

1 MiNALab, CMM – irst, Fondazione Bruno Kessler, Via Sommarive 18, 38123 Povo, Trento, Italy. E-mail: pepponi@fbk.eu

2 Institute of Biotechnology, Graiciuno 8, LT-02241 Vilnius, Lithuania. E-mail: grazulis@ibt.lt

3 CRISMAT, ENSICAEN, IUT-Caen, Université de Caen Basse-Normandie, 6 Boulevard du Maréchal Juin, 14050 Caen, France

E-mail: daniel.chateigner@ensicaen.fr

MOTIVATION

Crystallographic structures affect microscopic properties of the phases constituting a given material which has consequences at the macroscopic scale. Knowledge about the structure can also be used to make predictions about such properties, e.g. with a simulation approach (DFT, Molecular dynamics, ...). Knowledge about experimentally measured crystallite properties, however, is of key importance for counter-checking theoretical studies and also to better define fitting models for the structure determination itself.



Material Properties Open Database

[home](#) [datafiles](#) [dictionary](#)

[introduction](#)
[search](#)
[properties](#)
[submit](#)
[documentation](#)
[references](#)

Input search parameters

Phase Name:
Formula contains:
COD code:
Publication author:

Search results:

Found datafiles

code	filename	cod code	phase generic	phase name	chemical formula	publication
1000002	1000002.mpod	9008460	None	aluminum	Al	2
1000003	1000003.mpod	9008460	None	aluminum	Al	3
1000093	1000093.mpod	9008460	None	Aluminum	Al N	53
1000094	1000094.mpod	9008860	None	Aluminum nitride	Al N	54



Material Properties Open Database

[home](#) [datafiles](#) [dictionary](#)

[introduction](#)
[search](#)
[properties](#)
[submit](#)
[documentation](#)
[references](#)

Publication details

title	Anisotropy of the superconducting state parameters and intrinsic pinning in low-level Pr-doped YBa ₂ Cu ₃ O _{7-d} single crystals
authors	Kortyka, A.; Puzniak, R.; Wisniewski, A.; Zehetmayer, M.; Weber, H.W.; Cai, Y.Q.; Yao, X.
journal	Superconductor Science and Technology
year	2010
volume	23
issue	10
first page	None
last page	None
reference	065001
pages number	7

Associated datafiles

code	filename	cod code	phase generic	phase name	chemical formula	publication
1000107	1000107.mpod	None	None	YBCO	Y Ba ₂ Cu ₃ O _{6.915}	65

GET INVOLVED!!! SUBMIT YOUR DATA!

www.materialproperties.org



Material Properties Open Database

[home](#) [datafiles](#) [dictionary](#)

[introduction](#)
[search](#)
[properties](#)
[submit](#)
[documentation](#)
[references](#)

Property details

tag	_prop_superconducting_critical_field2_Hc2i
name	prop superconducting critical field2 Hc2i
description	_superconducting_critical_field2_Hc2i
tensor dimensions	3
units	T
units detail	tesla

Associated datafiles

code	filename	cod code	phase generic	phase name	chemical formula	publication
1000097	1000097.mpod	9088326	None	LiFeAs	Li Fe As	56
1000102	1000102.mpod	None	?	iron arsenide	Ba Fe ₂ As _{1.3} P _{0.7}	60
1000107	1000107.mpod	None	None	YBCO	Y Ba ₂ Cu ₃ O _{6.915}	65
1000108	1000108.mpod	None	None	YBCO	Y Ba ₂ Cu ₃ O _{6.973}	65
1000109	1000109.mpod	None	None	Pr-YBCO	Y _{0.992} Pr _{0.008} Ba ₂ Cu ₃ O _{6.934}	65



Material Properties Open Database

[home](#) [datafiles](#) [dictionary](#)

[introduction](#)
[search](#)
[properties](#)
[submit](#)
[documentation](#)
[references](#)

Datafile info

code	: 1000002
filename	: 1000002.mpod
cod code	: 9008460
phase generic	: None
phase name	: aluminum
chemical formula	: Al
publication	: 2

Property values

elastic stiffness c _{ij} [GPa]	106.75	60.41	60.41	-	-	-
	-	106.75	60.41	-	-	-
	-	-	106.75	-	-	-
	-	-	-	28.34	-	-
	-	-	-	-	28.34	-
	-	-	-	-	-	28.34

[measurement method](#) : RUS
[conditions temperature](#) [K] : 297

Property values

General experimental conditions/parameters

[measurement method](#) : RUS
[conditions temperature](#) [K] : 297

Properties' values

elastic stiffness c _{ij} [GPa]	106.75	60.41	60.41	-	-	-
	-	106.75	60.41	-	-	-
	-	-	106.75	-	-	-
	-	-	-	28.34	-	-
	-	-	-	-	28.34	-
	-	-	-	-	-	28.34

DISCUSSION and CONCLUSION

Inspired by the Crystallography Open Database, the Material Properties Open Database (MPOD) was given birth. MPOD aims at collecting and making publicly available at no charge tensorial properties (including scalar properties) of phases and linking such properties to structural information of the COD when available. MPOD files are written with the STAR file syntax, used and developed for the Crystallographic Information Files. A dictionary containing new definitions has been written according to the Dictionary Definition Language DDL1, although some tricks were adopted to allow for multiple entries still avoiding ambiguity.

The initial set includes mechanical properties, elastic stiffness and compliance, internal friction; electrical properties, resistivity, dielectric permittivity and stiffness, thermodynamic properties, heat capacity, thermal conductivity, diffusivity and expansion; electromechanical properties, piezoelectricity, electrostriction, electromechanical coupling; optical properties; piezooptic and photoelastic properties; superconducting properties, critical fields, penetration and coherence lengths.

Properties are reported in mpod files where the original published paper containing the data is cited and structural and experimental information is also given. One mpod file contains information relative to only one publication and one phase.

A significant set of experimental parameters and measurement methods are included in the dictionary.

The website provides not also the files but also the dictionary and information on the software used for the syntactic correctness of the files. Further validation algorithms will be implemented in the near future taking into account the validity of the matrix indexes.

The work has already been presented at conferences and has received appreciations and interest. The advantage for the authors in fact is visibility of their work and data that can be searched through the web interface of the MPOD.

The website in fact provides reader-friendly views of the properties values, with links to the properties' definitions and the details of the publication where the data are released. A form for submitting new MPOD files will be put online in the near future.

Acceptance of contributions at international conferences and academic collaborations show the scientific relevance of the activity carried out.

Acknowledgement

This research was partially carried out within the 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.