

Match! Phase Analysis Report

Indian Institute of Technology Delhi, Electrical Department

Sample: cvd testing-2

Sample Data

| | |
|-------------------------------|-----------------------|
| File name | cvd testing-2.UXD |
| File path | E:/CVD Leak Test |
| Data collected | Jul 18, 2018 15:09:07 |
| Data range | 9.770° - 79.773° |
| Number of points | 3602 |
| Step size | 0.019 |
| Rietveld refinement converged | No |
| Alpha2 subtracted | No |
| Background subtr. | No |
| Data smoothed | Yes |
| 2theta correction | -0.23° |
| Radiation | X-rays |
| Wavelength | 1.541874 Å |

Matched Phases

| Index | Amount (%) | Name | Formula sum |
|-------|------------|------------------------|-------------|
| A | 100.0 | Copper | Cu |
| | 4.7 | Unidentified peak area | |

A: Copper (100.0 %)

| | |
|------------------------|--|
| Formula sum | Cu |
| Entry number | 96-900-8469 |
| 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 |
| Calc. density | 8.935 g/cm ³ |
| 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 |
| | N2 | 96-901-1346 | 0.6174 |
| Nitrogen | H40 K1.56 Na4.32 O68 Si9 Ti12 | 96-901-3697 | 0.6123 |
| Ivanyukite-Na-T | 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] | I/I0 | FWHM | 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 | A |

| | | | | | |
|----|-------|--------|---------|--------|---|
| 8 | 47.92 | 1.8984 | 14.85 | 0.0778 | |
| 9 | 50.61 | 1.8037 | 167.47 | 0.0778 | A |
| 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 | A |
| 17 | 74.45 | 1.2744 | 453.29 | 0.0778 | A |

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



