XRD Measurement and Peaks evaluation

Outline

Objective

XRD measurement and Peak evaluation of powder samples

Samples:

- ✓ NaCl
- ✓ Fe powder
- ✓ ZnO
- ✓ PbO
- ✓ Lithium Carbonate
- ✓ CuO

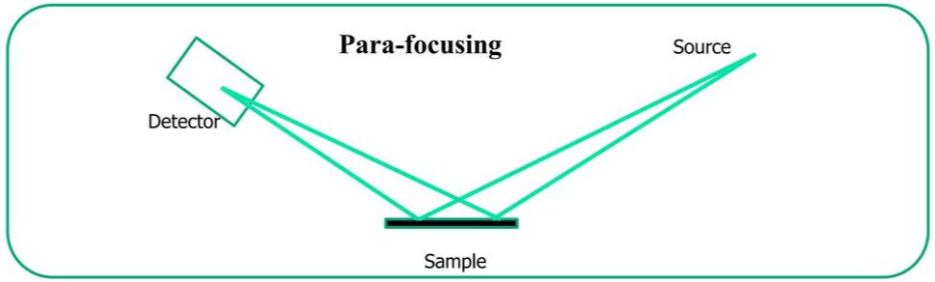
Equipment:

SmartLab SE

Software:

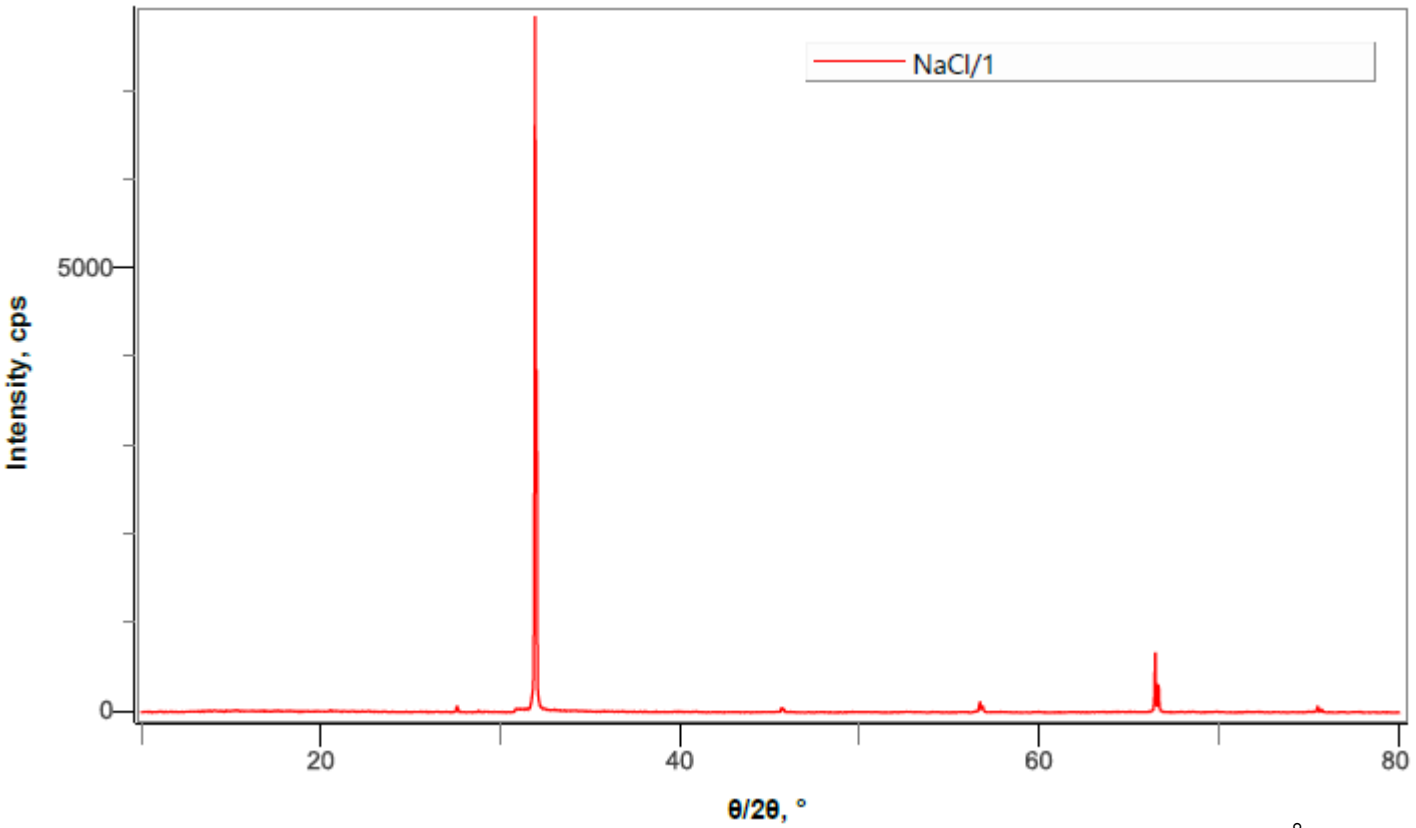
SmartLab Studio II

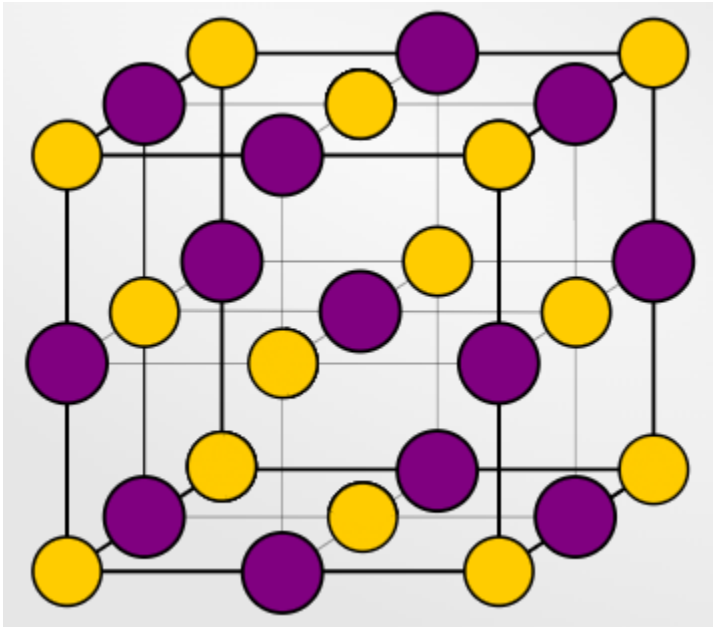
Parameter	Setting / Value
Scan Mode	θ/2θ scan
Incident Angle	10–80°
Scan Speed	2°/min
Step Width	0.02°
Receiving Slit 1	2 mm
Receiving Slit 2	5.025 mm
Filter	Kβ filter 1D for Cu



The same measurement conditions and identical optical alignment (BB) were maintained for all samples.

Peaks evaluation (NaCl)





NaCl adopts the halite (rock-salt) structure with cubic $Fm\bar{3}m$ symmetry, where Na^+ and Cl^- are each octahedrally coordinated.

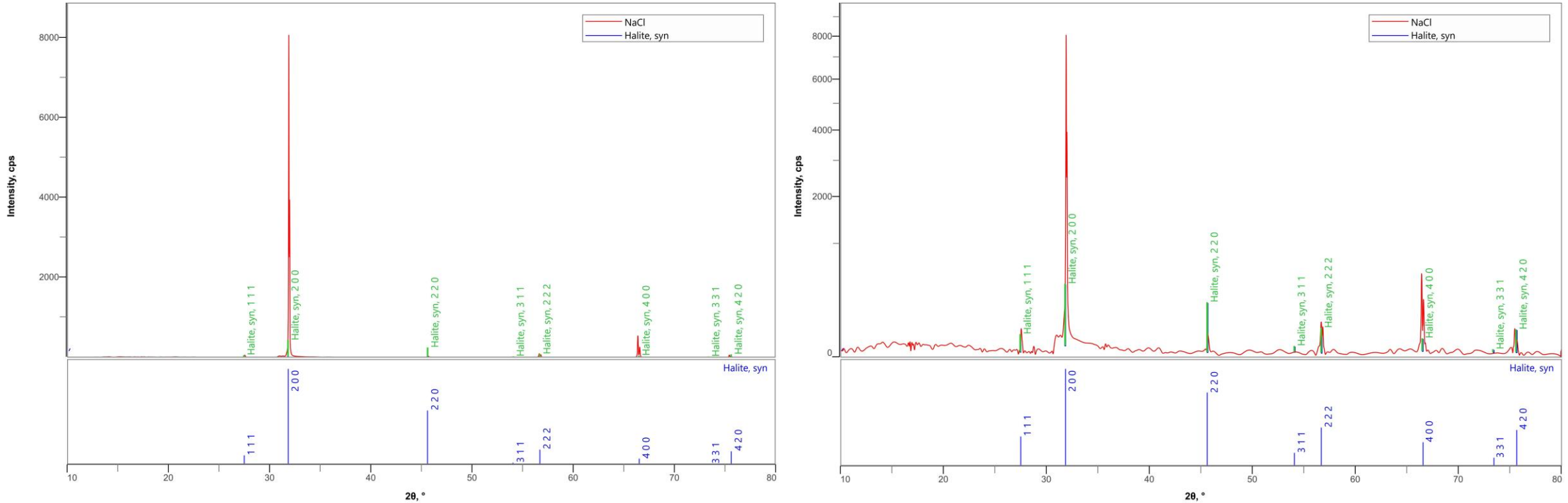
As-measured XRD pattern of NaCl using Cu-Kα radiation (λ = 1.54186 Å) with BB optics and D/teX Ultra 250 detector.

Peaks Searching and Matching (NaCl)

Qualitative Analysis Results

Phase name	Chemical formula	FOM	Phase reg. detail	Space Group	DB Card Number
Halite, syn	Na Cl	1.837	S/M:PDF-2 2026	225 : Fm-3m	01-088-2300

Phase Name	a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)
Halite, syn	5.61103	5.61103	5.61103	90.000	90.000	90.000



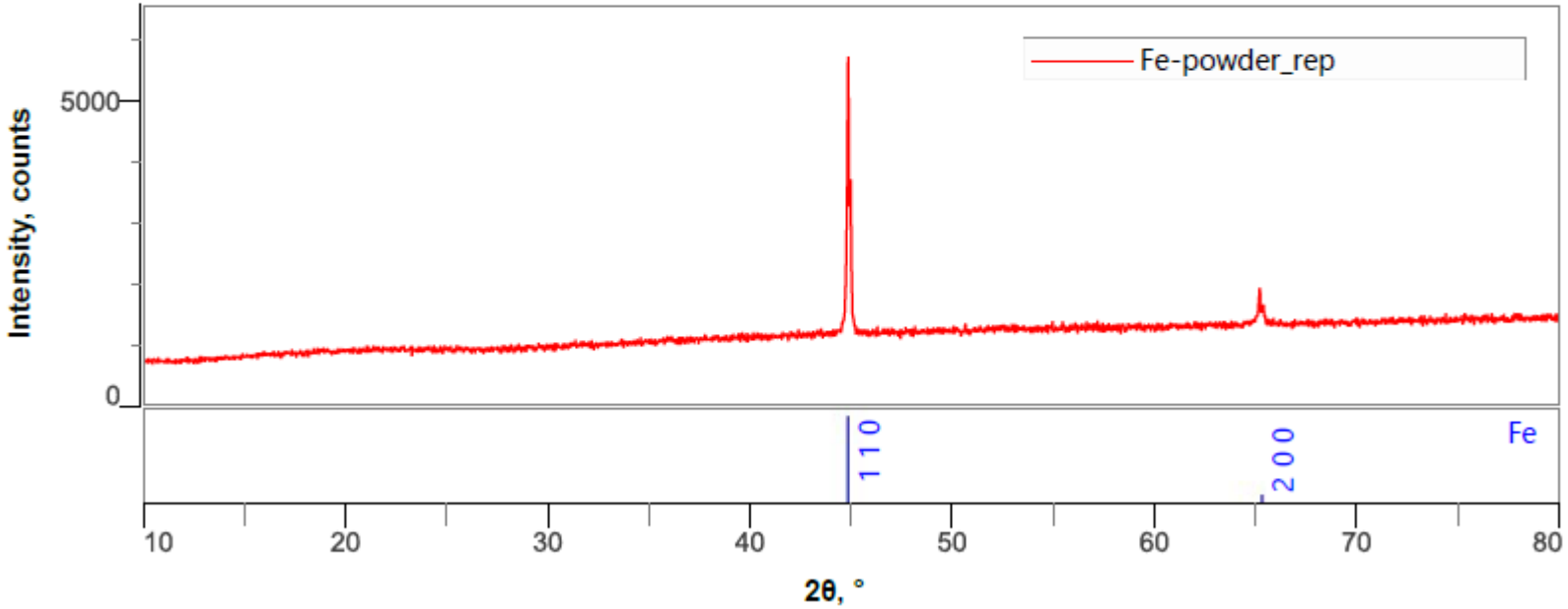
Peak matching of the NaCl XRD pattern: (a) linear scale and (b) square-root intensity scale to reveal weak peaks, confirming the Halite (Cubic) phase (PDF-2 No. 01-088-2300), cubic Fm-3m (No. 225; FOM = 1.837).

Peaks Searching and Matching (Fe)

Qualitative Analysis Results

Phase name	Chemical formula	FOM	Phase reg. detail	Space Group	DB Card Number
a-Fe	Fe	0.951	S/M:PDF-2 2026	229 : Im-3m	01-071-4648

Phase Data View



Phase Name	a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)
a-Fe	2.85665	2.85665	2.85665	90.000	90.000	90.000

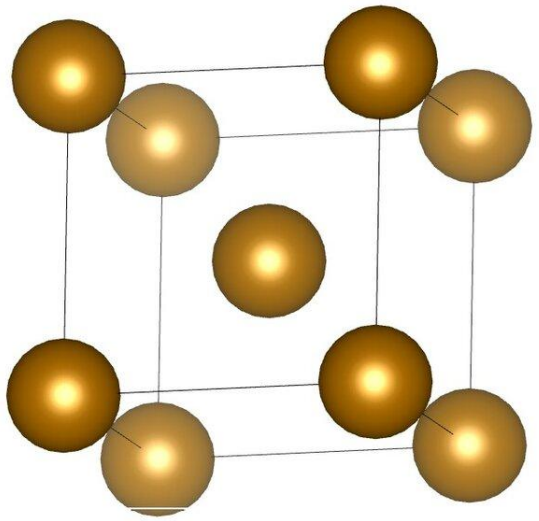


Fig: BCC Crystal Structure of Iron(Fe)

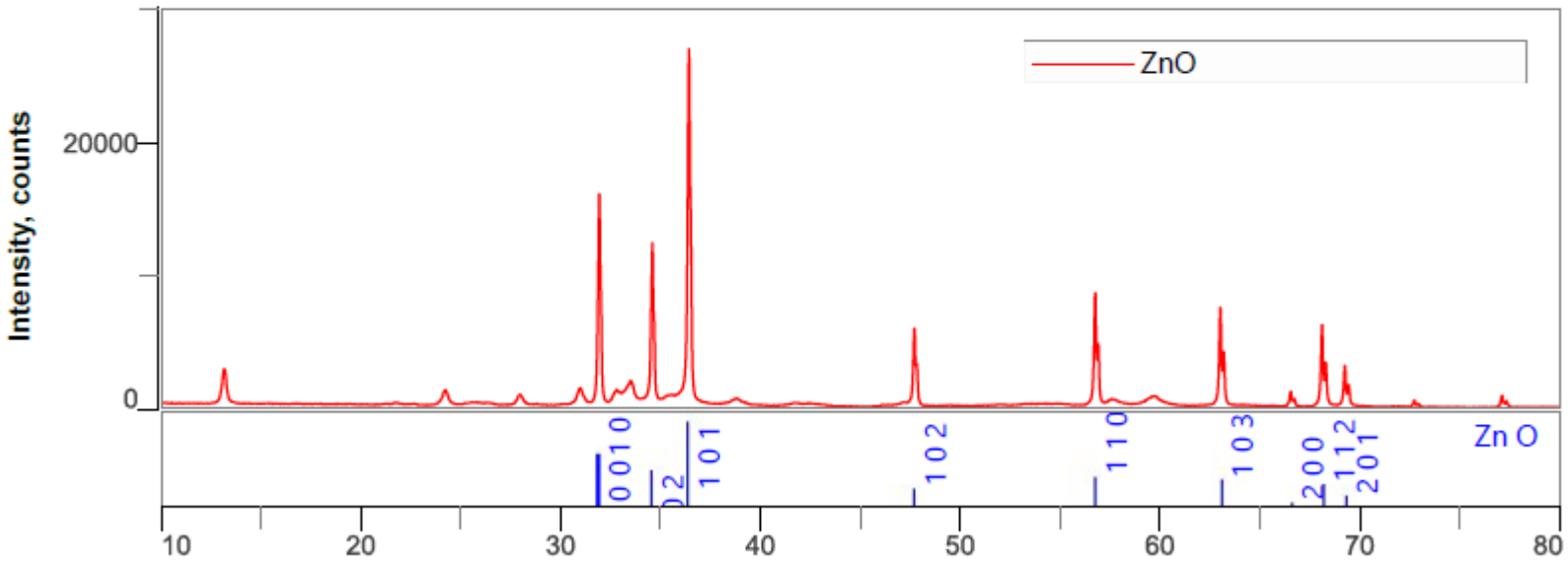
Peak matching of Fe powder confirming the α-Fe phase (PDF-2 No. 01-071-4648), cubic structure with space group Im-3m (No. 229), showing characteristic (110) and (200) reflections (FOM = 0.951).

Peaks Searching and Matching (ZnO)

Qualitative Analysis Results

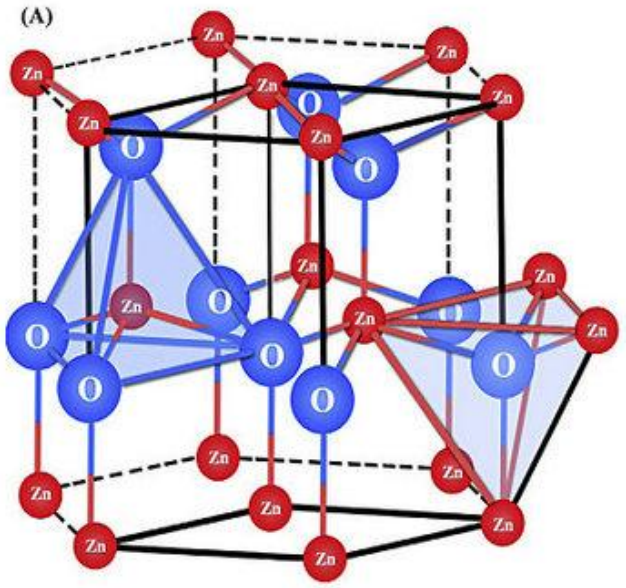
Phase name	Chemical formula	FOM	Phase reg. detail	Space Group	DB Card Number
Zinc Oxide	Zn O	0.595	S/M:PDF-2 2026	186 : P63mc	00-074-1112

Phase Data View



Lattice parameters

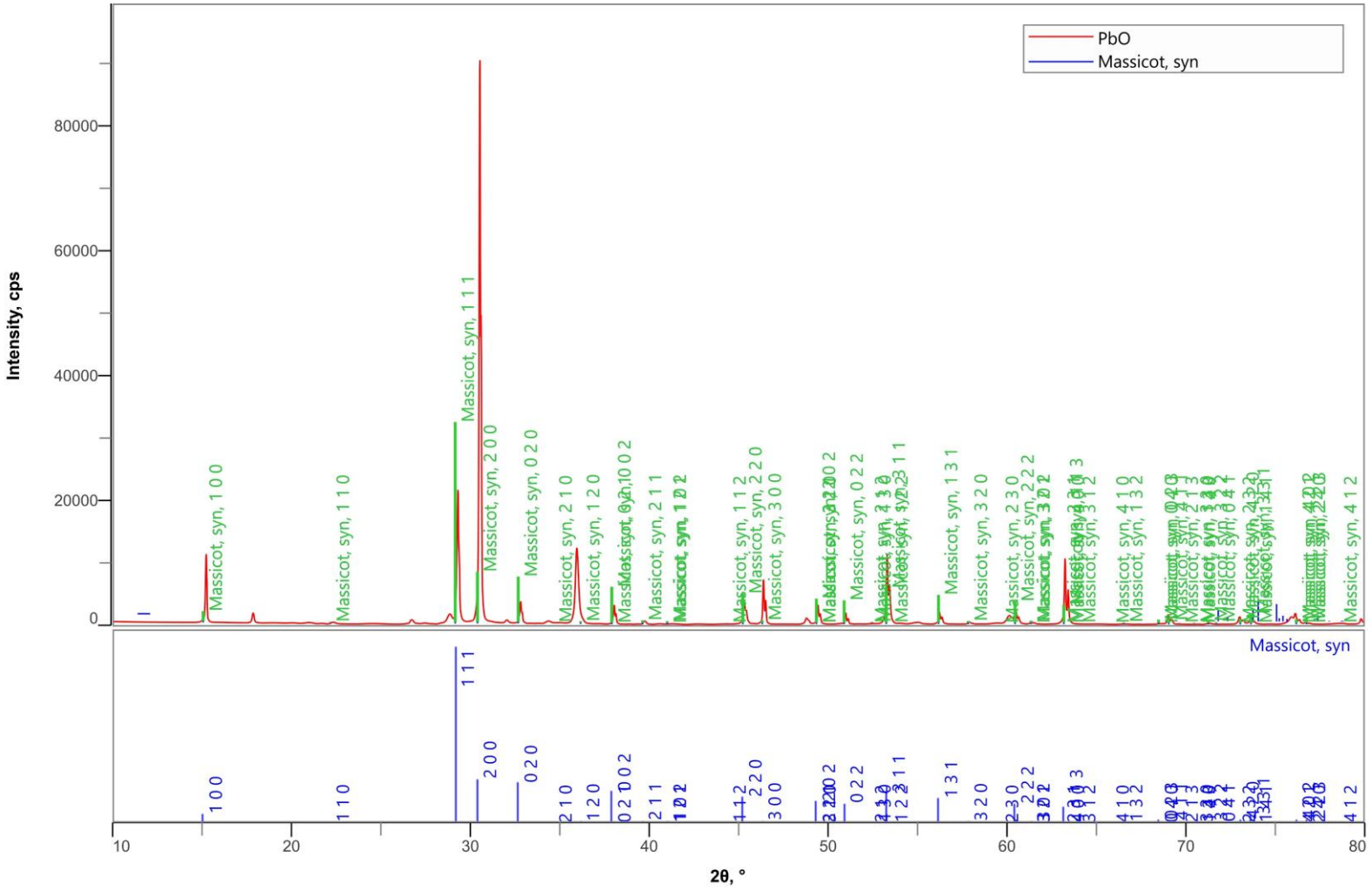
Phase name	a, Å	b, Å	c, Å	α, °	β, °	γ, °
Zinc Oxide	3.24183	3.24183	5.19262	90.000	90.000	120.000



Hexagonal wurtzite crystal structure of ZnO

Peak matching of ZnO powder shows the wurtzite Zinc Oxide phase (PDF-2 No. 00-074-1112, hexagonal $P6_3mc$, FOM = 0.595).

Peaks Searching and Matching (PbO)



Quantitative analysis

Peak matching of PbO powder shows the Massicot phase (PDF-2 No. 01-072-0093, orthorhombic Pbcm, FOM = 1.597)

Lattice parameters

a = 5.84867 Å, b = 5.44730 Å, c = 4.73643 Å,
α = β = γ = 90°.

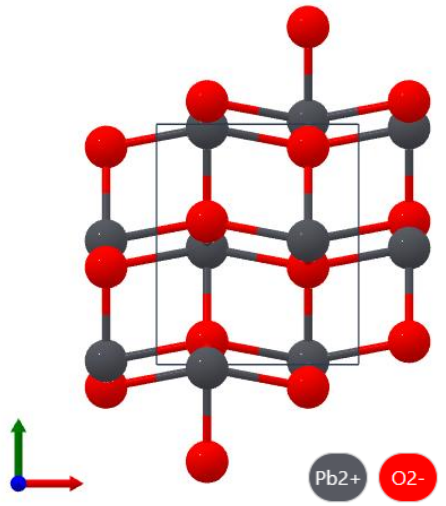
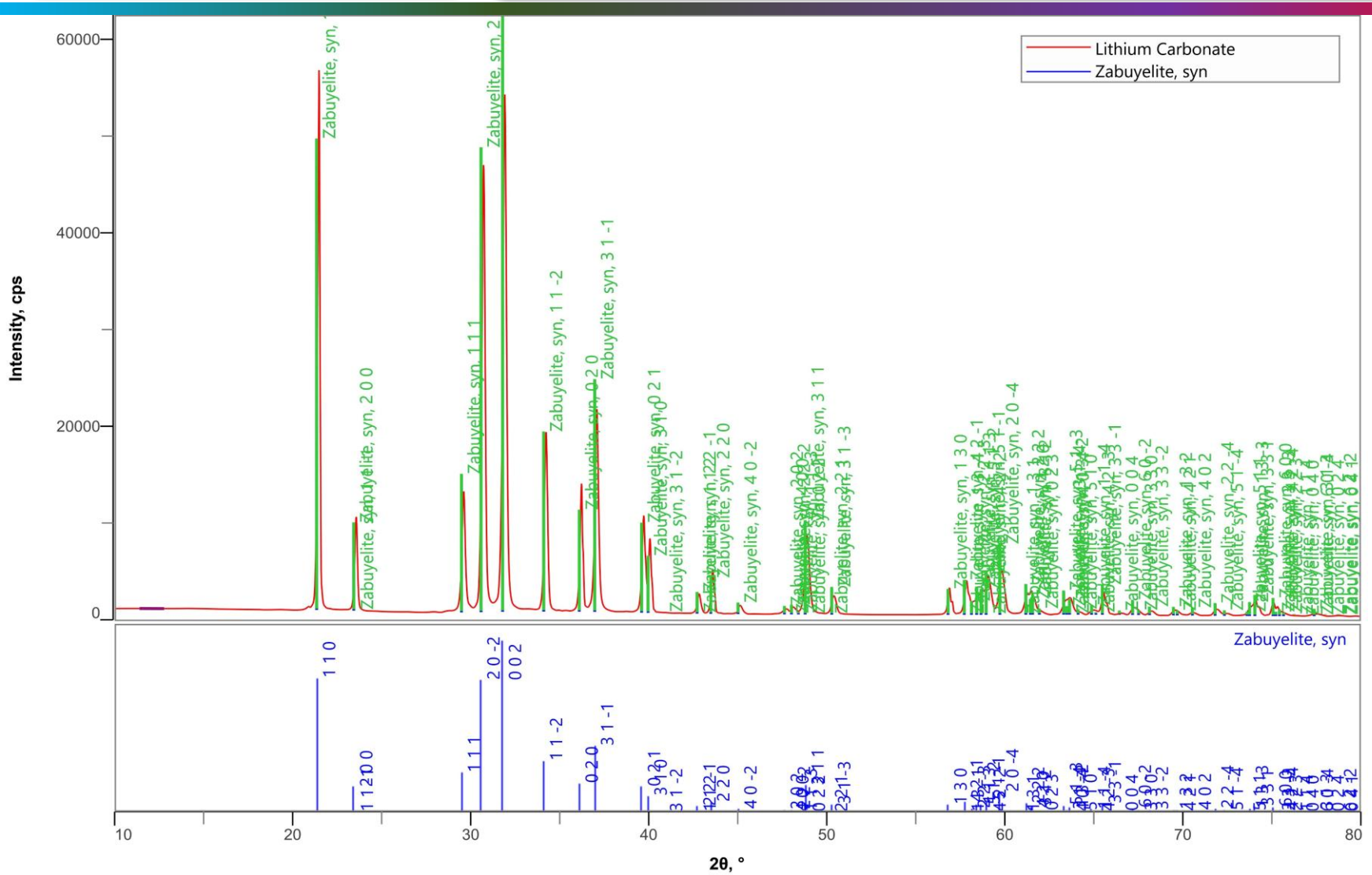


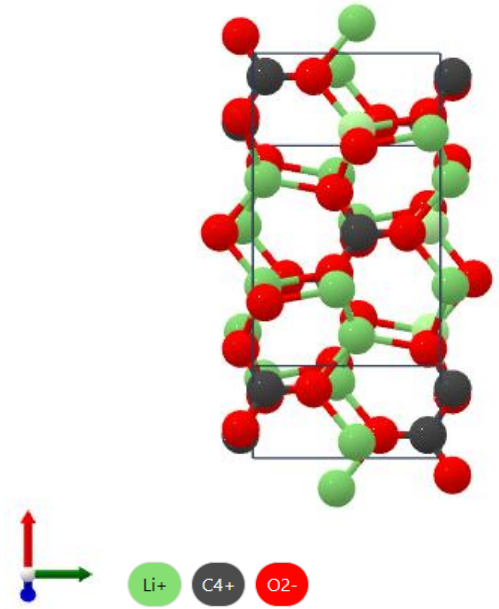
Fig: PbO crystallizes in the orthorhombic Pbcm structure.

Peaks Searching and Matching (Li2CO3)



Quantitative analysis

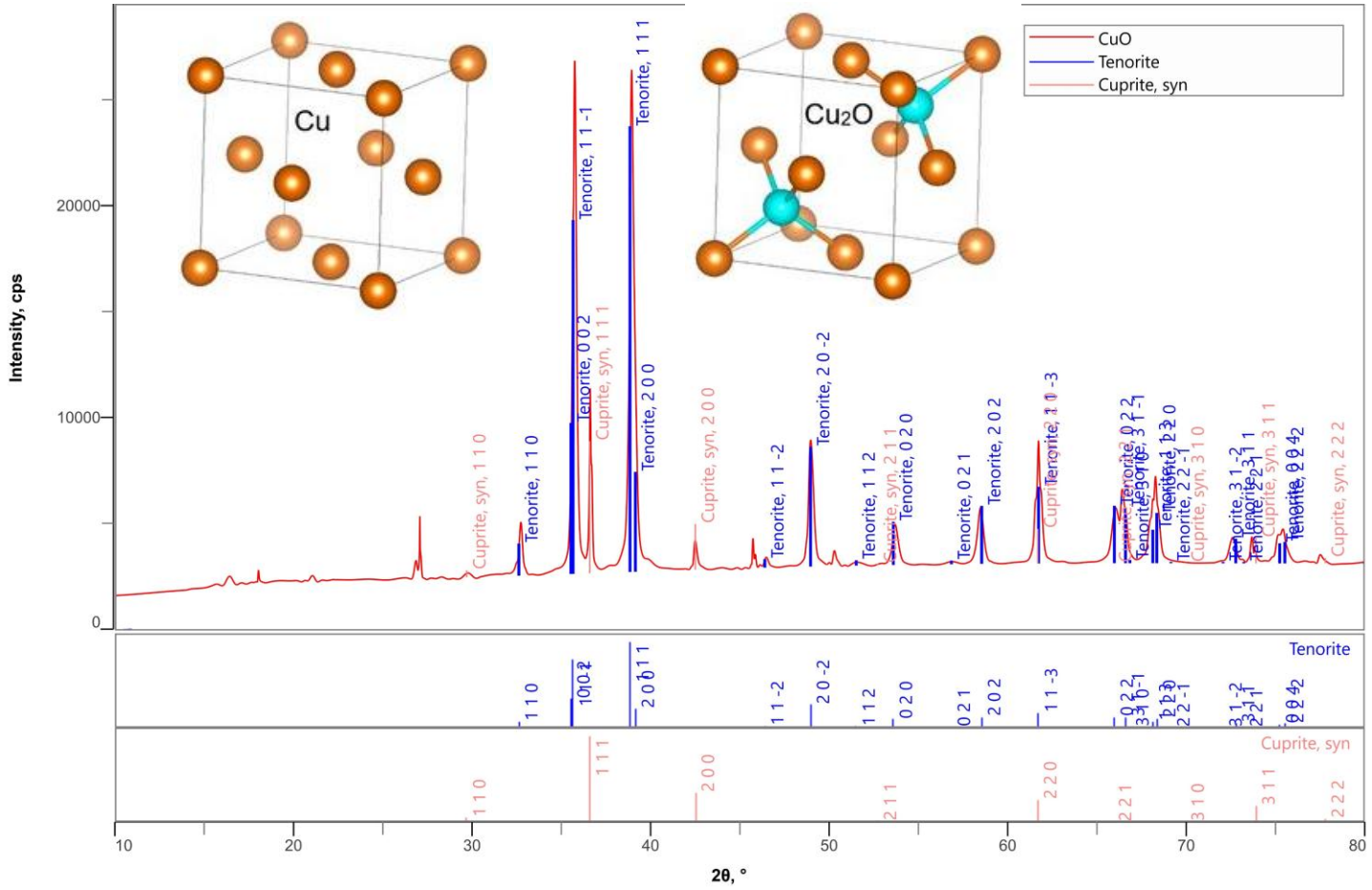
Li_2CO_3 powder shows the Zabuyelite phase (PDF-2 No. 01-083-1454, monoclinic C12/c1, FOM = 0.196



Lattice parameters

a = 8.36968 Å, b = 4.97868 Å,
c = 6.20520 Å, α = γ = 90°, β = 114.83°.

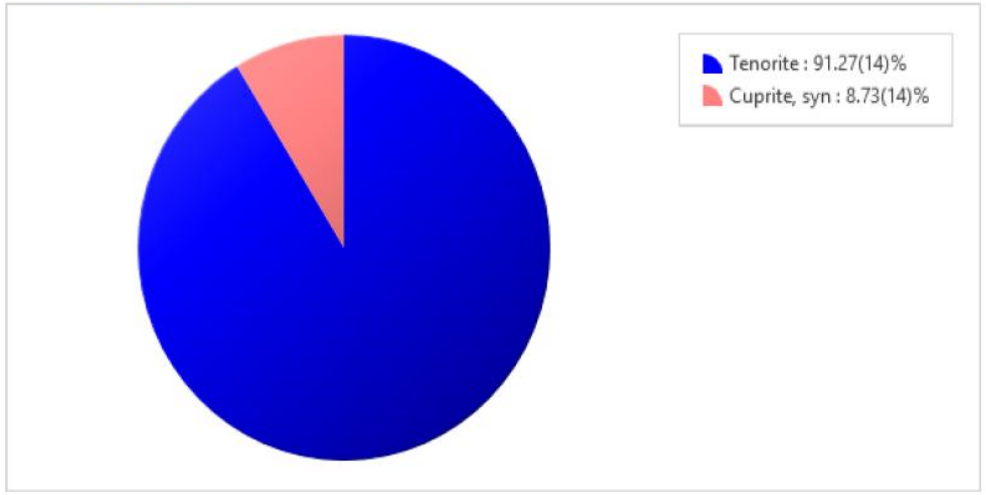
Peaks Searching and Matching (CuO)



Qualitative Analysis Results

Phase name	Chemical formula	FOM	Phase reg. detail	Space Group	DB Card Number
Tenorite	Cu O	0.545	S/M:PDF-2 2026	15 : C12/c1	01-073-6234
Cuprite, syn	Cu2 O	0.899	S/M:PDF-2 2026	224 : Pn-3m:2	01-071-4310

WPPF weight fraction



Lattice parameters

Phase name	a, Å	b, Å	c, Å	α, °	β, °	γ, °
Tenorite	4.6893(3)	3.42641(18)	5.1343(3)	90.000	99.447(2)	90.000
Cuprite, syn	4.2725(2)	4.2725(2)	4.2725(2)	90.000	90.000	90.000

Peak matching of CuO powder showing two phases: Tenorite (CuO, PDF-2 No. 01-073-6234, monoclinic C12/c1, FOM = 0.545) and Cuprite (Cu_2O, PDF-2 No. 01-071-4310, cubic Pn-3m, FOM = 0.899).

Conclusion

BB alignment XRD measurements were performed in θ–2θ geometry.

NaCl, α-Fe, and Li_2CO_3 peaks exactly matched the corresponding PDF database patterns.
All major peaks of ZnO and PbO were consistent with PDF references.

CuO sample showed two phases:
CuO: 91.27%
Cu_2O: 8.73%

Phase estimation was performed using SmartLab Studio II.