Supporting Information

for Adv. Mater., DOI: 10.1002/adma.202102301

Phase–Property Diagrams for Multicomponent Oxide Systems toward Materials Libraries

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Sample 1

Chemical Composition [at. %]

Cations

- Y
- Sm
- La
- Ce
- Pr

Intensity [a.u.]

Crystal structure (XS): Lattice Parameter (LP) - Crystallite Size (CS)

- XS Ia-3 (100%) 10.57291 Å
- CS 139.8 nm
- ICSD 23811

Linear Fit of Sheet3 B"Y\textsubscript{2}O\textsubscript{3}"

Equation y = a + b*x

Plot Y\textsubscript{2}O\textsubscript{3}

Weight No Weighting

Intercept -15.60416 ± 0.1833

Slope 2.72916 ± 0.03103

Adj. R-Square 0.99871
Sample 2

Chemical Composition [at. %]

Cations

Intensity [a.u.]

Crystal structure (XS) - Lattice Parameter (LP) - Crystallite Size (CS)

Linear Fit of Sheet3 F"Sm2O3"

Equation \( y = a + b \times x \)

Plot Sm-(2)O-(3)

Weight No Weighting

Intercept \(-15.25924 \pm 0.33123\)

Slope \(3.17123 \pm 0.06675\)

Adj. R-Square \(0.99383\)

\(E_g=4.81 \text{ eV}\)
Sample 5

Chemical Composition [at. %]

Y Sm La Ce Pr

0 20 40 60 80 100

Crystal structure (XS) - Lattice Parameter (LP) - Crystallite Size (CS)

XS Fm-3m(100%)

LP 5.44705 Å

CS 180.4 nm

ICSD 28786

PrO$_2$

Linear Fit of Sheet3 H"PrO$_2$"

Equation $y = a + b \times x$

Plot PrO$^-(2)$

Weight No Weighting

Intercept $-0.7686 \pm 0.02229$

Slope $0.3173 \pm 0.00664$

Adj. R-Square 0.98278

$E_g=2.46\,\text{eV}$
Sample 6

Chemical Composition [at. %]

Cations

Crystal structure (XS) - Lattice Parameter (LP) - Crystallite Size (CS)

Intensity [a.u.]

2q

XS Ia-3(100%)

LP 10.73466 Å

CS 124.7 nm

Linear Fit of Sheet3 L“6”

Equation

\[ y = a + b \times x \]

Plot

Weight No Weighting

Intercept -10.98417 ± 0.41781

Slope 2.20642 ± 0.08185

Adj. R-Square 0.98373

\[ E_g = 4.97 \text{ eV} \]
Sample 7

Chemical Composition [at. %]

Cations

Intensity [a.u.]

Crystal structure (XS) - Lattice Parameter (LP) - Crystallite Size (CS)

Linear Fit of Sheet3 T7

Equation $y = a + b \times x$

Plot 7

Weight No Weighting

Intercept $-5.55799 \pm 0.06891$

Slope $1.14937 \pm 0.01375$

Adj. R-Square $0.99786$

$E_g = 4.83$ eV
Sample 8

Chemical Composition [at. %]

Y  Sm  La  Ce  Pr
0  20  40  60

Crystal structure (XS) - Lattice Parameter (LP) - Crystallite Size (CS)

XS Fm-3m(95.1%), P321 (4.9%)
LP *5.51203 Å
CS *67.5 nm

Linear Fit of Sheet3 Z"8"

Equation \( y = a + b \times x \)

Plot 8

Weight No Weighting

Intercept -3.01963 ± 0.02413
Slope 0.93238 ± 0.00701
Adj. R-Square 0.99825

\( E_g = 3.23 \text{ eV} \)
Sample 11

Chemical Composition [at. %]

- Y
- Sm
- La
- Ce
- Pr

Intensities [a.u.]

Crystal structure (XS) - Lattice Parameter (LP) - Crystallite Size (CS)

- XS: Fm-3m (65.1%), P4/nmm (29%), P63/mmc (5.9%)
- LP: *a = 10.90395 Å
- CS: *D = 125.3 nm

Linear Fit of Sheet3 N"11"

- Equation: \( y = a + b \cdot x \)
- Intercept: \( a = -0.32435 \pm 0.01506 \)
- Slope: \( b = 0.06402 \pm 0.0029 \)
- Adj. R-Square: 0.9878

\( E_g = 5.06 \text{ eV} \)
Sample 12

Chemical Composition [at. %]

Cations

Y  Sm  La  Ce  Pr

0  20  40  60

Crystal structure (XS) - Lattice Parameter (LP) - Crystallite Size (CS)

Intensity [a.u.]

XS Ia-3(100%)
LP 10.7869 Å
CS 100.6 nm

Linear Fit of Sheet3 R"12"

Equation: \( y = a + b \cdot x \)

Plot

Weight: No Weighting

Intercept: -0.64415 ± 0.00237
Slope: 0.3197 ± 9.31615E-4
Adj. R-Square: 0.99888

\( Eg = 2.00 \) eV

Graphs showing chemical composition and intensity plots with various data points and lines.
Sample 13

Chemical Composition [at. %]

| Cations | 0 | 20 | 40 | 60 |
|---------|---|----|----|----|
| Y       |   |    |    |    |
| Sm      |   |    |    |    |
| La      |   |    |    |    |
| Ce      |   |    |    |    |
| Pr      |   |    |    |    |

Intensity [a.u.]

| 2q |
|----|
| 10 | 20 | 30 | 40 | 50 |
X-ray
Iα-3 (100%)
Lattice Parameter (LP) 10.88347 Å
Crystallite Size (CS) 169.1 nm

Linear Fit of Sheet3 X'13'
Equation y = a + b*x
Plot 13
Weight No Weighting
Intercept -1.03692 ± 0.00457
Slope 0.51109 ± 0.00175
Adj. R-Square 0.99805
Eg = 2.02 eV

Crystal structure (XS) - Lattice Parameter (LP) - Crystallite Size (CS)
Sample 14

Chemical Composition [at. %]

| Cations | 0 | 20 | 40 | 60 |
|---------|---|----|----|----|
| Y       |   |    |    |    |
| Sm      |   |    |    |    |
| La      |   |    |    |    |
| Ce      |   |    |    |    |
| Pr      |   |    |    |    |

Intensity [a.u.]

Crystal structure (XS) - Lattice Parameter (LP) - Crystallite Size (CS)

- XS: Fm-3m (100%)
- LP: 5.44442 Å
- CS: 110.5 nm

Linear Fit of $F(R)h_n^2$

- Equation: $y = a + b \times x$
- Plot: 14
- Weight: No Weighting
- Intercept: $-3.44189 \pm 0.04202$
- Slope: $1.0384 \pm 0.01207$
- Adj. R-Square: 0.99663

$E_g = 3.31 \text{ eV}$
Sample 15

Chemical Composition [at. %]

- Cations: Y, Sm, La, Ce, Pr

Intensity [a.u.]

- XS Fm-3m (100%)
- LP 5.36719 Å
- CS 101.5 nm

Crystal structure (XS) - Lattice Parameter (LP) - Crystallite Size (CS)

Linear Fit of Sheet3 P"15"

- Equation: \( y = a + b \times x \)
- Plot 15
- Weight No Weighting
- Intercept: \(-3.19485 \pm 0.03875\)
- Slope: \(0.96834 \pm 0.01108\)
- Adj. R-Square: \(0.99557\)

\( E_g = 3.30 \text{ eV} \)
Sample 16

Chemical Composition [at. %]

Cations

Intensity [a.u.]

Crystal structure (XS) - Lattice Parameter (LP) - Crystallite Size (CS)

E\textsubscript{g} = 2.01 eV

Linear Fit of Sheet3 BP"16"

Intercept: -1.15768 ± 0.00388
Slope: 0.57453 ± 0.0015
Adj. R-Square: 0.99872
Sample 19

Chemical Composition [at. %]

| Cations | Y  | Sm | La | Ce | Pr |
|---------|----|----|----|----|----|
|         | 0  | 20 | 40 | 20 | 0  |

Crystal structure (XS) - Lattice Parameter (LP) - Crystallite Size (CS)

- XS Fm-3m (100%)
- LP 5.4024 Å
- CS 77.5 nm

Linear Fit of Sheet3 CL"19"

- Equation: $y = a + b \cdot x$
- Plot 19
- Weight: No Weighting
- Intercept: $-3.0976 \pm 0.01561$
- Slope: $0.9399 \pm 0.00439$
- Adj. R-Square: 0.99913

Energy Gap ($E_g$) = 3.29 eV
Sample 20

Chemical Composition [at. %]

| Cations | Y  | Sm | La | Ce | Pr |
|---------|----|----|----|----|----|
|         | 0  | 20 | 40 | 20 | 0  |

Crystal structure (XS) - Lattice Parameter (LP) - Crystallite Size (CS)

- XS: Fm-3m (100%)
- LP: 5.48594 Å
- CS: 48.3 nm

Linear Fit of Sheet3 DH^20^:

- Equation: \( y = a + b \times x \)
- Intercept: \(-3.23089 \pm 0.02127\)
- Slope: \(0.97817 \pm 0.00601\)
- Adj. R-Square: 0.99876

Energy gap: \(E_g=3.30\) eV
Sample 22

Crystal structure (XS) - Lattice Parameter (LP) - Crystallite Size (CS)

Intensity [a.u.]

Crystal structure (XS):
- Ia-3 (41%)
- P4/nmm (27.4%)
- P63/m (16.6%)
- P-3C1 (15%)

Lattice Parameter (LP):
- *10.84606 Å

Crystallite Size (CS):
- *86.7 nm

Direct Band Gap [eV]:

| Single Phase | Single Phase Fm3m | Multiple Phase |
|--------------|-------------------|---------------|
| F(R)h^n | 1.800 | 1.887 | 1.975 | 2.062 | 2.150 | 2.237 | 2.300 |

Linear Fit of Sheet3 J"22":

- Equation: \( y = a + b \times x \)
- Intercept: -0.91557 ± 0.01476
- Slope: 0.18243 ± 0.00285
- Adj. R-Square: 0.99829

E_g = 5.01 eV
Sample 23

Chemical Composition [at. %]

Y Sm La Ce Pr

0
20
40

Crystal structure (XS): Fm-3m (98.9%), P4/nmm (1.1%)

Crystal lattice parameters:
- LP: 5.506 Å
- CS: 93.4 nm

Direct Band Gap [eV]:

1.800
1.887
1.975
2.062
2.150
2.237
2.300

(F(R)h_n)^2

hn [eV]

23

Linear Fit of Sheet3 DV"23"

Plot

Weight

No Weighting

Intercept

-2.64768 ± 0.02709

Slope

0.79307 ± 0.00758

Adj. R-Square

0.99663

E_g = 3.33 eV
Sample 24

**Chemical Composition [at. %]**

- **Cations**
  - Y
  - Sm
  - La
  - Ce
  - Pr

**Intensity [a.u.]**

- XS Ia-3(100%)
- LP 10.95435 Å
- CS 60.7 nm

**Linear Fit of Sheet3 EX**

- $E_g = 2.05 \text{ eV}$
- Equation: $y = a + b \times x$
- Plot

  - Weight: No Weighting
  - Intercept: $-0.33728 \pm 0.0019$
  - Slope: $0.16402 \pm 7.06997 \times 10^{-4}$
  - Adj. R-Square: 0.99711

**Direct Bang Gap [eV]**

- 1.800
- 1.887
- 1.975
- 2.062
- 2.150
- 2.237
- 2.300

---

**Crystal Structure (XS) - Lattice Parameter (LP) - Crystallite Size (CS)**

- XS Ia-3(100%)
- LP 10.95435 Å
- CS 60.7 nm

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**F(R)h**

- $h = 24$
- $eV$

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**Single Phase Ia$3$**

- Single Phase Fm$3m$
- Multiple Phase

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N.A.
Sample 25

Chemical Composition [at. %]

| Cations | Y  | Sm | La | Ce | Pr |
|---------|----|----|----|----|----|
|         | 0  | 20 | 40 | 0  | 0  |

Crystal structure (XS) - Lattice Parameter (LP) - Crystallite Size (CS)

- XS Ia-3(100%)
- LP 10.80213 Å
- CS 126.4 nm

Linear Fit of Sheet3 X"25"

- Equation: $y = a + b \times x$
- Plot: 25
- Weight: No Weighting
- Intercept: $-0.84872 \pm 0.00706$
- Slope: $0.42594 \pm 0.00307$
- Adj. R-Square: 0.99664

Direct Band Gap [eV]

- 1.800
- 1.887
- 1.975
- 2.062
- 2.150
- 2.237
- 2.300

Eg = 1.98 eV
Sample 26

Chemical Composition [at. %]

Cations

Y Sm La Ce Pr

0
20
40

Intensity [a.u.]

2q

XS Ia-3(100%)

LP 10.90459 Å

CS 83.2 nm

Crystal structure (XS) - Lattice Parameter (LP) - Crystallite Size (CS)

Linear Fit of Sheet3 B"26"

Equation $y = a + b \times x$

Intercept $-0.78114 \pm 0.00395$

Slope $0.37964 \pm 0.00148$

Adj. R-Square $0.99808$

$E_g=2.03 \text{ eV}$
Sample 27

- **Chemical Composition [at. %]**
  - Cations: Y, Sm, La, Ce, Pr
  - Graph showing Relative Composition

- **Crystal structure (XS) - Lattice Parameter (LP) - Crystallite Size (CS)**
  - XS: Fm-3m (100%)
  - LP: 5.49182 Å
  - CS: 94 nm

- **Direct Band Gap [eV]**
  - Scale: 1.300 to 2.300

- **Raman shift [cm⁻¹]**
  - Peaks: Fit Peak 1, Fit Peak 2, Cumulative Fit Peak
  - Graph showing Raman spectra

- **Linear Fit of Sheet3 CT**
  - Equation: \( y = a + b \times x \)
  - Intercepts:
    - Intercept: \(-0.48543 ± 0.00185\)
    - Slope: \(0.24048 ± 0.0072741\)
  - Adjusted R-Square: 0.99848

- **Eg = 2.01 eV**

- **Plot 27**
  - Graph showing Intensity [a.u.] vs. Energy [eV]
  - **Linear Fit of Sheet3 CT**
    - Equation: \( y = a + b \times x \)
    - Intercepts:
      - Intercept: \(-0.48543 ± 0.00185\)
      - Slope: \(0.24048 ± 0.0072741\)
    - Adjusted R-Square: 0.99848

- **Eg = 2.01 eV**

- **Crystal structure**
  - XS: Fm-3m (100%)
  - LP: 5.49182 Å
  - CS: 94 nm

- **Graph showing Intensity [a.u.] vs. Energy [eV]**
  - Trend line: Linear Fit of Sheet3 CT
  - **Eg = 2.01 eV**

- **Graph showing Intensity [a.u.] vs. Energy [eV]**
  - Trend line: Linear Fit of Sheet3 CT
  - **Eg = 2.01 eV**
Sample 28

Chemical Composition [at. %]

| Cations | Y | Sm | La | Ce | Pr |
|---------|---|----|----|----|----|
| 10      |   |    |    |    |    |
| 20      |   |    |    |    |    |
| 30      |   |    |    |    |    |
| 40      |   |    |    |    |    |
| 50      |   |    |    |    |    |

Crystal structure (XS) - Lattice Parameter (LP) - Crystallite Size (CS)

- XS: Fm-3m (100%)
- LP: 5.47679 Å
- CS: 70.2 nm

Linear Fit of Sheet3 BV "28"

Equation: $y = a + b \times x$

- Intercept: $-0.42479 \pm 0.00145$
- Slope: $0.216 \pm 5.51507E-4$
- Adj. R-Square: 0.99885

E$_g$ = 1.98 eV
Sample 30

Direct Band Gap [eV]

1.800 1.887 1.975 2.062 2.150 2.237 2.300

○ Single Phase $Ia\overline{3}$  ● Single Phase $Fm\overline{3}m$  ◇ Multiple Phase

Chemical Composition [at. %]

Y Sm La Ce Pr

0 20 40

Crystal structure (XS) - Lattice Parameter (LP) - Crystallite Size (CS)

XS $Fm\overline{3}m$ (100%)
LP 5.47701 Å
CS 53.4 nm

Intensity [a.u.]

2q

30

Linear Fit of Sheet3 Z"30"
Equation $y = a + b \times x$
Plot 30
Weight No Weighting
Intercept $-0.31941 \pm 0.0000760544$
Slope $0.14232 \pm 0.000027164$
Adj. R-Square 0.99951
$E_g = 2.24 \text{ eV}$

$F(R)h_n^2$

$hn$ [eV]

30

Raman shift [cm$^{-1}$]

400 600

Fit Peak 1
Fit Peak 2
Cumulative Fit Peak

400 600

Intensity [a.u.]

Raman shift [cm$^{-1}$]

Intensity [a.u.]
Sample 32

Crystal structure (XS) - Lattice Parameter (LP) - Crystallite Size (CS)
- XS Fm-3m(100%)
- LP 5.49655 Å
- CS 80.1 nm

Linear Fit of Sheet3 F"32"
- Equation: $y = a + b \times x$
- Plot 32
- Weight: No Weighting
- Intercept: $-0.55988 \pm 0.00242$
- Slope: $0.26443 \pm 9.37516 \times 10^{-4}$
- Adj. R-Square: 0.99847
- $E_g = 2.11$ eV

Direct Band Gap [eV]

Chemical Composition [at. %]
- Y 0
- Sm 10
- La 20
- Ce 30
- Pr 40

Intensity [a.u.]

Raman shift [cm$^{-1}$]

Cumulative Fit Peak

Fit Peak 1

Fit Peak 2

Fit Peak 3

Intensity [a.u.]

Weight
- No Weighting

(F(R)h$n$)$_2$

$hn$ [eV]

32
Sample 33

- **Chemical Composition [at. %]**
  - Cations: Y, Sm, La, Ce, Pr
- **Crystal structure (XS)**
  - Fm-3m (100%)
- **Lattice Parameter (LP)**
  - 5.48187 Å
- **Crystallite Size (CS)**
  - 71.8 nm

- **Raman shift [cm⁻¹]**
- **Intensity [a.u.]**

- **Linear Fit of Sheet3 H"33"**
  - Equation: \(y = a + b \cdot x\)
  - Intercept: \(-0.7279 ± 0.00178\)
  - Slope: \(0.34684 ± 6.61905 \times 10^{-4}\)
  - Adj. R-Square: 0.99941
  - \(E_g = 2.09\) eV

- **Direct Band Gap [eV]**

- **Weight No Weighting**
Sample 34

Intensity [a.u.]
Raman shift [cm$^{-1}$]
Fit Peak 1
Fit Peak 2
Cumulative Fit Peak

34

Chemical Composition [at. %]

Cations
Y Sm La Ce Pr

0
10
20
30

Crystal structure (XS) - Lattice Parameter (LP) - Crystallite Size (CS)

XS Fm-3m(100%)
LP 5.49139 Å
CS 90.9 nm

Linear Fit of Sheet 3 CV "43"
Equation $y = a + b \times x$
Plot 34
Weight No Weighting
Intercept $-0.44102 \pm 0.0014$
Slope $0.21853 \pm 5.37607 \times 10^{-4}$
Adj. R-Square 0.99888
$E_g = 2.02$ eV
Sample 35

Chemical Composition [at. %]

Cations

Y  Sm  La  Ce  Pr

Intensity [a.u.]

Raman shift [cm$^{-1}$]

Fit Peak 1

Fit Peak 2

Cumulative Fit Peak

Crystal structure (XS) - Lattice Parameter (LP) - Crystallite Size (CS)

XS Fm-3m(100%)
LP 5.48662 Å
CS 86.7 nm

Linear Fit of Sheet3 CX"44"

Equation $y = a + b \times x$

Plot 35

Weight No Weighting

Intercept $-0.60203 \pm 0.00336$

Slope $0.29332 \pm 0.00135$

Adj. R-Square 0.99734

$E_g = 2.05 \text{ eV}$
Sample 36

![Diagram showing chemical composition and crystal structure](image)

- **Chemical Composition [at. %]**
  - Y: 36%
  - Sm: 20%
  - La: 30%
  - Ce: 10%
  - Pr: 10%

- **Crystal Structure (XS) - Lattice Parameter (LP) - Crystallite Size (CS)**
  - XS: Fm-3m (100%)
  - LP: 5.48508 Å
  - CS: 81.9 nm

- **Linear Fit of Sheet3 CZ"45"**
  - Equation: $y = a + bx$
  - Intercept: $-0.56222 \pm 0.00335$
  - Slope: $0.27427 \pm 0.00131$
  - Adj. R-Square: 0.99677
  - $E_g = 2.04$ eV
Sample 38

- Direct Band Gap [eV]
  - 1.800
  - 1.887
  - 1.975
  - 2.062
  - 2.150
  - 2.237
  - 2.300

- Chemical Composition [at. %]
  - Cations: Y, Sm, La, Ce, Pr

- Raman shift [cm⁻¹]
  - Fit Peak 1
  - Fit Peak 2
  - Cumulative Fit Peak
  - 38

- Intensity [a.u.]

- Crystal structure (XS) - Lattice Parameter (LP) - Crystallite Size (CS)
  - XS: Fm-3m (100%) | LP: 5.48112 Å | CS: 75.5 nm

- Linear Fit of Sheet3 BZ

  Equation: \( y = a + b \times x \)
  - Intercept: \(-0.65714 ± 0.00431\)
  - Slope: \(0.32426 ± 0.00176\)
  - Adj. R-Square: 0.99635
  - \( E_g = 2.03 \text{ eV} \)
Sample 39

Chemical Composition [at. %]

Cations
- Y
- Sm
- La
- Ce
- Pr

Crystal structure (XS) - Lattice Parameter (LP) - Crystallite Size (CS)

- XS: Fm-3m (100%)
- LP: 5.47173 Å
- CS: 77.9 nm

Linear Fit of Sheet3 CB

Equation: \( y = a + b \times x \)

- Intercept: \(-0.59459 \pm 0.00292\)
- Slope: \(0.2884 \pm 0.00114\)
- Adj. R-Square: 0.99769

E\(_g\) = 2.06 eV
Sample 40

Chemical Composition [at. %]

- Y
- Sm
- La
- Ce
- Pr

Intensity [a.u.]

Raman shift [cm$^{-1}$]

Fit Peak 1
Fit Peak 2
Cumulative Fit Peak

Crystal structure (XS) - Lattice Parameter (LP) - Crystallite Size (CS)

- XS Fm-3m (100%)
- LP 5.43235 Å
- CS 89.7 nm

Linear Fit of Sheet3 AZ$^{37}$

Equation $y = a + b \times x$

- Intercept: $-0.59725 \pm 0.00597$
- Slope: $0.29611 \pm 0.00236$
- Adj. R-Square: 0.99271

$E_g = 2.02$ eV
Sample 41

Direct Band Gap [eV]

- Single Phase $Ia\bar{3}$
- Single Phase $Fm\bar{3}m$
- Multiple Phase

Chemical Composition [at. %]

- Y
- Sm
- La
- Ce
- Pr

Crystal structure (XS) - Lattice Parameter (LP) - Crystallite Size (CS)

- XS: Fm-3m (100%)
- LP: 5.45701 Å
- CS: 87.5 nm

Linear Fit of Sheet3 BB"38"

- Equation: $y = a + b \times x$
- Plot: 41
- Weight: No Weighting
- Intercept: $-0.56348 \pm 0.00234$
- Slope: $0.27926 \pm 8.96637E-4$
- Adj. R-Square: 0.99846

Eg = 2.02 eV

Raman shift [cm$^{-1}$]

- Fit Peak 1
- Fit Peak 2
- Fit Peak 3
- Cumulative Fit Peak

Intensity [a.u.]

- hν [eV]

$F(\mathbf{R})h\mathbf{n}$
Sample 42

Chemical Composition [at. %]

| Cations | Y | Sm | La | Ce | Pr |
|---------|---|----|----|----|----|
|         |   |    |    | 20 | 10 |

Intensity [a.u.]

Raman shift [cm$^{-1}$]

Fit Peak 3
Fit Peak 2
Fit Peak 1
Cumulative Fit Peak
42

Crystal structure (XS) - Lattice Parameter (LP) - Crystallite Size (CS)

- XS Fm-3m (100%)
- LP 5.45987 Å
- CS 84.2 nm

Linear Fit of Sheet3 BD:9

- Equation: $y = a + b \times x$
- Plot: 42
- Weight: No Weighting
- Intercept: $-0.65681 \pm 0.00325$
- Slope: $0.3212 \pm 0.00129$
- Adj. R-Square: 0.9979
Sample 43

- Chemical Composition [at. %]
  - Cations: Y, Sm, La, Ce, Pr

- Crystal structure (XS): Fm-3m (100%)
- Lattice Parameter (LP): 5.47296 Å
- Crystallite Size (CS): 57.5 nm

- Intensity [a.u.]
- Raman shift [cm\(^{-1}\)]

- Linear Fit of Sheet AB\(^{34}\)
  - Equation: \( y = a + b \times x \)
  - Plot: 43
  - Weight: No Weighting
  - Intercept: \(-0.49989 ± 0.0026\)
  - Slope: \(0.226 ± 9.57233 \times 10^{-4}\)
  - Adj. R-Square: 0.99826
- \( E_g = 2.21 \text{ eV} \)
Sample 44

![Diagram showing chemical composition and crystal structure analysis](image)

- **Chemical Composition [at. %]**
  - Y: 0, 10, 20, 30
  - Sm: 10, 20, 30
  - La: 0
  - Ce: 10, 20, 30
  - Pr: 0

- **Crystal Structure (XS)**
  - Lattice Parameter (LP): 5.48452 Å
  - Crystallite Size (CS): 62.1 nm

- **Linear Fit of Sheet3 AD35**
  - Equation: \( y = a + b \cdot x \)
  - Intercept: \(-0.64643 \pm 0.00288\)
  - Slope: \(0.29844 \pm 0.00112\)
  - Adjusted R-Square: 0.99855

- **E\(_g\) = 2.14 eV**
Sample 45

Chemical Composition [at. %]

- Y: 10
e- Sm: 20
e- Ce: 30
- Pr: 40
- La: 50

Crystal structure (XS): Fm-3m (100%)
- Lattice Parameter (LP): 5.49842 Å
- Crystallite Size (CS): 70.6 nm

Linear Fit of Sheet3 AF36
Equation: \( y = a + b \times x \)
- Intercept: \(-0.54554 \pm 0.00395\)
- Slope: \(0.25945 \pm 0.00148\)
- Adj. R-Square: 0.99582

\( E_g = 2.10 \text{ eV} \)
Sample 46

Chemical Composition [at. %]

| Cations | Y | Sm | La | Ce | Pr |
|---------|---|----|----|----|----|
|         | 0 | 20 | 40 | 30 | 50 |

Crystal structure (XS) - Lattice Parameter (LP) - Crystallite Size (CS)

- XS Fm-3m (100%)
- LP 5.48942 Å
- CS 88.7 nm

\[ E_g = 2.02 \text{ eV} \]

Linear Fit of Sheet3 BR"46"

Equation: \[ y = a + b \times x \]

- Intercept: \(-0.67328 ± 0.00254\)
- Slope: \(0.32877 ± 0.88986E-\)
- Adj. R-Square: 0.99853

Raman shift [cm\(^{-1}\)]

Intensity [a.u.]

- Fit Peak 3
- Fit Peak 2
- Fit Peak 1
- Cumulative Fit Peak
Sample 49

- Chemical Composition [at. %]
  - Y: 0
  - Sm: 20
  - La: 30
  - Ce: 40
  - Pr: 50

- Crystal structure (XS): Lattice Parameter (LP) - Crystallite Size (CS)
  - XS Fm-3m (100%)
  - LP 5.49675 Å
  - CS 84.9 nm

- Linear Fit of Sheet3 CF "49"
  - Equation: \( y = a + b \times x \)
  - Plot 49
  - Weight: No Weighting
  - Intercept: \(-0.62876 \pm 0.00253\)
  - Slope: \(0.30062 \pm 9.65801 \times 10^{-4}\)
  - Adj. R-Square: 0.99836
  - \( E_g = 2.08 \text{ eV} \)

- Direct Bang Gap [eV]
  - Single Phase \( Ia \bar{3} \)
  - Single Phase \( Fm \bar{3}m \)
  - Multiple Phase

- Intensity [a.u.]
  - Raman shift [cm\(^{-1}\)]
  - Fit Peak 1
  - Fit Peak 2
  - Fit Peak 3
  - Cumulative Fit Peak
Sample 51

Chemical Composition [at. %]

- Y
- Sm
- La
- Ce
- Pr

Crystal structure (XS): Lattice Parameter (LP): Crystallite Size (CS)
- XS Fm-3m (100%)
- LP 5.48862 Å
- CS 85.4 nm

Linear Fit of Sheet3 CJ"51"
- Equation: \( y = a + b \times x \)
- Intercept: -0.55157 ± 0.00296
- Slope: 0.27395 ± 0.00111
- Adj. R-Square: 0.99751

Direct Band Gap [eV]

- Single Phase \( l a \bar{3} \)
- Single Phase \( Fm\bar{3} m \)
- Multiple Phase

Intensity [a.u.]

Raman shift [cm\(^{-1}\)]

Fit Peak 3
Fit Peak 2
Fit Peak 1
Cumulative Fit Peak

Int. [eV]

\( E_g = 2.01 \ eV \)
Sample 57

Chemical Composition [at. %]

Cations

- Y
- Sm
- La
- Ce
- Pr

Crystal structure (XS) - Lattice Parameter (LP) - Crystallite Size (CS)

- XS Fm-3m (100%)
- LP 5.48685 Å
- CS 75.5 nm

Linear Fit of Sheet3 FX"57"

Equation: $y = a + b \cdot x$

- Intercept: $-0.38263 \pm 9.82352 \times 10^{-4}$
- Slope: $0.18964 \pm 3.76692 \times 10^{-4}$
- Adj. R-Square: 0.99927

Energy Gap ($E_g$): 2.02 eV

Direct Bang Gap [eV]

- Single Phase $Ia\bar{3}$
- Single Phase $Fm\bar{3}m$
- Multiple Phase

Intensity [a.u.]

Intensity vs. Raman shift [cm$^{-1}$]

- Fit Peak 1
- Fit Peak 2
- Cumulative Fit Peak

$F(R)h_n$ vs. $hn$ [eV]

- 57

Plot 57

Weight: No Weighting

$E_g = 2.02$ eV
Sample 58

Chemical Composition [at. %]

| Cations | Y | Sm | La | Ce | Pr |
|---------|---|----|----|----|----|
| Chemical Composition [at. %] | 0 | 20 | 40 | 50 |

Crystal structure (XS) - Lattice Parameter (LP) - Crystallite Size (CS)

- **XS**: Fm-3m (100%)
- **LP**: 5.44105 Å
- **CS**: 80.7 nm

Linear Fit of Sheet3 EP"60"

- Equation: $y = a + b \times x$
- Plot: 58
- Weight: No Weighting
- Intercept: $-0.48421 \pm 0.00139$
- Slope: $0.2517 \pm 5.09767 \times 10^{-4}$
- Adj. R-Square: 0.99919

Direct Band Gap [eV]

Intensity [a.u.]

- Intensity vs. Raman shift [cm$^{-1}$]
- Intensity vs. $h_n$ [eV]

$E_g = 1.96$ eV

---

**Legend:**
- **Single Phase $La_3**
- **Single Phase Fm$3m**
- **Multiple Phase**
Sample 59

- **Chemical Composition [at. %]**
  - Y: 0
  - Sm: 20
  - La: 40
  - Ce: 40
  - Pr: 0

- **Crystal structure (XS)**: Fm-3m (100%)
- **Lattice Parameter (LP)**: 5.46116 Å
- **Crystallite Size (CS)**: 74.3 nm

- **Linear Fit of Sheet3 ET**: $E_g = 1.97$ eV
- **Equation** $y = a + b \times x$
- **Plot 59**
  - **Intercept**: $-0.45793 \pm 0.00171$
  - **Slope**: $0.23253 \pm 6.46386 \times 10^{-4}$
  - **Adj. R-Square**: 0.99866
Sample 61

Chemical Composition [at. %]

Cations

Y, Sm, La, Ce, Pr

Crystal structure (XS): Lattice Parameter (LP) - Crystallite Size (CS)

XS Fm-3m(100%)

LP 5.46363 Å

CS 81.8 nm

Equation $y = a + b \times x$

Plot 61

Weight No Weighting

Intercept $-0.59203 \pm 0.00295$

Slope $0.29594 \pm 0.00121$

Adj. R-Square 0.99811

Direct Band Gap [eV]

1.800 1.887 1.975 2.062 2.150 2.237 2.300
Sample 64

Chemical Composition [at. %]

Cations

Y  Sm  La  Ce  Pr

Intensity [a.u.]

Raman shift [cm\(^{-1}\)]

Fit Peak 1
Fit Peak 2
Cumulative Fit Peak

64

Crystal structure (XS) - Lattice Parameter (LP) - Crystallite Size (CS)

10 20 30 40 50

Intensity [a.u.]

\(2q\)

XS Fm-3m (100%)
LP 5.42222 Å
CS 75.3 nm

\(E_g = 2.15\) eV

Linear Fit of Sheet3 CR"66"

Equation

\(y = a + b \times x\)

Plot

64

Weight

No Weighting

Intercept

-0.66681 ± 0.00386

Slope

0.30811 ± 0.00146

Adj. R-Square

0.99705

\(E_g = 2.15\) eV
Sample 65

Chemical Composition [at. %]

Cations

Y Sm La Ce Pr
0
20
40

Crystal structure (XS) - Lattice Parameter (LP) - Crystallite Size (CS)

Intensities [a.u.]

2q
XS Fm-3m(100%)
LP 5.44468 Å
CS 80.2 nm

Linear Fit of Sheet3 DD"68"

Equation

\[ y = a + b \times x \]

Plot

Intercept

-0.3922 ± 0.0022

Slope

0.18392 ± 7.97621E-4

Adj. R-Square

0.99661

Eg = 2.10 eV

Direct Bang Gap [eV]

1.800 1.887 1.975 2.062 2.150 2.237 2.300

○ Single Phase łą3 ● Single Phase Fm3m ◇ Multiple Phase

Fit Peak 1

Fit Peak 2

Cumulative Fit Peak

65

Intensity [a.u.]

Raman shift [cm⁻¹]

400 600

Intensity [a.u.]

Raman shift [cm⁻¹]

65

Intensity [a.u.]

hv [eV]
Sample 66

Chemical Composition [at. %]

| Cations | Y | Sm | La | Ce | Pr |
|---------|---|----|----|----|----|
| 0       | 20| 40 | 60 | 80 | 0  |

Crystal structure (XS) - Lattice Parameter (LP) - Crystallite Size (CS)

- XS: Fm-3m (100%)
- LP: 5.44681 Å
- CS: 67.8 nm

Linear Fit of Sheet3 CN"64"
Equation: \( y = a + b \cdot x \)
- Intercept: \(-0.48718 \pm 0.00269\)
- Slope: \(0.21884 \pm 9.85908 \times 10^{-4}\)
- Adj. R-Square: 0.99771

\( E_g = 2.22 \text{ eV} \)
Sample 68

Chemical Composition [at. %]
- Y: 0, 20, 40
- Sm: 0, 20, 40
- La: 0
- Ce: 10, 20, 30, 40, 50
- Pr: 0

Crystal structure (XS) - Lattice Parameter (LP) - Crystallite Size (CS)
- XS: Fm-3m (100%)
- LP: 5.46367 Å
- CS: 67.9 nm

Spectroscopic Measurements
- Raman shift [cm⁻¹]
- Intensity [a.u.]

Linear Fit of Sheet3 CP"65"
- Equation: \( y = a + b \times x \)
- Plot: 68
- Weight: No Weighting
- Intercepts: 68
- Slopes: 68
- Adj. R-Square: 0.99932
- \( E_g = 2.26 \, \text{eV} \)
Sample 73

Chemical Composition [at. %]

Cations

Y Sm La Ce Pr

Intensity [a.u.]

Raman shift [cm$^{-1}$]

Fit Peak 1

Fit Peak 2

Cumulative Fit Peak

Crystal structure (XS) - Lattice Parameter (LP) - Crystallite Size (CS)

Crystal structure (XS) - Lattice Parameter (LP) - Crystallite Size (CS)

Fit Peak 1

Fit Peak 2

Cumulative Fit Peak

Linear Fit of Sheet3 DP"73"

Equation $y = a + b \times x$

Plot 73

Weight No Weighting

Intercept $-0.69319 \pm 0.00449$

Slope $0.31608 \pm 0.00174$

Adj. R-Square $0.99727$

$E_g = 2.16 \, \text{eV}$
Sample 76

- Chemical Composition [at. %]: Y, Sm, La, Ce, Pr
- Crystal structure (XS) - Fm-3m (100%)
- Lattice Parameter (LP): 5.49203 Å
- Crystallite Size (CS): 78.7 nm

Linear Fit of Sheet3 BH"78"
- Equation: \( y = a + b \times x \)
- Intercept: \(-0.50073 \pm 0.00193\)
- Slope: \(0.24817 \pm 7.25794 \times 10^{-4}\)
- Adj. R-Square: 0.99862

Direct Band Gap [eV]: 1.800, 1.887, 1.975, 2.062, 2.150, 2.237, 2.300

- Single Phase \(Ia\bar{3}\)
- Single Phase \(Fm\bar{3}m\)
- Multiple Phase
Sample 78

Chemical Composition [at. %]

| Cations | 0 | 20 | 40 |
|----------|---|----|----|
| Y        |   |    |    |
| Sm       |   |    |    |
| La       |   |    |    |
| Ce       |   |    |    |
| Pr       |   |    |    |

Intensity [a.u.]

Fit Peak 1
Fit Peak 2
Fit Peak 3
Cumulative Fit Peak

78

Crystal structure (XS): Fm-3m (100%)
Lattice Parameter (LP): 5.48839 Å
Crystallite Size (CS): 83.2 nm

Linear Fit of Sheet3 AV
Equation: y = a + b*x
Plot 78
Weight: No Weighting
Intercept: -0.68512 ± 0.00244
Slope: 0.32338 ± 9.00874E-4
Adj. R-Square: 0.99874

E g = 2.09 eV
Sample 79

Chemical Composition [at. %]

Cations

Intensity [a.u.]

Fit Peak 3
Fit Peak 2
Fit Peak 1
Cumulative Fit Peak

Crystal structure (XS) - Lattice Parameter (LP) - Crystallite Size (CS)

Linear Fit of Sheet3 BN81

Equation

Plot

Weight
No Weighting

Intercept
-0.57333 ± 0.00263

Slope
0.2803 ± 0.00107

Adj. R-Square
0.99825

Eg = 2.04 eV

Direct Band Gap [eV]

1.800 1.887 1.975 2.062 2.150 2.237 2.300

Single Phase Ia3 • Single Phase Fm-3m • Multiple Phase

Linear Fit of Sheet3 BN81

Equation

Plot

Weight
No Weighting

Intercept
-0.57333 ± 0.00263

Slope
0.2803 ± 0.00107

Adj. R-Square
0.99825

Eg = 2.04 eV
Sample 82

Chemical Composition [at. %]

Cations

Y  Sm  La  Ce  Pr

Intensity [a.u.]

XS Ia-3(100%)
LP 10.94121 Å
CS 67.3 nm

Crystal structure (XS) - Lattice Parameter (LP) - Crystallite Size (CS)

Linear Fit of Sheet3 L"82"
Equation $y = a + b \cdot x$
Plot 82
Weight No Weighting
Intercept $-0.67914 \pm 0.00262$
Slope $0.30584 \pm 8.96017 \times 10^{-4}$
Adj. R-Square $0.99864$

$E_g = 2.22 \text{ eV}$
Sample 86

Chemical Composition [at. %]

- Y
- Sm
- La
- Ce
- Pr

Intensity [a.u.]
Raman shift [cm\(^{-1}\)]
Fit Peak 3
Fit Peak 2
Fit Peak 1
Cumulative Fit Peak

Crystal structure (XS) - Lattice Parameter (LP) - Crystallite Size (CS)

- XS Fm-3m (100%)
- LP 5.48653 Å
- CS 59.3 nm

Linear Fit of Sheet3 T"86"

Equation: \( y = a + b \times x \)

- Plot 86
- Weight: No Weighting
- Intercept: -0.50087 ± 0.00159
- Slope: 0.22318 ± 5.71269E-4
- Adj. R-Square: 0.99907

\( E_g = 2.24 \text{ eV} \)

Direct Band Gap [eV]
Sample 87

- Chemical Composition [at. %]
  - Cations: Y, Sm, La, Ce, Pr

- Crystal structure (XS): Lattice Parameter (LP) = 5.48005 Å
  - Crystallite Size (CS) = 66 nm

- Intensity [a.u.]

- Raman shift [cm\(^{-1}\)]

- Fit Peak 1
- Fit Peak 2
- Fit Peak 3
- Cumulative Fit Peak

- Equation: \( y = a + b \times x \)
  - Intercept: \(-0.46693 \pm 0.00236\)
  - Slope: \(0.21782 \pm 8.86292 \times 10^{-4}\)
  - Adj. R-Square: 0.99807

- Linear Fit of Sheet3 V"87"
- \( E_g = 2.14 \text{ eV} \)

- Direct Bang Gap [eV]
  - 1.8000
  - 1.8875
  - 1.9750
  - 2.0625
  - 2.1500
  - 2.2375
  - 2.3000

- Single Phase \( \text{Ia\text{3}} \) • Single Phase \( \text{Fm\text{3m}} \) • Multiple Phase

- Intensity [a.u.]
- Raman shift [cm\(^{-1}\)]
- Fit Peak 1
d- Fit Peak 2
d- Fit Peak 3
d- Cumulative Fit Peak
Sample 88

Chemical Composition [at. %]

| Cations | Y | Sm | La | Ce | Pr |
|---------|---|----|----|----|----|

Intensity [a.u.]

Raman shift [cm⁻¹]

Fit Peak 1
Fit Peak 2
Cumulative Fit Peak

Fit Peak 3

Linear Fit of Sheet3 DX“88”

Equation

y = a + b*x

Plot

Intercept
-0.46167 ± 0.00213
Slope
0.20575 ± 8.03422E-4
Adj. R-Square
0.99845

Crystal structure (XS) - Lattice Parameter (LP) - Crystallite Size (CS)

XS Fm-3m(98.5%), P4/nmm(1.5%)
LP *5.49497 Å
CS *63.6 nm

Direct Bang Gap [eV]

1.800 1.887 1.975 2.062 2.150 2.237 2.300

Direct Bang Gap [eV]
Sample 89

Chemical Composition [at. %]

| Cations | Y | Sm | La | Ce | Pr |
|---------|---|----|----|----|----|
| At. %   | 30| 40 | 20 | 10 | 0  |

Intensity [a.u.]

Crystal structure (XS) - Lattice Parameter (LP) - Crystallite Size (CS)

| XS | LP 10.95435 Å | CS 60.7 nm |

Linear Fit of Sheet3 DZ89

\[ E_g = 2.25 \text{ eV} \]

Equation

\[ y = a + b \times x \]

| Intercept | Slope | Adj. R-Square |
|-----------|-------|---------------|
| -0.30048 ± 8.16161E-4 | 0.13377 ± 2.95861E-4 | 0.99932 |

(F(R)h)n \[ \text{eV} \]

89

Weight | No Weighting

Intercept

Slope

Adj. R-Square

1.800 | 1.975 | 2.062 | 2.150 | 2.237 | 2.300

Direct Bang Gap [eV]

Single Phase \( \text{Ia}\overline{3} \)● Single Phase \( \text{Fm}\overline{3}m \) ● Multiple Phase

N.A.
Sample 90

Chemical Composition [at. %]
- Y: 0, 20, 40, 50
- Sm: 0, 20, 40, 50
- La: 0, 20, 40, 50
- Ce: 0, 20, 40, 50
- Pr: 0, 20, 40, 50

Crystal structure (XS) - Lattice Parameter (LP) - Crystallite Size (CS)
- XS Fm-3m(100%)
- LP 5.49823 Å
- CS 71.5 nm

Intensity [a.u.]
- 400 600

Linear Fit of Sheet3 EB"90"
- Equation: $y = a + b \times x$
- Plot 90
- Weight No Weighting
- Intercept: $-0.5142 \pm 0.00296$
- Slope: $0.24813 \pm 0.00115$
- Adj. R-Square: 0.99766

Direct Bang Gap [eV]
- 1.800
- 1.975
- 2.062
- 2.150
- 2.237
- 2.300

Single Phase $Ia\bar{3}$  •  Single Phase Fm$\bar{3}m$  •  Multiple Phase
Sample 91

Chemical Composition [at. %]

| Cations | 0 | 20 | 40 |
|---------|---|----|----|
| Y       |   |    |    |
| Sm      |   |    |    |
| La      |   |    |    |
| Ce      |   |    |    |
| Pr      |   |    |    |

Crystal structure (XS) - Lattice Parameter (LP) - Crystallite Size (CS)

- XS: Fm-3m (100%)
- LP: 5.47675 Å
- CS: 70.5 nm

Direct Band Gap [eV]

- Single Phase $Ia\bar{3}$
- Single Phase $Fm\bar{3}m$
- Multiple Phase

Linear Fit of Sheet3 ED"91"

- Equation: $y = a + b \times x$
- Plot: 91
- Weight: No Weighting
- Intercept: $-0.56825 \pm 0.0031$
- Slope: $0.26257 \pm 0.00123$
- Adj. R-Square: 0.99787

Raman shift [cm$^{-1}$]

- Fit Peak 1
- Fit Peak 2
- Cumulative Fit Peak

Intensity [a.u.]

- $E_g = 2.16$ eV

Equation

- $y = a + b \times x$

Plot

Intensity [a.u.]

- 91
- No Weighting

Intercept

- $-0.56825 \pm 0.0031$

Slope

- $0.26257 \pm 0.00123$

Adj. R-Square

- 0.99787
Sample 92

**Chemical Composition [at. %]**

- Y
- Sm
- La
- Ce
- Pr

**Crystal Structure (XS)**

- Fm-3m (100%)
- Lattice Parameter (LP)
  - 5.4952 Å
- Crystallite Size (CS)
  - 63.2 nm

**Linear Fit of Sheet3 EF**

- \( E_g = 2.06 \text{ eV} \)

**Equation**

- \( y = a + b \times x \)

**Plot**

- Weighted
- No Weighting

**Fit Parameters**

- Intercept: \(-0.45634 \pm 0.00303\)
- Slope: \(0.22105 \pm 0.00117\)
- Adjusted R-Square: 0.99665

**Raman Shift [cm\(^{-1}\)]**

- Fit Peak 1
- Fit Peak 2
- Fit Peak 3
- Cumulative Fit Peak

**Intensity [a.u.]**

- Y
- Sm
- La
- Ce
- Pr

**Direct Bang Gap [eV]**

- 1.800
- 1.887
- 1.975
- 2.062
- 2.150
- 2.37
- 2.300

**Single Phase**

- Lal3
- Single Phase Fm\(^{3}m\)
- Multiple Phase
Sample 95

Chemical Composition [at. %]
- Y: 0%
- Sm: 20%
- La: 30%
- Ce: 40%
- Pr: 50%

Direct Bang Gap [eV]
- 1.800
- 1.887
- 1.975
- 2.062
- 2.150
- 2.237
- 2.300

Crystal structure (XS) - Lattice Parameter (LP) - Crystallite Size (CS)
- XS Fm-3m (100%)
- LP 5.46736 Å
- CS 90.2 nm

Linear Fit of Sheet3 FH"98"
- $E_g = 1.95$ eV
- Equation: $y = a + b \times x$
- Weight: No Weighting
- Intercept: $-0.43045 \pm 0.00153$
- Slope: $0.22213 \pm 0.000629$
- Adj. R-Square: 0.99879
Sample 96

Crystal structure (XS) - Lattice Parameter (LP) - Crystallite Size (CS)

- Chemical Composition [at. %]
  - Y: 20
  - Sm: 40
  - La: 20
  - Ce: 20
  - Pr: 0

- Intensity [a.u.]
  - 2q: 96
  - XS: Fm-3m (100%)
  - LP: 5.44692 Å
  - CS: 99.1 nm

- Linear Fit of Sheet 3 EZ'
  - Equation: \( y = a + b \times x \)
  - Plot 96
  - Weight: No Weighting
  - Intercept: \(-0.57792 \pm 0.00418\)
  - Slope: \(0.29802 \pm 0.00178\)
  - Adj. R-Square: 0.9961
  - \(E_g = 1.94\) eV

- Energy vs. Raman shift
  - \(h\nu\) vs. \(E_F\)
  - \(E_F = 1.94\) eV

- Raman shift [cm\(^{-1}\)]
  - Fit Peak 1
  - Fit Peak 2
  - Cumulative Fit Peak

- Direct Bang Gap [eV]
  - Single Phase \(Ia\bar{3}\)
  - Single Phase \(Fm\bar{3}m\)
  - Multiple Phase
Sample 98

Chemical Composition [at. %]
- Y
- Sm
- La
- Ce
- Pr

Intensities [a.u.]
- Raman shift [cm⁻¹]

Fit Peak 1
Fit Peak 2
Cumulative Fit Peak

Intensity [a.u.]

Crystal structure (XS) - Lattice Parameter (LP) - Crystallite Size (CS)
- XS Fm-3m (100%)
- LP 5.43249 Å
- CS 98.2 nm

Linear Fit of Sheet3 FB'95'
- Equation: $y = a + b \times x$
- Plot 98
- Intercept: $-0.67277 \pm 0.00418$
- Slope: $0.33806 \pm 0.00173$
- Adj. R-Square: 0.99662

Direct Band Gap [eV]

Equation $E_g = 1.99$ eV
Sample 99

Chemical Composition [at. %]

- Cations: Y, Sm, La, Ce, Pr

Crystal structure (XS) - Lattice Parameter (LP) - Crystallite Size (CS)

- XS: Fm-3m (100%)
- LP: 5.45781 Å
- CS: 83.7 nm

Linear Fit of Sheet 3 FF"97"

- Equation: \( y = a + b \times x \)
- \( E_g = 1.98 \, \text{eV} \)
- Intercept: \(-0.5131 \pm 0.00236\)
- Slope: \(0.25793 \pm 9.22786 \times 10^{-4}\)
- Adj. R-Square: 0.99812

Direct Bang Gap [eV]

- Color Scale: 1.800, 1.887, 1.975, 2.062, 2.150, 2.237, 2.300

E -- g = 1.98 eV
Sample 100

Crystal structure (XS) - Lattice Parameter (LP) - Crystallite Size (CS)

XS la-3(100%)
LP 10.85715 Å
CS 101.5 nm

Intensity [a.u.]

2q

Linear Fit of Sheet3 AL"102"

Equation: \( y = a + b \times x \)

Plot 100

Weight No Weighting

Intercept: -0.59394 ± 0.00213

Slope: 0.30073 ± 8.15838E-4

Adj. R-Square: 0.9985

Eg = 1.97 eV
Sample 101

**Chemical Composition [at. %]**

- Y: 0
- Sm: 20
- La: 40
- Ce: 50
- Pr: 100

**Crystal Structure (XS) - Lattice Parameter (LP) - Crystallite Size (CS)**

- Fm-3m (100%)
- LP: 5.42465 Å
- CS: 93.4 nm

**Eg = 2.03 eV**

- Equation: \( y = a + b \times x \)
  - Intercept: \(-0.59354 \pm 0.00383\)
  - Slope: \(0.29257 \pm 0.00146\)
  - Adj. R-Square: 0.99594
Sample 102

Chemical Composition [at. %]

| Cations | Chemical Composition |
|---------|----------------------|
| Y       | 120                  |
| Sm      | 80                   |
| La      | 20                   |
| Ce      | 10                   |
| Pr      | 5                    |

Crystal structure (XS) - Lattice Parameter (LP) - Crystallite Size (CS)

- XS: Ia-3(100%)
- LP: 10.89865 Å
- CS: 98 nm

Intensity [a.u.]

- 2θ: 20° to 50°

Linear Fit of Sheet3 AH"100"

Equation: \( y = a + b \times x \)

- Intercept: \(-0.76291 \pm 0.0032\)
- Slope: \(0.3638 \pm 0.00116\)
- Adj. R-Square: 0.99811

\( E_g = 2.09 \text{ eV} \)
Sample 104

Chemical Composition [at. %]

- Y
- Sm
- La
- Ce
- Pr

Intensity [a.u.]

Crystal structure (XS) - Lattice Parameter (LP) - Crystallite Size (CS)

- XS Ia-3 (100%)
- LP: 10.93557 Å
- CS: 87.9 nm

Linear Fit of Sheet 3

Equation: \( y = a + b \cdot x \)

- Intercept: \(-0.7887 \pm 0.0029\)
- Slope: \(0.37055 \pm 9.94382 \times 10^{-4}\)
- Adj. R-Square: 0.99858

Eg = 2.00 eV
Sample 106

Chemical Composition [at. %]

| Cations | Y | Sm | La | Ce | Pr |
|---------|---|----|----|----|----|
| 0       | 10| 20 | 30 | 40 | 50 |

Crystal structure (XS) - Lattice Parameter (LP) - Crystallite Size (CS)

| 106 |
|-----|
| XS Fm-3m(100%) |
| LP 5.46832 Å |
| CS 76.2 nm |

Linear Fit of Sheet3 GB

Equation: $y = a + b \times x$

- Intercept: $-0.52114 \pm 0.00167$
- Slope: $0.25168 \pm 6.18744 \times 10^{-4}$
- Adj. R-Square: 0.99897
- $E_g = 2.07 \text{ eV}$