.org/s_mrs/sec.asp?CID=10891&DID=201200. Note that the PI of this project is actually the organizer of this symposium.

The screenshot shows a web browser window with the URL <http://nanocrystallography.research.pdx.edu/search.py/index>. The page title is "Interactive Crystallography Databases". A left-hand navigation menu includes: Home, Nano-Crystallography Group, Interactive Databases (with sub-links for COD Subset, Nano-Crystallography Database, Crystal Morphology Database, and Wiki Crystallography Database), Tools, Login, Main Sponsor, and Links. The main content area displays four database tiles:

- COD Subset⁽²⁰²⁶⁴⁾**: Includes a logo with letters C, O, D in colored spheres and a link for "Search and view".
- Nano-Crystallography Database⁽²⁾**: Includes a logo with letters N, C, D in colored spheres and links for "Search and view" and "Login/Register for upload".
- Crystal Morphology Database⁽⁴⁾**: Includes a logo with letters C, M, D in colored diamonds and a link for "Search and view".
- Wiki Crystallography Database⁽⁸⁹³⁰⁾**: Includes a circular logo with various actions (Learn, Teach, Share, Create, Edit, Crystal, World) and links for "Search and view" and "Upload data".

Below the tiles, a paragraph states: "Several crystallography databases are offered for browsing, each of which having a slightly different purpose. You can search the databases, display the contained CIFs, view 3D models of the crystal structure and morphology or compute and display their lattice fringe fingerprint plots." Below this, it notes: "The [COD Subset](#) available here is a mainly inorganic and educational subset of the...".

The footer contains logos for "Project made possible by assistance from:" including Portland State University, NWACC, ONAMI, and NanoMEGAS. It also includes the text "Page maintained by consultants@pdx.edu © Portland State University 2008" and a "Visits since January 1st, 2008: 15836" counter.

Fig. 1. Access page to our interactive open-access crystallography databases. Note the more than 15,800 hits on these websites since January 1st, 2008.

http://nanocrystallography.research.pdx.edu/test/match.py/match?d

Lattice Fringe-Fingerprint Matching

Home

Nano-Crystallography Group

Interactive Databases

- COD Subset
- Nano-Crystallography Database
- Crystal Morphology Database
- Wiki Crystallography Database
- LFFP Matching

Tools

Login

Main Sponsor

Links

Narrow match search by these properties:

With these elements

Without these elements

Minimum and Maximum volume

Strict number of elements

Symmetry cell setting

a (min, max) [Å]

b (min, max) [Å]

c (min, max) [Å]

alpha (min, max) [deg]

beta (min, max) [deg]

gamma (min, max) [deg]


Smallest reciprocal vector [nm⁻¹]

2nd smallest reciprocal vector in the pair [nm⁻¹]

Their angle [deg]

Input your LFFP in specified format here.

Project made possible by assistance from:



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 Visits since January 1st, 2008: 1

Fig. 2. Interface to the Lattice-fringe Fingerprinting Module on our development web site, <http://nanocrystallography.research.pdx.edu/test>