

Match! Phase Analysis Report

Indian Institute of Technology Delhi, Electrical Department

Sample: cvd testing-1

Sample Data

File name	cvd testing-1.UXD
File path	C:/Users/SOUMEN/Downloads
Data collected	Jul 17, 2018 13:32:59
Data range	10.020° - 80.023°
Number of points	3602
Step size	0.019
Rietveld refinement converged	No
Alpha2 subtracted	No
Background subtr.	Yes
Data smoothed	Yes
2theta correction	0.02°
Radiation	X-rays
Wavelength	1.541874 Å

Candidates

Name	Formula	Entry No.	FoM
Copper(I) oxide (Cuprite)	Cu ₂ O	96-101-0942	0.8116
Cerium palladium antimonide (8/24/1)	Ce ₈ Pd ₂₄ Sb	96-100-5034	0.7831
Cuprite	Cu ₂ O	96-900-7498	0.7775
Cuprite	Cu ₂ O	96-900-5770	0.7772
Copper(I) oxide (Cuprite)	Cu ₂ O	96-100-0064	0.7746
Copper(I) oxide (Cuprite)	Cu ₂ O	96-101-0927	0.7746
Tetrataenite	Fe Ni	96-901-0018	0.7730
La Pd ₃	La Pd ₃	96-152-3423	0.7703
La Pd ₃	La Pd ₃	96-153-8083	0.7701
Mn Ni ₃	Mn Ni ₃	96-152-3339	0.7678
Copper(I) oxide (Cuprite)	Cu ₂ O	96-101-0964	0.7677
La Pd ₃ B	B La Pd ₃	96-151-1208	0.7646
	Rh	96-210-0455	0.7636
(Ga _{0.85} Zn _{0.15}) Ni ₃	Ga _{0.85} Ni ₃ Zn _{0.15}	96-152-2544	0.7634
copper	Cu	96-410-5041	0.7614
(Fe _{0.3} Ga _{0.7}) Ni ₃	Fe _{0.3} Ga _{0.7} Ni ₃	96-152-4943	0.7607
(Fe _{0.08} Ti _{0.092} V _{0.828})	Fe _{0.08} Ti _{0.092} V _{0.828}	96-152-2405	0.7602
La Pd ₃	La Pd ₃	96-153-8988	0.7601
Helium	He	96-901-1637	0.7601
(Cr _{0.3} Ga _{0.7}) Ni ₃	Cr _{0.3} Ga _{0.7} Ni ₃	96-152-4941	0.7595
Ru ₃ Th B _{0.9}	B _{0.9} Ru ₃ Th	96-151-1380	0.7588
(Cu _{0.8} Ga _{0.2}) Ni ₃	Cu _{0.8} Ga _{0.2} Ni ₃	96-152-4942	0.7586
(Ga _{0.85} Mo _{0.15}) Ni ₃	Ga _{0.85} Mo _{0.15} Ni ₃	96-152-2541	0.7582
(Cu _{0.9} Ga _{0.1}) Y	Cu _{0.9} Ga _{0.1} Y	96-152-4621	0.7552
Cd _{0.025} Li _{0.975}	Cd _{0.025} Li _{0.975}	96-152-4667	0.7549
La Rh ₃ B	B La Rh ₃	96-151-1211	0.7536
Lithium	Li	96-900-8542	0.7532
Lithium	Li	96-901-1005	0.7532
(Co _{2.1} Fe _{0.9}) V	Co _{2.1} Fe _{0.9} V	96-152-5300	0.7531
(Ga _{0.5} Ti _{0.5}) Ni ₃	Ga _{0.5} Ni ₃ Ti _{0.5}	96-152-2543	0.7507
(Li Mg)	Li Mg	96-152-2372	0.7488
Dy Ga ₃	Dy Ga ₃	96-152-4227	0.7481
Co O	Co O	96-152-8839	0.7481
Ga ₂ Sc	Ga ₂ Sc	96-152-2721	0.7438
	Dy ₄ Fe Ga ₁₂	96-431-4514	0.7438
La Rh ₃ B	B La Rh ₃	96-151-1212	0.7436
Dy Pd	Dy Pd	96-152-7911	0.7433
Ga ₃ Ho	Ga ₃ Ho	96-152-3405	0.7420
Periclase	Mg O	96-900-0497	0.7398
Periclase	Mg O	96-900-6755	0.7398
(Hf _{0.93} Mo _{0.07})	Hf _{0.93} Mo _{0.07}	96-152-2717	0.7390
Periclase	Mg O	96-900-6754	0.7384
Cd Li ₃	Cd Li ₃	96-152-5522	0.7383
	Cu F	96-900-8844	0.7359
(Os _{0.1} U _{0.9})	Os _{0.1} U _{0.9}	96-152-2082	0.7358
Tetrataenite	Fe _{0.507} Ni _{0.493}	96-901-1507	0.7355
(Co _{0.5} Ni _{0.5}) Ti	Co _{0.5} Ni _{0.5} Ti	96-152-4742	0.7336
Ga ₃ Ho	Ga ₃ Ho	96-152-2287	0.7321
	Er ₄ Fe _{0.67} Ga ₁₂	96-431-4517	0.7319
Ru V	Ru V	96-152-7981	0.7304
Periclase	Mg O	96-900-6460	0.7293
	Ga ₆ Ge ₆ Mn Y ₄	96-410-2611	0.7288

and 150 others...

Search-Match

Settings

Reference database used	COD-Inorg REV208743 2018.07.02
Automatic zeropoint adaptation	Yes
Minimum figure-of-merit (FoM)	0.60
2theta window for peak corr.	0.30 deg.
Minimum rel. int. for peak corr.	1
Parameter/influence 2theta	0.50
Parameter/influence intensities	0.50
Parameter multiple/single phase(s)	0.50

Peak List

No.	2theta [°]	d [Å]	h/k/l	FWHM
1	16.82	5.2697	25.87	0.3441
2	29.72	3.0059	101.22	0.2333
3	32.07	2.7908	22.33	0.4277
4	32.34	2.7681	16.13	0.9720
5	36.05	2.4914	18.76	0.2333
6	36.62	2.4538	1000.00	0.3499
7	42.13	2.1447	13.16	0.6086
8	42.49	2.1274	118.52	0.4755
9	42.68	2.1186	4.91	0.2802
10	43.31	2.0890	0.00	0.0022
11	43.61	2.0754	0.00	0.1893
12	43.75	2.0693	898.13	0.2722
13	50.75	1.7991	0.00	0.0901
14	50.77	1.7984	0.00	0.1289
15	50.90	1.7941	488.64	0.2488
16	52.59	1.7403	23.06	0.9796
17	58.36	1.5813	18.19	0.5054
18	58.60	1.5752	20.97	0.2722
19	61.15	1.5157	175.33	0.3110
20	61.73	1.5027	97.11	0.4277
21	62.04	1.4960	30.39	0.1944
22	62.31	1.4902	20.50	0.2333
23	72.85	1.2983	25.01	0.6287
24	73.42	1.2897	63.84	0.5023
25	73.63	1.2865	0.00	0.1940
26	74.44	1.2745	417.55	0.2777
27	74.77	1.2697	307.77	0.3436
28	74.79	1.2694	0.00	0.2484

Rietveld Refinement using FullProf

Calculation was not run or did not converge.

Crystallite Size Estimation using Scherrer Formula

Calculation was not run.

Integrated Profile Areas

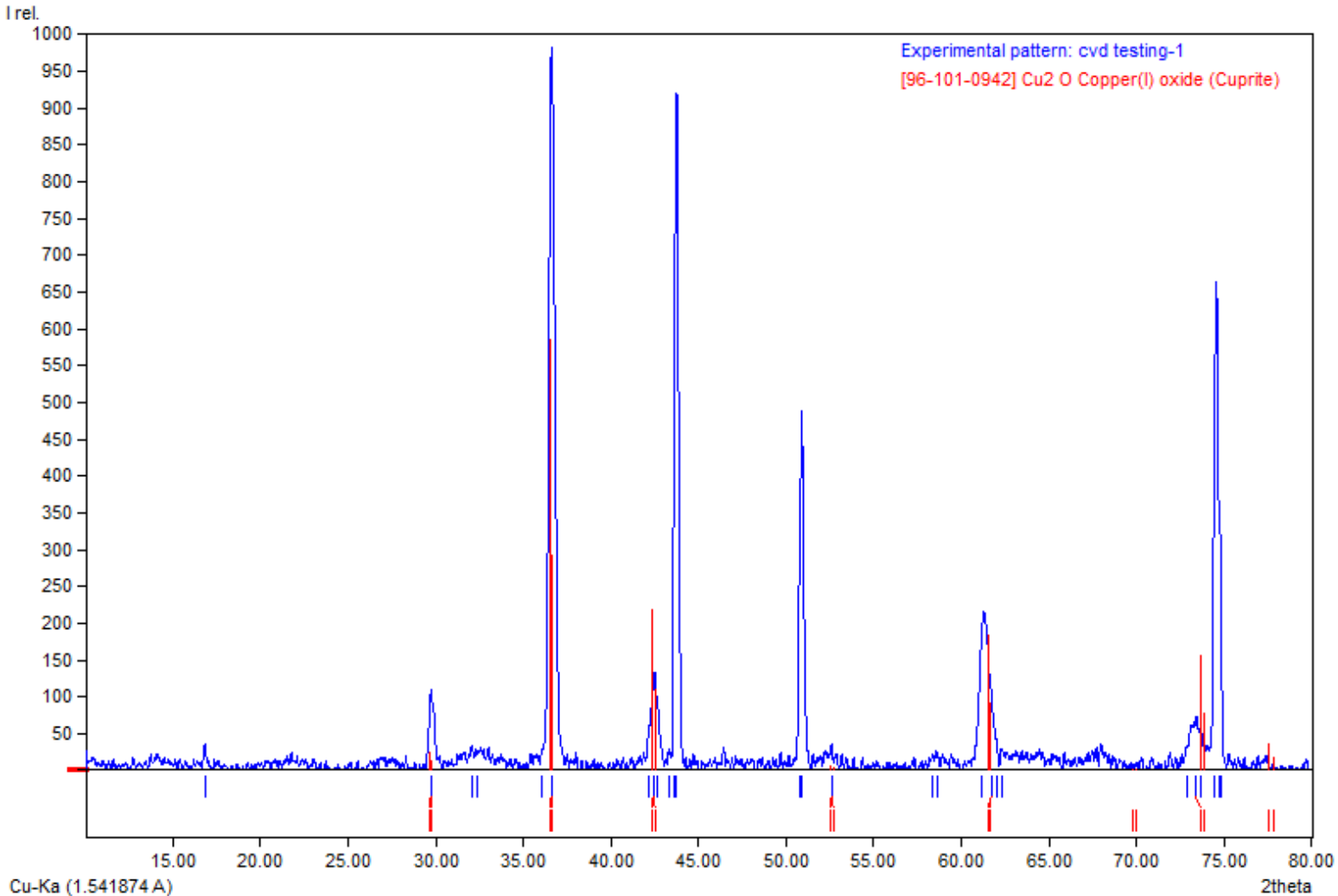
Based on calculated profile

Profile area	Counts	Amount
Overall diffraction profile	192528	100.00%
Background radiation	22594	11.74%
Diffraction peaks	169933	88.26%
Peak area belonging to selected phases	0	0.00%
Unidentified peak area	167819	87.17%

Peak Residuals

Peak data	Counts	Amount
Overall peak intensity	3084	100.00%
Peak intensity belonging to selected phases	1676	54.34%
Unidentified peak intensity	1408	45.66%

Diffraction Pattern Graphics



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