# **Match! Phase Analysis Report**

#### Indian Institute of Technology Delhi, Electrical Department

Sample: cvd testing-2

#### Sample Data

Number of points

File name cvd testing-2.UXD File path E:/CVD Leak Test Data collected Jul 18, 2018 15:09:07 9.770° - 79.773° Data range

Step size 0.019 Rietveld refinement converged No Alpha2 subtracted No Background subtr. No Data smoothed Yes -0.23° 2theta correction Radiation X-rays Wavelength 1.541874 Å

#### **Matched Phases**

Index	Amount (%)	Name	Formula sum
Α	100.0	Copper	Cu
	4.7	Unidentified peak area	

3602

#### A: Copper (100.0 %)

Calc. density

Formula sum Cu 96-900-8469 Entry number Figure-of-Merit (FoM) 0.763235 Total number of peaks 16 Peaks in range 16 Peaks matched 6 Intensity scale factor 0.33 Space group F m -3 m Crystal system cubic Unit cell a= 3.6150 Å I/Ic 11.93

8.935 g/cm<sup>3</sup> Reference Wyckoff R. W. G., "Second edition. Interscience Publishers, New York, New YorkCubic closest packed, ccp,

structure", Crystal Structures 1, 7-83 (1963)

#### **Candidates**

Name	Formula	Entry No.	FoM
Hydrogen	H2	96-901-3083	0.6941
, ,	Ba Ce0.8 O3 Pr0.2	96-210-6632	0.6240
	Ba Ce0.8 O3 Pr0.2	96-210-6633	0.6220
Ce0.22 La0.78 Nb O3.92	Ce0.22 La0.78 Nb O3.92	96-152-8783	0.6204
Nitrogen	N2	96-901-1346	0.6174
lvanyukite-Na-T	H40 K1.56 Na4.32 O68 Si9	Гі1296-901-3697	0.6123
-	Ba Ce0.4 O3 Pr0.6	96-210-6642	0.6035
	Ba Ce0.4 O3 Pr0.6	96-210-6643	0.6004

#### 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]	1/10	<b>FWHM</b>	Matched
1	11.08	7.9874	13.17	0.1555	
2	27.32	3.2644	22.32	0.0389	
3	28.11	3.1746	16.68	0.0778	
4	28.92	3.0879	15.44	0.1166	
5	32.79	2.7312	24.89	0.1944	
6	32.99	2.7153	15.59	0.0778	
7	43.47	2.0821	232.11	0.1166	Α

8	47.92	1.8984	14.85	0.0778	
9	50.61	1.8037	167.47	0.0778	Α
10	60.54	1.5294	15.76	0.0778	
11	65.95	1.4164	14.42	0.0778	
12	68.74	1.3656	17.39	0.1166	
13	69.19	1.3578	22.56	0.0389	
14	72.06	1.3106	21.96	0.1166	
15	72.53	1.3033	23.57	0.0389	
16	74.24	1.2775	1000.00	0.0778	Α
17	74.45	1.2744	453.29	0.0778	Α

## **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**

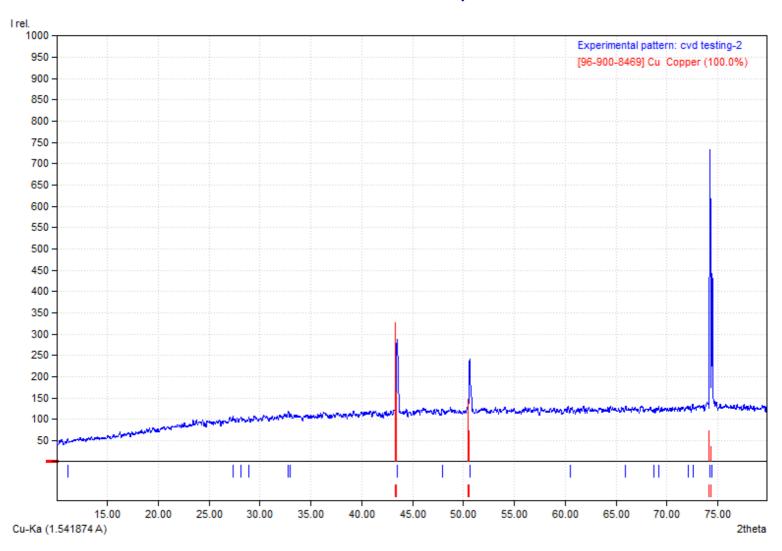
#### Based on calculated profile

Profile area	Counts	Amount
Overall diffraction profile	757625	100.00%
Background radiation	718487	94.83%
Diffraction peaks	39138	5.17%
Peak area belonging to selected phases	3578	0.47%
Peak area of phase A (Copper)	3578	0.47%
Unidentified peak area	35560	4.69%

#### **Peak Residuals**

Peak data	Counts	Amount
Overall peak intensity	371	100.00%
Peak intensity belonging to selected phases	344	92.66%
Unidentified peak intensity	27	7.34%

### **Diffraction Pattern Graphics**



Match! Copyright © 2003-2018 CRYSTAL IMPACT, Bonn, Germany