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Supporting information for article:

The influence of XRD pattern angular range on Rietveld refinement results used for quantitative analysis, crystallite size calculation and unit cell parameters refinement

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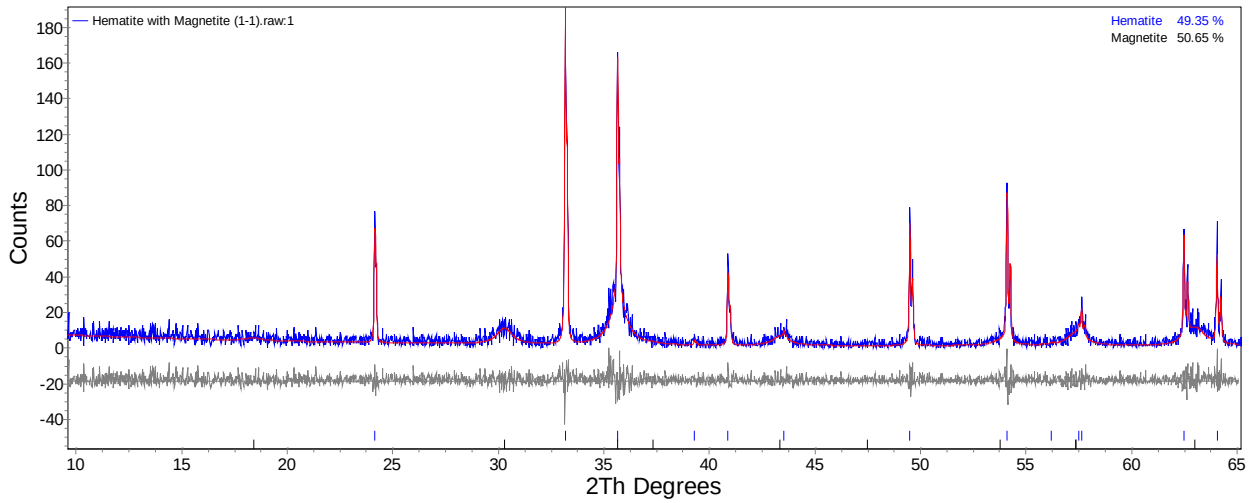
Examples of Rietveld refinement

1. Hematite-Magnetite (1:1) mixture

Parameters	Angular range at Rietveld refinement, 2θ°							
	10-65	10-70	10-75	10-80	10-90	10-100	10-110	10-120
Rwp	39.94	40.79	41.51	42.05	42.95	43.98	44.66	45.63
Hematite, %	51.05 (59)	50.78 (61)	51.03 (59)	51.08 (57)	51.10 (54)	51.44 (52)	51.44 (52)	51.49 (48)
a=b, Å	5.03249 (30)	5.03249 (28)	5.03250 (29)	5.03249 (27)	5.03243 (24)	5.03233 (23)	5.03219 (20)	5.03220 (19)
c, Å	13.7438 (11)	13.7442 (11)	13.74361 (91)	13.74363 (91)	13.74318 (82)	13.74272 (76)	13.74207 (72)	13.74242 (61)
d, nm	241 (49)	251 (38)	245 (36)	244 (36)	243 (34)	243 (33)	242 (33)	237 (30)
Magnetite, %	49.95 (59)	49.22 (61)	48.97 (59)	48.92 (57)	48.90 (54)	48.56 (52)	48.57 (49)	48.51 (48)
a=b=c, Å	8.3459 (24)	8.3445 (24)	8.3449 (24)	8.3449 (23)	8.3450 (23)	8.3458 (21)	8.3458 (21)	8.3452 (21)
d, nm	10.20 (50)	9.84 (45)	9.75 (44)	9.74 (43)	9.65 (42)	9.74 (41)	9.75 (40)	9.73 (40)



10-65

File 1 : Hematite with Magnetite (1-1).raw

R-Values

Rexp : 37.54 Rwp : 39.60 Rp : 28.84 GOF : 1.05
Rexp`: 48.88 Rwp`: 51.56 Rp` : 40.60 DW : 1.90

Quantitative Analysis - Rietveld

Phase 1 : Hematite		49.35(72) %
Phase 2 : Magnetite		50.65(72) %

Background

Chebychev polynomial, Coefficient	0	2.875(68)
	1	-2.67(11)
	2	1.437(96)
	3	-0.413(83)
	4	0.022(80)
	5	0.031(71)
	6	0.074(66)

Instrument

Primary radius (mm)	217.5
Secondary radius (mm)	217.5
Receiving slit width (mm)	0.2
Divergence angle (°)	1
Full Axial Convolution	
Filament Length (mm)	12
Sample Length (mm)	15
Receiving Slit Length (mm)	12
Primary Sollers (°)	2.3
Secondary Sollers (°)	2.3

Corrections

Specimen displacement	-0.0150(48)
LP Factor	26.4

Structure 1

Phase name	Hematite
R-Bragg	4.298
Space group	R-3cH
Scale	0.00000677(26)
Cell Mass	958.149
Cell Volume (Å^3)	301.462(36)
Wt% - Rietveld	49.35(72)
Crystallite Size	
k: 1 LVol-IB (nm)	245(23)
Crystal Density (g/cm^3)	5.27777(64)
Preferred Orientation Spherical Harmonics	
Order	4
y00	1
y20	-0.094(73)
y40	-0.109(87)
y43m	0.043(35)
Lattice parameters	
a (Å)	5.03266(23)
c (Å)	13.7438(11)

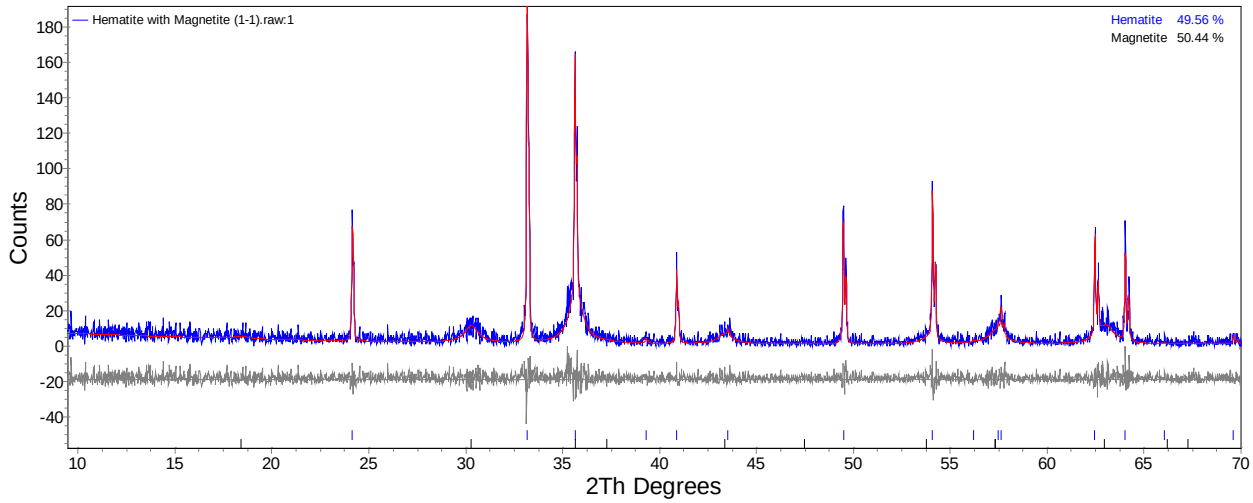
Site	Np	x	y	z	Atom	Occ	Beq
Fe1	12	0.00000	0.00000	0.35510	Fe+3	1	0.70(29)
O1	18	0.30400	0.00000	0.25000	O-2	1	1.17(54)

Structure 2

Phase name	Magnetite
R-Bragg	16.109
Space group	Fd-3mZ
Scale	0.00000212(13)

Cell Mass				1628.914		
Cell Volume (Å^3)				580.73(51)		
Crystallite Size						
k: 0.89 LVol-FWHM (nm)				9.81(49)		
Crystal Density (g/cm^3)				4.6577(41)		
Lattice parameters						
a (Å)				8.3431(25)		

Site	Np	x	y	z	Atom	Occ	Beq
Fe1	8	0.12500	0.12500	0.12500	Fe+3	0.9	0.35(65)
Fe2	16	0.50000	0.50000	0.50000	Fe+3	0.8	1.82(69)
O1	32	0.25600	0.25600	0.25600	O-2	1	1.00



10-70
File 1 : Hematite with Magnetite (1-1).raw

R-Values

Rexp : 38.59 Rwp : 40.53 Rp : 29.74 GOF : 1.05
Rexp`: 50.58 Rwp`: 53.13 Rp` : 42.13 DW : 1.90

Quantitative Analysis - Rietveld

Phase 1	: Hematite	49.56(71) %
Phase 2	: Magnetite	50.44(71) %

Background

Chebychev polynomial, Coefficient	0	2.816(55)
	1	-2.563(85)
	2	1.479(83)
	3	-0.475(75)
	4	0.039(73)
	5	0.049(67)
	6	0.021(63)

Instrument

Primary radius (mm)	217.5
Secondary radius (mm)	217.5
Receiving slit width (mm)	0.2
Divergence angle (°)	1

Full Axial Convolution	
Filament Length (mm)	12
Sample Length (mm)	15
Receiving Slit Length (mm)	12
Primary Sollers (°)	2.3
Secondary Sollers (°)	2.3

Corrections

Specimen displacement	-0.0160(47)
LP Factor	26.4

Structure 1

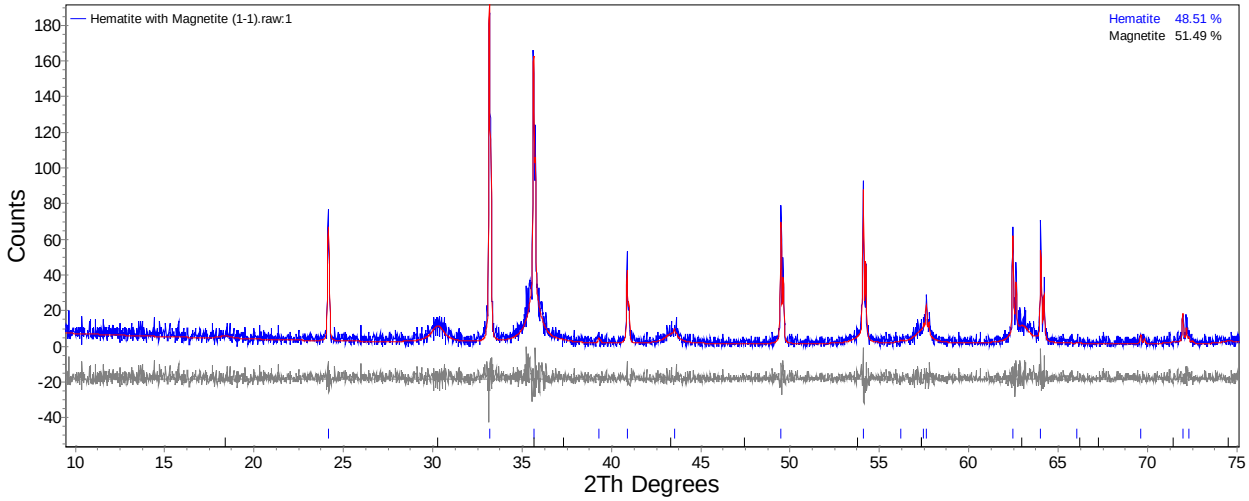
Phase name	Hematite
R-Bragg	4.514
Space group	R-3cH
Scale	0.00000680(26)
Cell Mass	958.149
Cell Volume (Å^3)	301.473(36)
Crystallite Size	
k: 1 LVol-IB (nm)	245(22)
Crystal Density (g/cm^3)	5.27758(63)
Preferred Orientation Spherical Harmonics	
Order	4
y00	1
y20	-0.100(73)
y40	-0.113(87)
y43m	0.041(35)
Lattice parameters	
a (Å)	5.03264(23)
c (Å)	13.7444(10)

Site	Np	x	y	z	Atom	Occ	Beq
Fe1	12	0.00000	0.00000	0.35510	Fe+3	1	0.76(28)
O1	18	0.30400	0.00000	0.25000	O-2	1	1.09(53)

Structure 2

Phase name	Magnetite
R-Bragg	16.294
Space group	Fd-3mZ
Scale	0.00000211(13)
Cell Mass	1628.914
Cell Volume (Å^3)	580.72(51)
Crystallite Size	
k: 0.89 LVol-FWHM (nm)	9.96(47)
Crystal Density (g/cm^3)	4.6578(41)
Lattice parameters	
a (Å)	8.3430(24)

Site	Np	x	y	z	Atom	Occ	Beq
Fe1	8	0.12500	0.12500	0.12500	Fe+3	0.9	0.38(64)
Fe2	16	0.50000	0.50000	0.50000	Fe+3	0.8	1.92(68)
O1	32	0.25600	0.25600	0.25600	O-2	1	1



10-75
File 1 : Hematite with Magnetite (1-1).raw

R-Values

Rexp : 39.32 Rwp : 41.25 Rp : 30.42 GOF : 1.05
Rexp`: 51.62  Rwp`: 54.15 Rp` : 43.06 DW : 1.90

Quantitative Analysis - Rietveld

Phase 1 : Hematite	48.51(71) %
Phase 2 : Magnetite	51.49(71) %

Background

Chebychev polynomial, Coefficient	0	2.726(57)
	1	-2.520(90)
	2	1.482(85)
	3	-0.588(70)
	4	0.046(69)
	5	0.054(62)
	6	0.009(61)

Instrument

Primary radius (mm)	217.5
Secondary radius (mm)	217.5
Receiving slit width (mm)	0.2
Divergence angle (°)	1
Full Axial Convolution	
Filament Length (mm)	12
Sample Length (mm)	15
Receiving Slit Length (mm)	12
Primary Sollers (°)	2.3
Secondary Sollers (°)	2.3

Corrections

Specimen displacement	-0.0150(45)
LP Factor	26.4

Structure 1

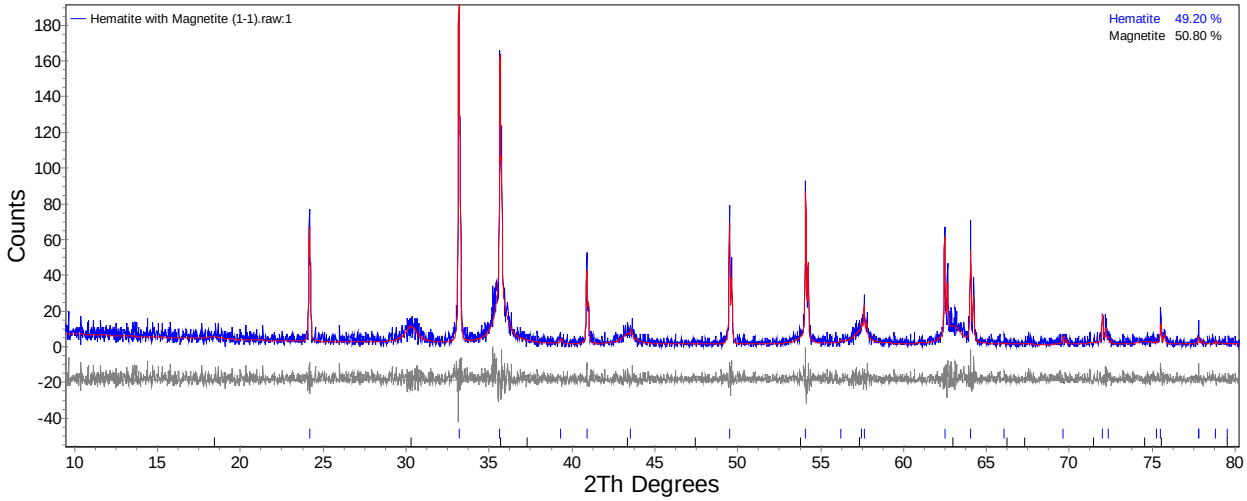
Phase name	Hematite
R-Bragg	5.634
Space group	R-3cH
Scale	0.00000680(25)
Cell Mass	958.149
Cell Volume (Å^3)	301.461(33)
Crystallite Size	
k: 1 LVol-IB (nm)	241(21)
Crystal Density (g/cm^3)	5.27778(58)
Preferred Orientation Spherical Harmonics	
Order	4
y00	1
y20	-0.036(51)
y40	-0.040(64)
y43m	0.024(32)
Lattice parameters	
a (Å)	5.03264(23)
c (Å)	13.74386(82)

Site	Np	x	y	z	Atom	Occ	Beq
Fe1	12	0.00000	0.00000	0.35510	Fe+3	1	0.68(27)
O1	18	0.30400	0.00000	0.25000	O-2	1	0.85(46)

Structure 2

Phase name	Magnetite
R-Bragg	17.096
Space group	Fd-3mZ
Scale	0.00000220(13)
Cell Mass	1628.914
Cell Volume (Å^3)	580.91(50)
Crystallite Size	
k: 0.89 LVol-FWHM (nm)	9.87(45)
Crystal Density (g/cm^3)	4.6563(40)
Lattice parameters	
a (Å)	8.3439(24)

Site	Np	x	y	z	Atom	Occ	Beq
Fe1	8	0.12500	0.12500	0.12500	Fe+3	0.9	0.94(59)
Fe2	16	0.50000	0.50000	0.50000	Fe+3	0.8	2.32(63)
O1	32	0.25600	0.25600	0.25600	O-2	1	1



10-80
File 1 : Hematite with Magnetite (1-1).raw

R-Values

Rexp : 40.08 Rwp : 41.86 Rp : 30.99 GOF : 1.04
Rexp`: 52.72  Rwp`: 55.06 Rp` : 43.90 DW : 1.89

Quantitative Analysis - Rietveld

Phase 1 : Hematite	49.20(66) %
Phase 2 : Magnetite	50.80(66) %

Background

Chebychev polynomial, Coefficient	0	2.685(51)
	1	-2.407(81)
	2	1.560(75)
	3	-0.595(67)
	4	0.132(65)
	5	0.086(57)
	6	-0.001(56)

Instrument

Primary radius (mm)	217.5
Secondary radius (mm)	217.5
Receiving slit width (mm)	0.2
Divergence angle (°)	1
Full Axial Convolution	
Filament Length (mm)	12
Sample Length (mm)	15
Receiving Slit Length (mm)	12
Primary Sollers (°)	2.3
Secondary Sollers (°)	2.3

Corrections

Specimen displacement	-0.0154(44)
LP Factor	26.4

Structure 1

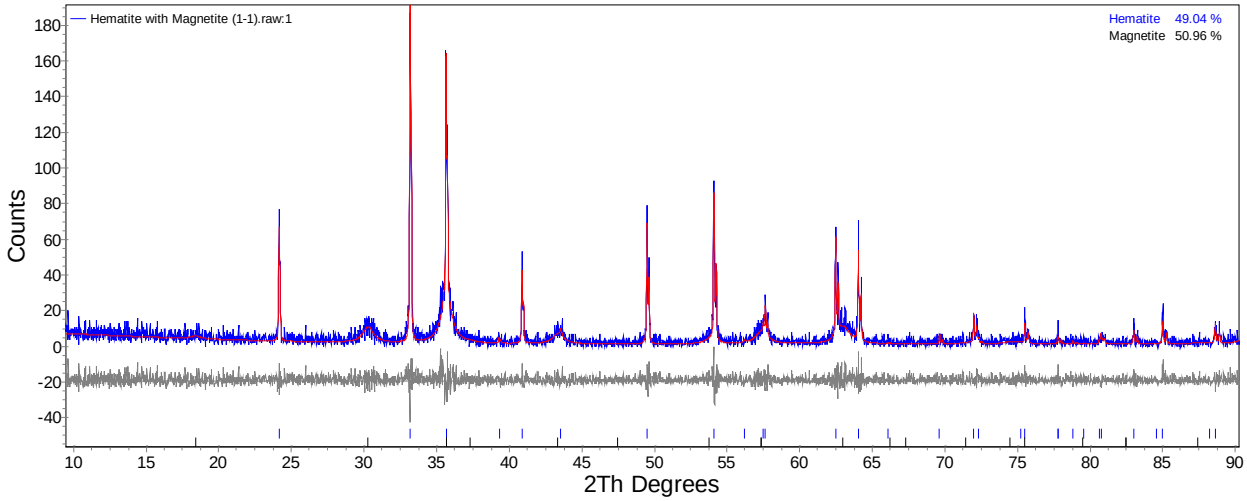
Phase name	Hematite
R-Bragg	5.634
Space group	R-3cH
Scale	0.00000689(24)
Cell Mass	958.149
Cell Volume (Å^3)	301.465(31)
Crystallite Size	
k: 1 LVol-IB (nm)	239(21)
Crystal Density (g/cm^3)	5.27771(55)
Preferred Orientation Spherical Harmonics	
Order	4
y00	1
y20	-0.036(49)
y40	-0.013(62)
y43m	0.022(31)
Lattice parameters	
a (Å)	5.03266(22)
c (Å)	13.74393(81)

Site	Np	x	y	z	Atom	Occ	Beq
Fe1	12	0.00000	0.00000	0.35510	Fe+3	1	0.76(23)
O1	18	0.30400	0.00000	0.25000	O-2	1	0.83(40)

Structure 2

Phase name	Magnetite
R-Bragg	17.229
Space group	Fd-3mZ
Scale	0.00000217(12)
Cell Mass	1628.914
Cell Volume (Å^3)	580.88(50)
Crystallite Size	
k: 0.89 LVol-FWHM (nm)	9.75(47)
Crystal Density (g/cm^3)	4.6566(40)
Lattice parameters	
a (Å)	8.3437(24)

Site	Np	x	y	z	Atom	Occ	Beq
Fe1	8	0.12500	0.12500	0.12500	Fe+3	0.9	0.90(50)
Fe2	16	0.50000	0.50000	0.50000	Fe+3	0.8	2.14(57)
O1	32	0.25600	0.25600	0.25600	O-2	1	1.00(89)



10-90
File 1 : Hematite with Magnetite (1-1).raw

R-Values

Rexp : 41.36 Rwp : 42.81 Rp : 31.97 GOF : 1.04
Rexp`: 54.61  Rwp`: 56.52 Rp` : 45.33 DW : 1.89

Quantitative Analysis - Rietveld

Phase 1 : Hematite	49.04(59) %
Phase 2 : Magnetite	50.96(59) %

Background

Chebychev polynomial, Coefficient	0	2.570(50)
	1	-2.309(81)
	2	1.558(73)
	3	-0.729(63)
	4	0.197(62)
	5	0.057(55)
	6	-0.040(51)

Instrument

Primary radius (mm)	217.5
Secondary radius (mm)	217.5
Receiving slit width (mm)	0.2
Divergence angle (°)	1
Full Axial Convolution	
Filament Length (mm)	12
Sample Length (mm)	15
Receiving Slit Length (mm)	12
Primary Sollers (°)	2.3
Secondary Sollers (°)	2.3

Corrections

Specimen displacement	-0.0138(40)
LP Factor	26.4

Structure 1

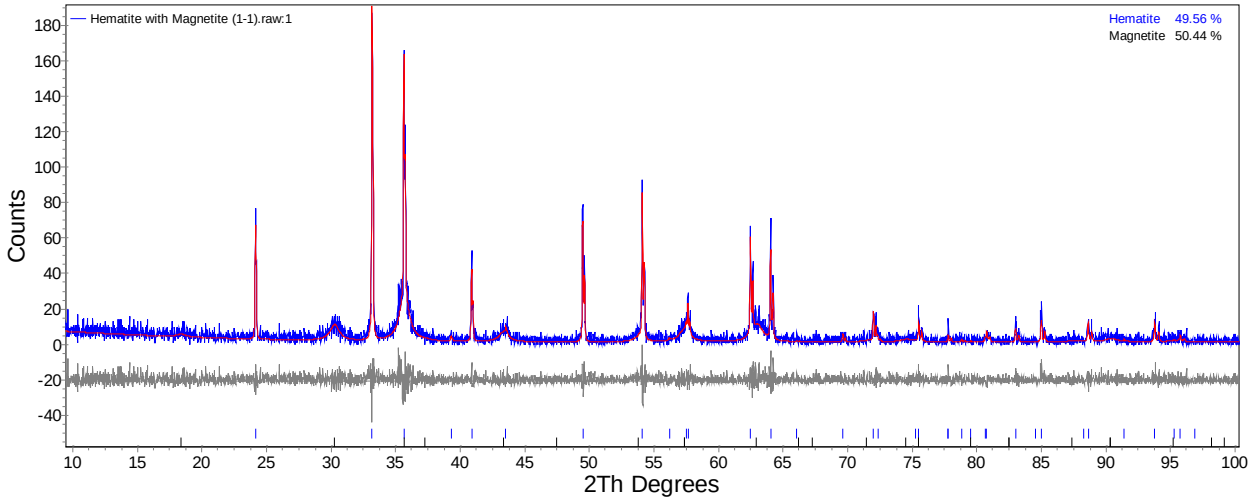
Phase name	Hematite
R-Bragg	6.654
Space group	R-3cH
Scale	0.00000690(21)
Cell Mass	958.149
Cell Volume (Å^3)	301.448(27)
Crystallite Size	
k: 1 LVol-IB (nm)	236(19)
Crystal Density (g/cm^3)	5.27801(48)
Preferred Orientation Spherical Harmonics	
Order	4
y00	1
y20	-0.041(47)
y40	-0.003(58)
y43m	0.018(30)
Lattice parameters	
a (Å)	5.03259(19)
c (Å)	13.74351(72)

Site	Np	x	y	z	Atom	Occ	Beq
Fe1	12	0.00000	0.00000	0.35510	Fe+3	1	0.74(17)
O1	18	0.30400	0.00000	0.25000	O-2	1	0.88(38)

Structure 2

Phase name	Magnetite
R-Bragg	18.039
Space group	Fd-3mZ
Scale	0.00000219(11)
Cell Mass	1628.914
Cell Volume (Å^3)	580.99(49)
Crystallite Size	
k: 0.89 LVol-FWHM (nm)	9.72(45)
Crystal Density (g/cm^3)	4.6556(39)
Lattice parameters	
a (Å)	8.3443(23)

Site	Np	x	y	z	Atom	Occ	Beq
Fe1	8	0.12500	0.12500	0.12500	Fe+3	0.9	1.24(52)
Fe2	16	0.50000	0.50000	0.50000	Fe+3	0.8	2.03(53)
O1	32	0.25600	0.25600	0.25600	O-2	1	0.81(78)



10-100
File 1 : Hematite with Magnetite (1-1).raw

R-Values

Rexp : 42.61 Rwp : 43.87 Rp : 33.06 GOF : 1.03
Rexp`: 56.54  Rwp`: 58.21 Rp` : 47.05 DW : 1.89

Quantitative Analysis - Rietveld

Phase 1 : Hematite	49.56(54) %
Phase 2 : Magnetite	50.44(54) %

Background

Chebychev polynomial, Coefficient	0	2.498(41)
	1	-2.217(68)
	2	1.576(64)
	3	-0.804(58)
	4	0.306(53)
	5	0.013(44)
	6	-0.031(47)

Instrument

Primary radius (mm)	217.5
Secondary radius (mm)	217.5
Receiving slit width (mm)	0.2
Divergence angle (°)	1
Full Axial Convolution	
Filament Length (mm)	12
Sample Length (mm)	15
Receiving Slit Length (mm)	12
Primary Sollers (°)	2.3
Secondary Sollers (°)	2.3

Corrections

Specimen displacement	-0.0113(37)
LP Factor	26.4

Structure 1

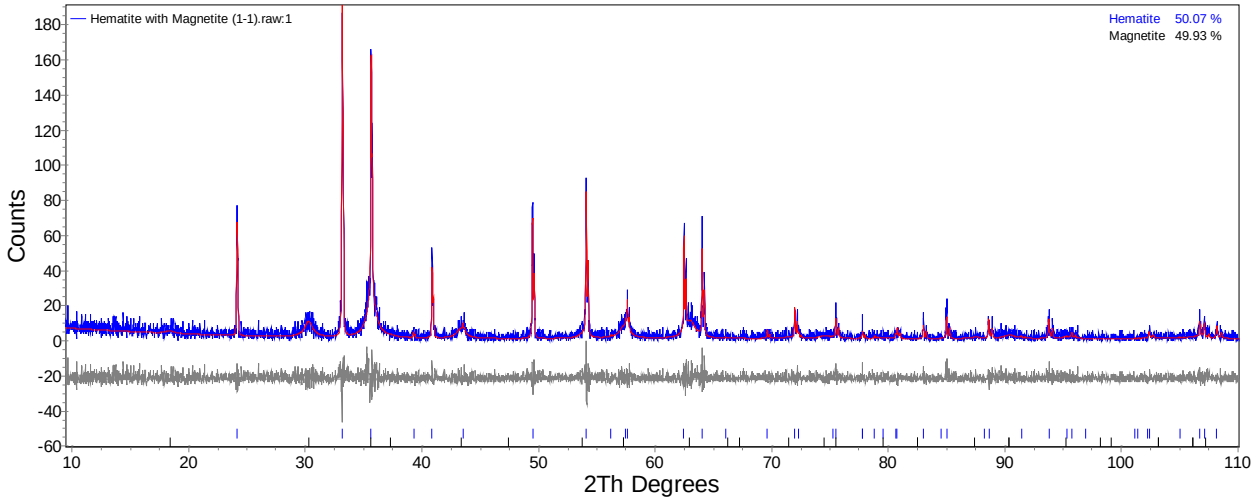
Phase name	Hematite
R-Bragg	7.274
Space group	R-3cH
Scale	0.00000693(20)
Cell Mass	958.149
Cell Volume (Å^3)	301.423(26)
Crystallite Size	
k: 1 LVol-IB (nm)	236(19)
Crystal Density (g/cm^3)	5.27845(45)
Preferred Orientation Spherical Harmonics	
Order	4
y00	1
y20	-0.039(46)
y40	-0.001(57)
y43m	0.013(30)
Lattice parameters	
a (Å)	5.03248(18)
c (Å)	13.74297(66)

Site	Np	x	y	z	Atom	Occ	Beq
Fe1	12	0.00000	0.00000	0.35510	Fe+3	1	0.79(15)
O1	18	0.30400	0.00000	0.25000	O-2	1	0.91(37)

Structure 2

Phase name	Magnetite
R-Bragg	18.225
Space group	Fd-3mZ
Scale	0.00000215(10)
Cell Mass	1628.914
Cell Volume (Å^3)	581.09(46)
Crystallite Size	
k: 0.89 LVol-FWHM (nm)	9.84(43)
Crystal Density (g/cm^3)	4.6548(37)
Lattice parameters	
a (Å)	8.3448(22)

Site	Np	x	y	z	Atom	Occ	Beq
Fe1	8	0.12500	0.12500	0.12500	Fe+3	0.9	1.10(43)
Fe2	16	0.50000	0.50000	0.50000	Fe+3	0.8	1.92(46)
O1	32	0.25600	0.25600	0.25600	O-2	1	0.84(75)



10-110
File 1 : Hematite with Magnetite (1-1).raw

R-Values

Rexp : 43.59 Rwp : 44.57 Rp : 33.85 GOF : 1.02
Rexp`: 58.04  Rwp`: 59.36 Rp` : 48.26 DW : 1.88

Quantitative Analysis - Rietveld

Phase 1 : Hematite	50.07(50) %
Phase 2 : Magnetite	49.93(50) %

Background

Chebychev polynomial, Coefficient	0	2.432(40)
	1	-2.125(65)
	2	1.581(61)
	3	-0.861(55)
	4	0.370(50)
	5	-0.052(41)
	6	-0.053(41)

Instrument

Primary radius (mm)	217.5
Secondary radius (mm)	217.5
Receiving slit width (mm)	0.2
Divergence angle (°)	1
Full Axial Convolution	
Filament Length (mm)	12
Sample Length (mm)	15
Receiving Slit Length (mm)	12
Primary Sollers (°)	2.3
Secondary Sollers (°)	2.3

Corrections

Specimen displacement	-0.0081(34)
LP Factor	26.4

Structure 1

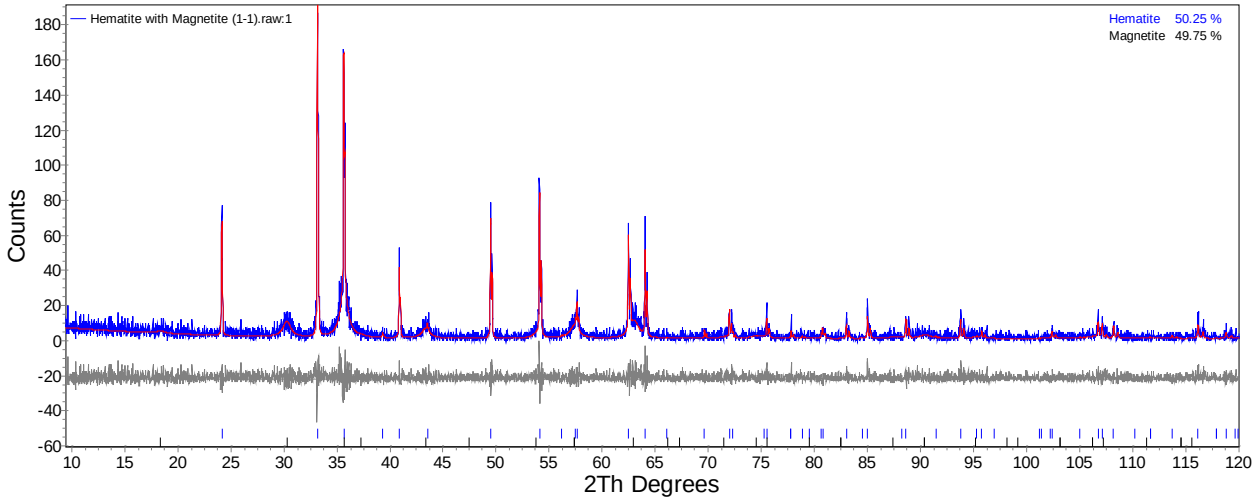
Phase name	Hematite
R-Bragg	7.911
Space group	R-3cH
Scale	0.00000697(18)
Cell Mass	958.149
Cell Volume (Å^3)	301.393(23)
Crystallite Size	
k: 1 LVol-IB (nm)	234(18)
Crystal Density (g/cm^3)	5.27898(40)
Preferred Orientation Spherical Harmonics	
Order	4
y00	1
y20	-0.027(45)
y40	0.010(55)
y43m	0.008(29)
Lattice parameters	
a (Å)	5.03234(15)
c (Å)	13.74241(62)

Site	Np	x	y	z	Atom	Occ	Beq
Fe1	12	0.00000	0.00000	0.35510	Fe+3	1	0.82(13)
O1	18	0.30400	0.00000	0.25000	O-2	1	1.03(36)

Structure 2

Phase name	Magnetite
R-Bragg	18.593
Space group	Fd-3mZ
Scale	0.000002121(91)
Cell Mass	1628.914
Cell Volume (Å^3)	580.99(45)
Crystallite Size	
k: 0.89 LVol-FWHM (nm)	9.83(43)
Crystal Density (g/cm^3)	4.6556(36)
Lattice parameters	
a (Å)	8.3443(22)

Site	Np	x	y	z	Atom	Occ	Beq
Fe1	8	0.12500	0.12500	0.12500	Fe+3	0.9	1.03(39)
Fe2	16	0.50000	0.50000	0.50000	Fe+3	0.8	1.72(41)
O1	32	0.25600	0.25600	0.25600	O-2	1	0.88(71)



10-120
File 1 : Hematite with Magnetite (1-1).raw

R-Values

Rexp : 44.66 Rwp : 45.51 Rp : 34.81 GOF : 1.02
Rexp`: 59.72  Rwp`: 60.84 Rp` : 49.77 DW : 1.88

Quantitative Analysis - Rietveld

Phase 1 : Hematite	50.25(48) %
Phase 2 : Magnetite	49.75(48) %

Background

Chebychev polynomial, Coefficient	0	2.365(37)
	1	-2.082(59)
	2	1.550(58)
	3	-0.943(53)
	4	0.420(47)
	5	-0.130(39)
	6	-0.035(37)

Instrument

Primary radius (mm)	217.5
Secondary radius (mm)	217.5
Receiving slit width (mm)	0.2
Divergence angle (°)	1
Full Axial Convolution	
Filament Length (mm)	12
Sample Length (mm)	15
Receiving Slit Length (mm)	12
Primary Sollers (°)	2.3
Secondary Sollers (°)	2.3

Corrections

Specimen displacement	-0.0089(32)
LP Factor	26.4

Structure 1

Phase name	Hematite
R-Bragg	8.801
Space group	R-3cH
Scale	0.00000700(18)
Cell Mass	958.149
Cell Volume (Å^3)	301.399(21)
Crystallite Size	
k: 1 LVol-IB (nm)	232(18)
Crystal Density (g/cm^3)	5.27886(38)
Preferred Orientation Spherical Harmonics	
Order	4
y00	1
y20	-0.067(44)
y40	-0.035(54)
y43m	0.015(29)
Lattice parameters	
a (Å)	5.03234(15)
c (Å)	13.74270(55)

Site	Np	x	y	z	Atom	Occ	Beq
Fe1	12	0.00000	0.00000	0.35510	Fe+3	1	0.87(11)
O1	18	0.30400	0.00000	0.25000	O-2	1	1.20(34)

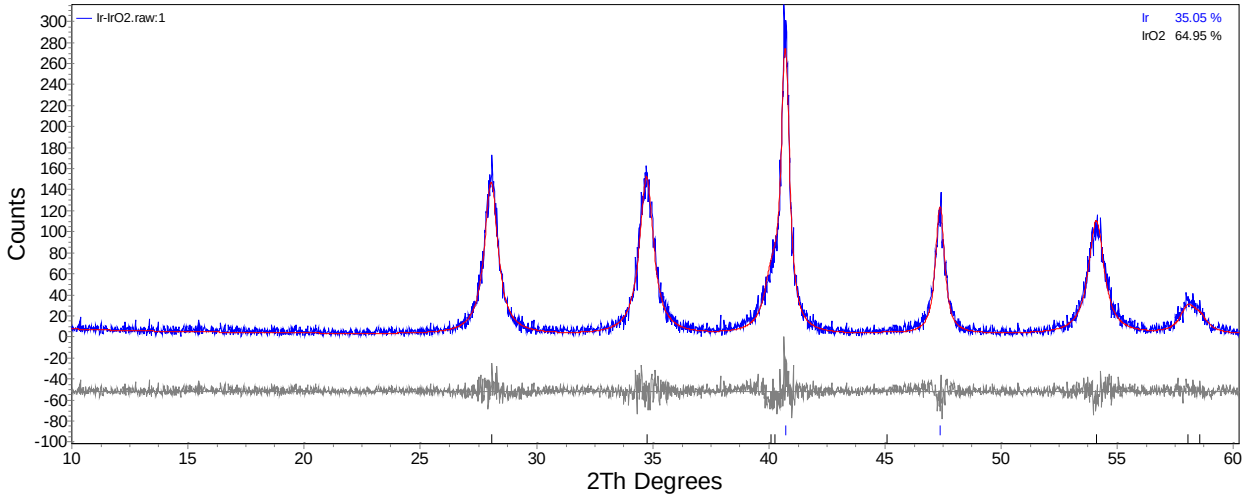
Structure 2

Phase name	Magnetite
R-Bragg	18.822
Space group	Fd-3mZ
Scale	0.000002114(89)
Cell Mass	1628.914
Cell Volume (Å^3)	580.91(45)
Crystallite Size	
k: 0.89 LVol-FWHM (nm)	9.82(43)
Crystal Density (g/cm^3)	4.6563(36)
Lattice parameters	
a (Å)	8.3439(21)

Site	Np	x	y	z	Atom	Occ	Beq
Fe1	8	0.12500	0.12500	0.12500	Fe+3	0.9	0.76(35)
Fe2	16	0.50000	0.50000	0.50000	Fe+3	0.8	1.90(41)
O1	32	0.25600	0.25600	0.25600	O-2	1	0.93(70)

2. Ir-IrO2 (1:2)

Parameter	Angular range at Rietveld refinement, 2θ°							
	10-60	10-70	10-80	10-85	10-90	10-100	10-110	10-120
Rwp	25.48	25.71	27.04	26.56	26.87	27.53	28.60	29.39
Iridium oxide,%	64.9 1.9	65.5 1.6	65.89 0.83	64.9 1.9	67.0 1.5	67.2 1.2	66.6 1.1	67.0 1.0
a=b, Å	4.4921 0.0017	4.4951 0.00020	4.4939 0.0017	4.4941 0.0017	4.4940 0.0012	4.4948 0.0010	4.49503 0.00093	4.49505 0.00087
c, Å	3.1507 0.0014	3.1520 0.0016	3.1511 0.0013	3.1512 0.0014	3.1510 0.0011	3.15089 0.00095	3.15063 0.00087	3.15068 0.00069
d, nm	12.22 0.24	12.12 0.20	11.99 0.20	12.09 0.19	11.98 0.18	11.87 0.17	11.87 0.17	11.84 0.17
Iridium,%	35.1 1.9	34.5 1.6	34.11 0.83	35.1 1.9	33.0 1.5	32.8 1.2	33.4 1.1	33.0 1.0
a=b=c, Å	3.8346 0.0014	3.8372 0.0017	3.8367 0.0017	3.8369 0.0015	3.83648 0.00094	3.83668 0.00057	3.83652 0.00077	3.83658 0.00069
d, nm	22.95 0.88	22.45 0.77	21.80 0.69	20.67 0.52	21.61 0.56	21.46 0.54	21.50 0.52	21.46 0.54



10-60

File 1 : " Ir-IrO2.raw"

R-Values

```
Rexp : 22.60    Rwp : 25.48     Rp  : 16.80  GOF : 1.13
Rexp`: 24.76    Rwp`: 27.91     Rp` : 18.86  DW  : 1.89
```

Quantitative Analysis - Rietveld

```
   Phase 1  : Ir                              35.1(19) %
   Phase 2  : IrO2                            64.9(19) %
```

Background

```
   Chebychev polynomial, Coefficient  0       2.89(11)
                                      1       -2.18(15)
                                      2       1.68(14)
                                      3       -0.67(11)
```

4	-0.10(11)
5	0.05(11)
6	0.26(11)

Instrument

Primary radius (mm)	217.5
Secondary radius (mm)	217.5
Receiving slit width (mm)	0.2
Divergence angle (°)	1
Full Axial Convolution	
Filament Length (mm)	12
Sample Length (mm)	15
Receiving Slit Length (mm)	12
Primary Sollers (°)	2.3
Secondary Sollers (°)	2.3

Corrections

Specimen displacement	0.008(36)
LP Factor	26.4
Surface Roughness Pitschke et al	0.0780(69)

Structure 1

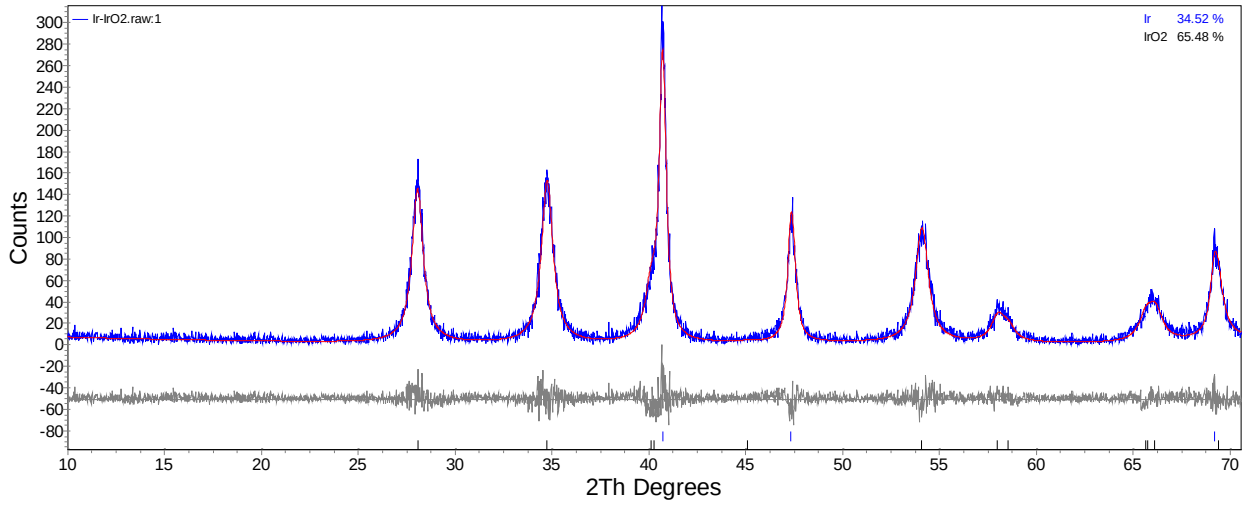
Phase name	Ir
R-Bragg	3.639
Space group	Fm-3m
Scale	0.0000402(34)
Cell Mass	768.885
Cell Volume (Å^3)	56.387(63)
Crystallite Size	
k: 0.89 LVol-FWHM (nm)	22.95(88)
Crystal Density (g/cm^3)	22.643(25)
Preferred Orientation Spherical Harmonics	
Order	2
k00	1
Lattice parameters	
a (Å)	3.8346(14)

Site	Np	x	y	z	Atom	Occ	Beq
Ir1	4	0.00000	0.00000	0.00000	Ir	1	1.34(71)

Structure 2

Phase name	IrO2
R-Bragg	4.912
Space group	P42/mnm
Scale	0.0001134(30)
Cell Mass	448.440
Cell Volume (Å^3)	63.580(55)
Crystallite Size	
k: 0.89 LVol-FWHM (nm)	12.22(24)
Crystal Density (g/cm^3)	11.712(10)
Preferred Orientation Spherical Harmonics	
Order	2
y00	1
y20	0.02942391
Lattice parameters	
a (Å)	4.4921(17)
c (Å)	3.1507(14)

Site	Np	x	y	z	Atom	Occ	Beq
Ir1	2	0.00000	0.00000	0.00000	Ir+4	1	0.5
O1	4	0.30800	0.30800	0.00000	O-2	1	0.5



10-70

File 1 “Ir-IrO2.raw"

R-Values

Rexp : 22.81 Rwp : 25.55 Rp : 17.10 GOF : 1.12
Rexp`: 25.16  Rwp`: 28.18 Rp` : 19.28 DW : 1.87

Quantitative Analysis - Rietveld

Phase 1 : Ir	34.5(16) %
Phase 2 : IrO2	65.5(16) %

Background

Chebychev polynomial, Coefficient	0	3.23(12)
	1	-1.03(19)
	2	2.52(18)
	3	-0.06(14)
	4	0.69(13)
	5	0.64(10)
	6	0.29(10)

Instrument

Primary radius (mm)	217.5
Secondary radius (mm)	217.5
Receiving slit width (mm)	0.2
Divergence angle (°)	1
Full Axial Convolution	
Filament Length (mm)	12
Sample Length (mm)	15
Receiving Slit Length (mm)	12
Primary Sollers (°)	2.3
Secondary Sollers (°)	2.3

Corrections

Specimen displacement	-0.010(26)
LP Factor	26.4
Surface Roughness Pitschke et al	0.091(17)

Structure 1

Phase name	Ir
R-Bragg	3.590
Space group	Fm-3m
Scale	0.0000431(30)

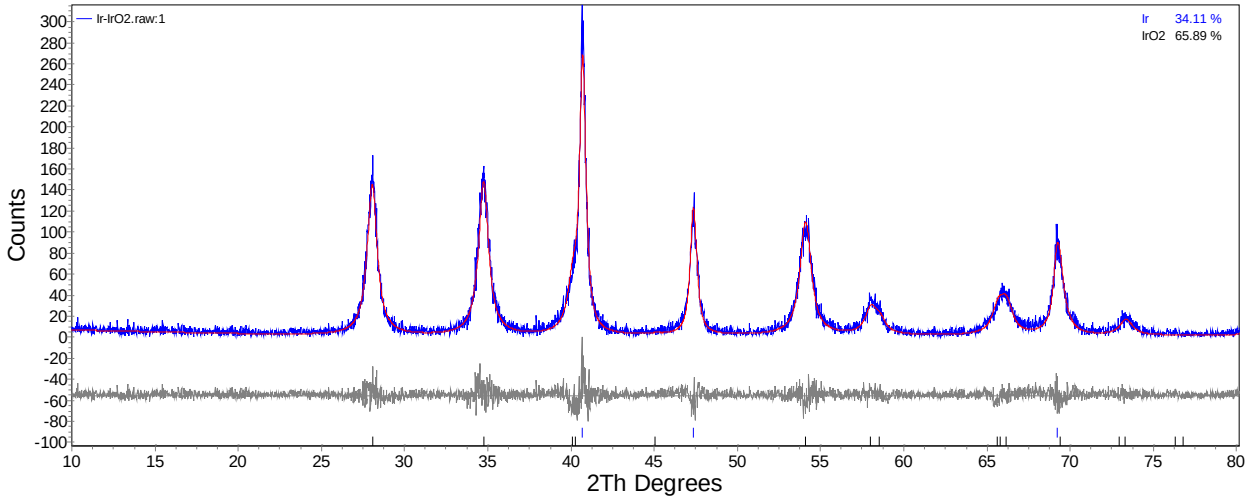
Cell Mass	768.885
Cell Volume (Å^3)	56.500(75)
Crystallite Size	
k: 0.89 LVol-FWHM (nm)	22.45(77)
Crystal Density (g/cm^3)	22.597(30)
Preferred Orientation Spherical Harmonics	
Order	2
k00	1
Lattice parameters	
a (Å)	3.8372(17)

Site	Np	x	y	z	Atom	Occ	Beq
Ir1	4	0.00000	0.00000	0.00000	Ir	1	1.60(29)

Structure 2

Phase name	IrO2
R-Bragg	5.161
Space group	P42/mnm
Scale	0.000124(13)
Cell Mass	448.440
Cell Volume (Å^3)	63.688(64)
Crystallite Size	
k: 0.89 LVol-FWHM (nm)	12.12(20)
Crystal Density (g/cm^3)	11.692(12)
Preferred Orientation Spherical Harmonics	
Order	2
y00	1
y20	0.03554592
Lattice parameters	
a (Å)	4.4951(20)
c (Å)	3.1520(16)

Site	Np	x	y	z	Atom	Occ	Beq
Ir1	2	0.00000	0.00000	0.00000	Ir+4	1	1.01(41)
O1	4	0.30800	0.30800	0.00000	O-2	1	0.5



10-80

File 1 : " Ir-IrO2.raw"

R-Values

Rexp : 23.98 Rwp : 27.04 Rp : 18.21 GOF : 1.13
Rexp`: 26.31  Rwp`: 29.67 Rp` : 20.42 DW : 1.87

Quantitative Analysis - Rietveld

Phase 1 : Ir	34.11(83) %
Phase 2 : IrO2	65.89(83) %

Background

Chebychev polynomial, Coefficient	0	2.661(72)
	1	-1.738(91)
	2	1.76(10)
	3	-0.698(86)
	4	0.382(85)
	5	0.267(84)
	6	-0.072(77)

Instrument

Primary radius (mm)	217.5
Secondary radius (mm)	217.5
Receiving slit width (mm)	0.2
Divergence angle (°)	1
Full Axial Convolution	
Filament Length (mm)	12
Sample Length (mm)	15
Receiving Slit Length (mm)	12
Primary Sollers (°)	2.3
Secondary Sollers (°)	2.3

Corrections

Specimen displacement	0.003(26)
LP Factor	26.4
Surface Roughness Pitschke et al	0.0804(51)

Structure 1

Phase name	Ir
R-Bragg	4.000
Spacegroup	Fm-3m
Scale	0.0000387(14)
Cell Mass	768.885

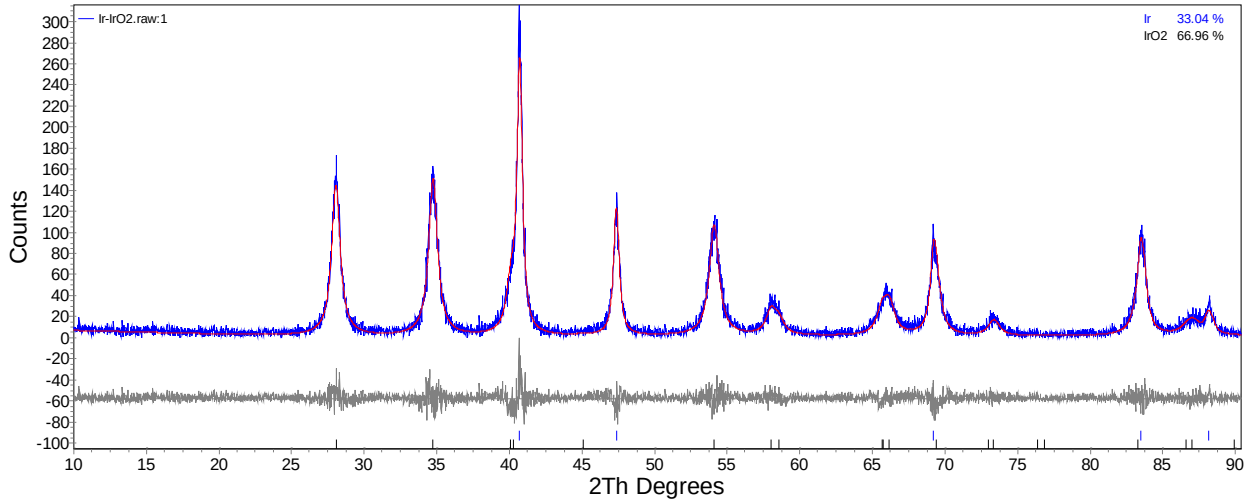
Cell Volume (Å^3)	56.478(73)
Crystallite Size	
k: 0.89 LVol-FWHM (nm)	21.80(69)
Crystal Density (g/cm^3)	22.606(29)
Preferred Orientation Spherical Harmonics	
Order	2
k00	1
Lattice parameters	
a (Å)	3.8367(17)

Site	Np	x	y	z	Atom	Occ	Beq
Ir1	4	0.00000	0.00000	0.00000	Ir	1	0.85(21)

Structure 2

Phase name	IrO2
R-Bragg	5.747
Spacegroup	P42/mnm
Scale	0.0001125(82)
Cell Mass	448.440
Cell Volume (Å^3)	63.638(55)
Wt% - Rietveld	65.8(19)
Crystallite Size	
k: 0.89 LVol-FWHM (nm)	11.99(20)
Crystal Linear Absorption Coeff. (1/cm)	1919.5(17)
Crystal Density (g/cm^3)	11.701(10)
Lattice parameters	
a (Å)	4.4939(17)
c (Å)	3.1511(13)

Site	Np	x	y	z	Atom	Occ	Beq
Ir1	2	0.00000	0.00000	0.00000	Ir+4	1	0.45(28)
O1	4	0.30800	0.30800	0.00000	O-2	1	0.5



10-90

File 1 : "Ir-IrO2.raw"

R-Values

Rexp : 23.99 Rwp : 26.87 Rp : 18.16 GOF : 1.12
Rexp`: 26.33  Rwp`: 29.49 Rp` : 20.31 DW : 1.88

Quantitative Analysis - Rietveld

Phase 1 : Ir	33.0(15) %
Phase 2 : IrO2	67.0(15) %

Background

Chebychev polynomial, Coefficient	0	2.547(72)
	1	-1.69(10)
	2	1.63(10)
	3	-0.886(85)
	4	0.398(76)
	5	0.060(73)
	6	-0.241(80)

Instrument

Primary radius (mm)	217.5
Secondary radius (mm)	217.5
Receiving slit width (mm)	0.2
Divergence angle (°)	1
Full Axial Convolution	
Filament Length (mm)	12
Sample Length (mm)	15
Receiving Slit Length (mm)	12
Primary Sollers (°)	2.3
Secondary Sollers (°)	2.3

Corrections

Specimen displacement	0.008(25)
LP Factor	26.4
Surface Roughness Pitschke et al	0.072(12)

Structure 1

Phase name	Ir
R-Bragg	4.281
Spacegroup	Fm-3m
Scale	0.0000361(14)
Cell Mass	768.885

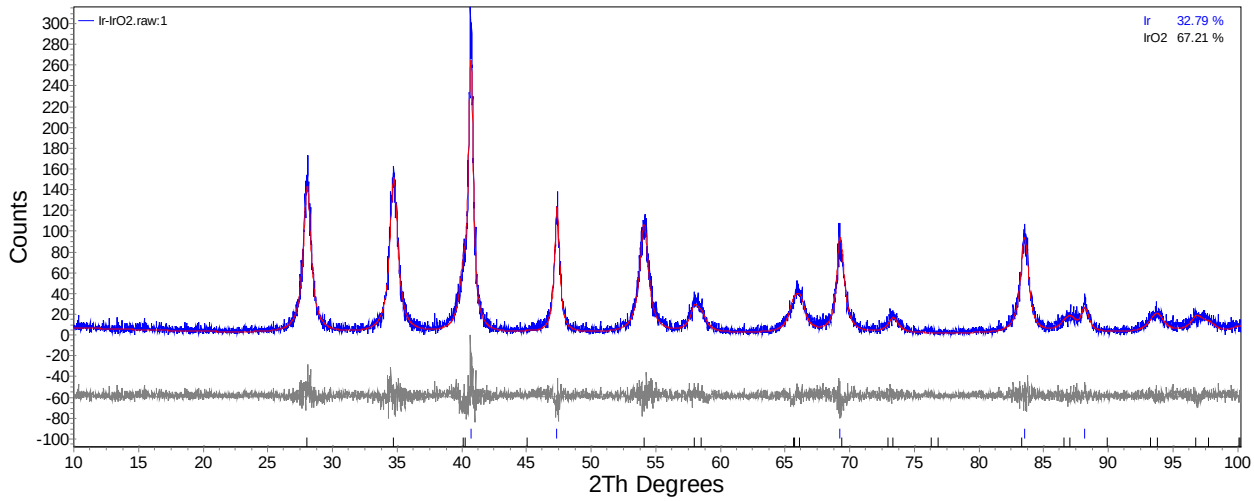
Cell Volume (Å^3)	56.468(42)
Crystallite Size	
k: 0.89 LVol-FWHM (nm)	21.61(56)
Crystal Density (g/cm^3)	22.611(17)
Preferred Orientation Spherical Harmonics	
Order	2
k00	1
Lattice parameters	
a (Å)	3.83648 (94)

Site	Np	x	y	z	Atom	Occ	Beq
Ir1	4	0.00000	0.00000	0.00000	Ir	1	0.38(12)

Structure 2

Phase name	IrO2
R-Bragg	5.892
Spacegroup	P42/mnm
Scale	0.0001113(67)
Cell Mass	448.440
Cell Volume (Å^3)	63.636(40)
Crystallite Size	
k: 0.89 LVol-FWHM (nm)	11.98(18)
Crystal Density (g/cm^3)	11.7017(73)
Preferred Orientation Spherical Harmonics	
Order	2
y00	1
y20	0.04273933
Lattice parameters	
a (Å)	4.4940(12)
c (Å)	3.1510(11)

Site	Np	x	y	z	Atom	Occ	Beq
Ir1	2	0.00000	0.00000	0.00000	Ir+4	1	0.53(21)
O1	4	0.30800	0.30800	0.00000	O-2	1	0.5



10-100

File 1 : " Ir-IrO2.raw"

R-Values

Rexp : 24.50 Rwp : 27.53 Rp : 18.74 GOF : 1.12
Rexp`: 27.02  Rwp`: 30.36 Rp` : 21.04 DW : 1.87

Quantitative Analysis - Rietveld

Phase 1 : Ir	32.8(12) %
Phase 2 : IrO2	67.2(12) %

Background

Chebychev polynomial, Coefficient	0	2.523(83)
	1	-1.54(13)
	2	1.64(12)
	3	-0.998(95)
	4	0.435(84)
	5	-0.123(76)
	6	-0.273(70)

Instrument

Primary radius (mm)	217.5
Secondary radius (mm)	217.5
Receiving slit width (mm)	0.2
Divergence angle (°)	1
Full Axial Convolution	
Filament Length (mm)	12
Sample Length (mm)	15
Receiving Slit Length (mm)	12
Primary Sollers (°)	2.3
Secondary Sollers (°)	2.3

Corrections

Specimen displacement	0.001(25)
LP Factor	26.4
Surface Roughness Pitschke et al	0.0765(99)

Structure 1

Phase name	Ir
R-Bragg	4.343
Spacegroup	Fm-3m
Scale	0.0000367(13)
Cell Mass	768.885

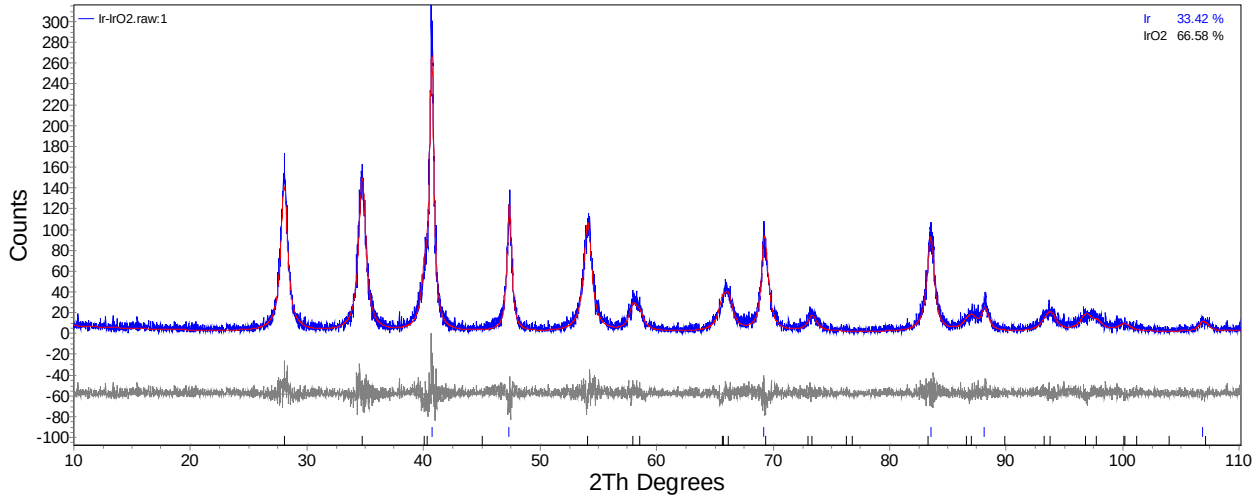
Cell Volume (Å^3)	56.476(38)
Wt% - Rietveld	32.8(12)
Crystallite Size	
k: 0.89 LVol-FWHM (nm)	21.46(54)
Crystal Density (g/cm^3)	22.607(15)
Preferred Orientation Spherical Harmonics	
Order	2
k00	1
Lattice parameters	
a (Å)	3.83668(87)

Site	Np	x	y	z	Atom	Occ	Beq
Ir1	4	0.00000	0.00000	0.00000	Ir	1	0.39(11)

Structure 2

Phase name	IrO2
R-Bragg	6.480
Spacegroup	P42/mnm
Scale	0.0001143(53)
Cell Mass	448.440
Cell Volume (Å^3)	63.657(35)
Crystallite Size	
k: 0.89 LVol-FWHM (nm)	11.87(17)
Crystal Density (g/cm^3)	11.6978(64)
Preferred Orientation Spherical Harmonics	
Order	2
y00	1
y20	0.055(20)
Lattice parameters	
a (Å)	4.4948(10)
c (Å)	3.15089(95)

Site	Np	x	y	z	Atom	Occ	Beq
Ir1	2	0.00000	0.00000	0.00000	Ir+4	1	0.65(14)
O1	4	0.30800	0.30800	0.00000	O-2	1	0.5



10-110

File 1 : " Ir-IrO2.raw"

R-Values

Rexp : 25.39 Rwp : 28.60 Rp : 19.49 GOF : 1.13
Rexp`: 28.14  Rwp`: 31.69 Rp` : 22.03 DW : 1.85

Quantitative Analysis - Rietveld

Phase 1 : Ir	33.4(11) %
Phase 2 : IrO2	66.6(11) %

Background

Chebychev polynomial, Coefficient	0	2.550(60)
	1	-1.445(78)
	2	1.744(83)
	3	-0.939(79)
	4	0.674(75)
	5	-0.119(64)
	6	0.021(65)

Instrument

Primary radius (mm)	217.5
Secondary radius (mm)	217.5
Receiving slit width (mm)	0.2
Divergence angle (°)	1
Full Axial Convolution	
Filament Length (mm)	12
Sample Length (mm)	15
Receiving Slit Length (mm)	12
Primary Sollers (°)	2.3
Secondary Sollers (°)	2.3

Corrections

Specimen displacement	0.003(24)
LP Factor	26.4
Surface Roughness Pitschke et al	0.0779(92)

Structure 1

Phase name	Ir
R-Bragg	4.770
Spacegroup	Fm-3m
Scale	0.0000373(12)
Cell Mass	768.885

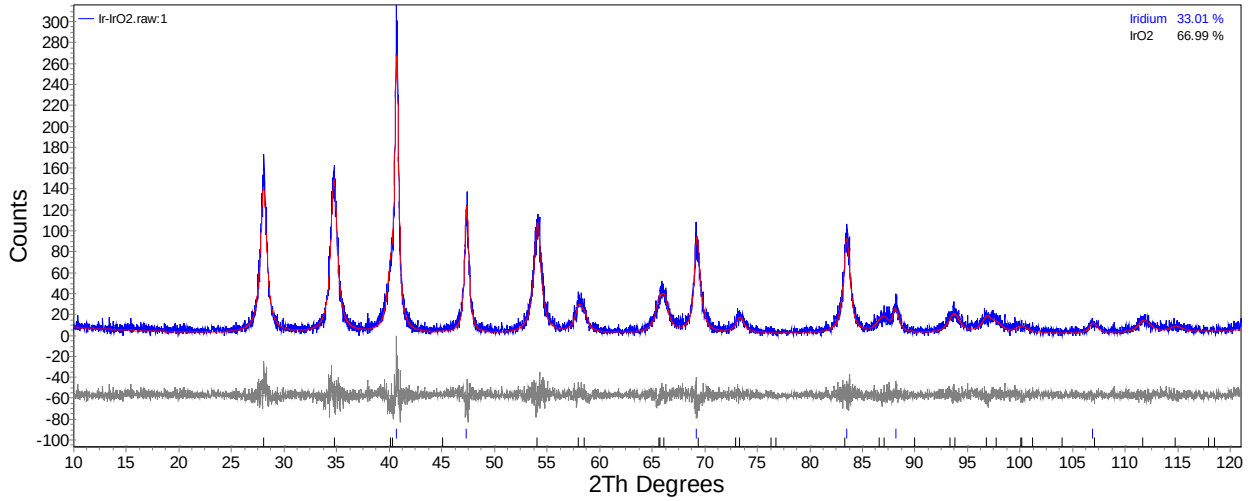
Cell Volume (Å^3)	56.469(34)
Wt% - Rietveld	33.4(11)
Crystallite Size	
Cry Size Lorentzian (nm)	24.15(58)
k: 1 LVol-IB (nm)	15.38(37)
k: 0.89 LVol-FWHM (nm)	21.50(52)
Crystal Linear Absorption Coeff. (1/cm)	4283.0(26)
Crystal Density (g/cm^3)	22.610(14)
Preferred Orientation Spherical Harmonics	
Order	2
k00	1
Lattice parameters	
a (Å)	3.83652(77)

Site	Np	x	y	z	Atom	Occ	Beq
Ir1	4	0.00000	0.00000	0.00000	Ir	1	0.50(10)

Structure 2

Phase name	IrO2
R-Bragg	6.714
Spacegroup	P42/mnm
Scale	0.0001132(48)
Cell Mass	448.440
Cell Volume (Å^3)	63.659(32)
Wt% - Rietveld	66.6(11)
Crystallite Size	
k: 0.89 LVol-FWHM (nm)	11.87(17)
Crystal Linear Absorption Coeff. (1/cm)	1918.81(95)
Crystal Density (g/cm^3)	11.6974(58)
Preferred Orientation Spherical Harmonics	
Order	2
y00	1
y20	0.049(19)
Lattice parameters	
a (Å)	4.49503(93)
c (Å)	3.15063(87)

Site	Np	x	y	z	Atom	Occ	Beq
Ir1	2	0.00000	0.00000	0.00000	Ir+4	1	0.55(12)
O1	4	0.30800	0.30800	0.00000	O-2	1	1



10-120

File 1 : "Ir-IrO2.raw"

R-Values

Rexp : 26.05 Rwp : 29.39 Rp : 20.14 GOF : 1.13
Rexp`: 29.21  Rwp`: 32.95 Rp` : 23.09 DW : 1.83

Quantitative Analysis - Rietveld

Phase 1 : Iridium	33.0(10) %
Phase 2 : IrO2	67.0(10) %

Background

Chebychev polynomial, Coefficient	0	2.846(58)
	1	-0.791(81)
	2	2.222(81)
	3	-0.592(75)
	4	1.029(69)
	5	-0.016(59)
	6	0.239(65)

Instrument

Primary radius (mm)	217.5
Secondary radius (mm)	217.5
Receiving slit width (mm)	0.2
Divergence angle (°)	1
Full Axial Convolution	
Filament Length (mm)	12
Sample Length (mm)	15
Receiving Slit Length (mm)	12
Primary Sollers (°)	2.3
Secondary Sollers (°)	2.3

Corrections

Specimen displacement	0.001(23)
LP Factor	26.4
Surface Roughness Pitschke et al	0.0869(81)

Structure 1

Phase name	Iridium
R-Bragg	4.734
Spacegroup	Fm-3m
Scale	0.0000382(12)

Cell Mass	768.885
Cell Volume (Å^3)	56.472(31)
Wt% - Rietveld	33.0(10)
Crystallite Size	
k: 0.89 LVol-FWHM (nm)	21.68(50)
Crystal Density (g/cm^3)	22.609(12)
Preferred Orientation Spherical Harmonics	
Order	2
k00	1
Lattice parameters	
a (Å)	3.83658(69)

Site	Np	x	y	z	Atom	Occ	Beq
Ir1	4	0.00000	0.00000	0.00000	Ir	1	0.56(10)

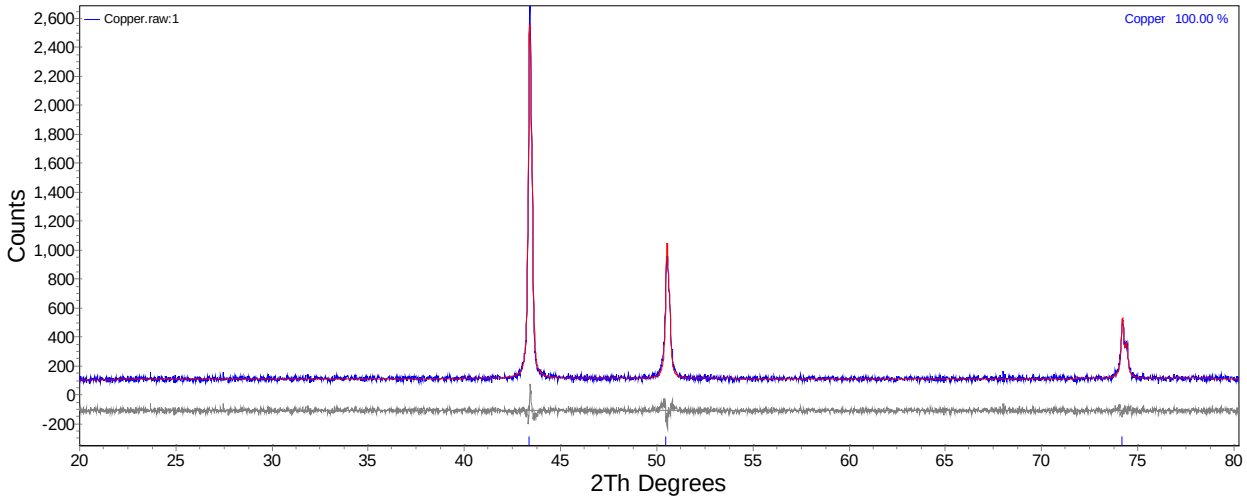
Structure 2

Phase name	IrO2
R-Bragg	7.070
Spacegroup	P42/mnm
Scale	0.0001180(45)
Cell Mass	448.440
Cell Volume (Å^3)	63.661(28)
Wt% - Rietveld	67.0(10)
Crystallite Size	
k: 0.89 LVol-FWHM (nm)	11.84(17)
Crystal Linear Absorption Coeff. (1/cm)	1918.77(85)
Crystal Density (g/cm^3)	11.6972(52)
Preferred Orientation Spherical Harmonics	
Order	2
y00	1
y20	0.03694792
Lattice parameters	
a (Å)	4.49505(87)
c (Å)	3.15068(69)

Site	Np	x	y	z	Atom	Occ	Beq
Ir1	2	0.00000	0.00000	0.00000	Ir+4	1	0.661(97)
O1	4	0.30800	0.30800	0.00000	O-2	1	1

3. Copper

Parameters	Angular range at Rietveld refinement, 2θ°			
	20-80	20-92	20-100	20-120
Rwp	9.25	9.23	9.24	9.31
a, Å	3.61314	3.61292	3.612832	3.612861
e.s.d.	0.00018	0.00010	0.000093	0.000090
d, nm	93.2	87.5	87.9	87.1
e.s.d.	2.4	2.1	2.1	2.0



20-80
File 1 : Copper.raw

R-Values

```
Rexp : 8.70    Rwp : 9.25     Rp  : 7.28   GOF : 1.06
Rexp`: 25.48   Rwp`: 27.10    Rp` : 36.70  DW  : 1.87
```

Quantitative Analysis - Rietveld

```
   Phase 1  : Copper                          100.000 %
```

Background

```
   Chebychev polynomial, Coefficient  0       111.31(26)
                                      1       2.95(44)
                                      2       -2.00(42)
                                      3       1.41(38)
                                      4       -0.18(39)
                                      5       -0.77(35)
                                      6       -1.30(34)
```

Instrument

```
   Primary radius (mm)                        217.5
   Secondary radius (mm)                      217.5
   Receiving slit width (mm)                  0.2
   Divergence angle (°)                       1
   Full Axial Convolution
      Filament Length (mm)                    12
      Sample Length (mm)                      15
```

Receiving Slit Length (mm)	12
Primary Sollers (°)	2.3
Secondary Sollers (°)	2.3

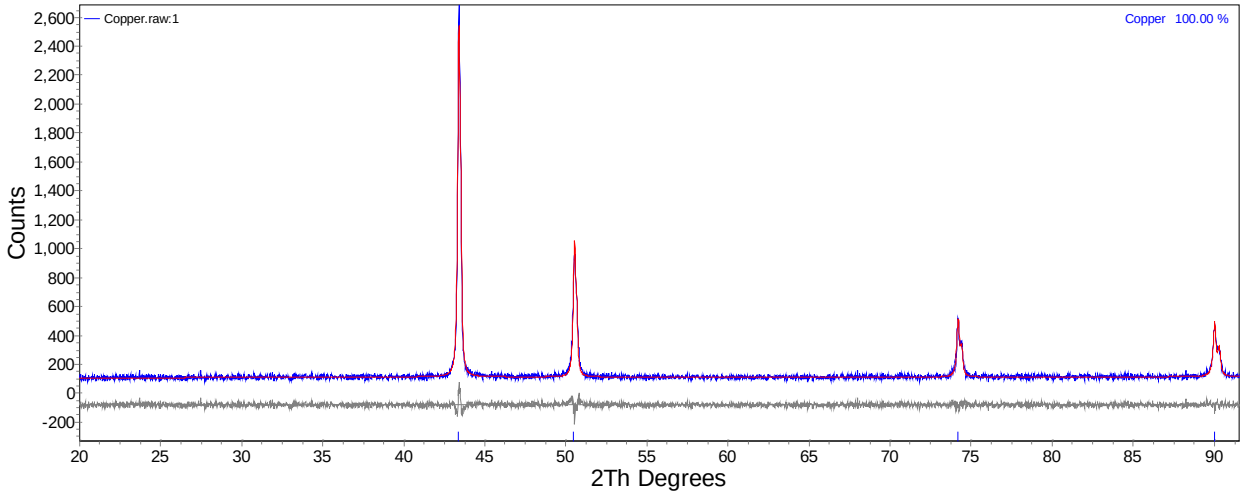
Corrections

Specimen displacement	-0.1609(96)
LP Factor	26.4
Absorption (1/cm)	37.8(67)
Sample Thickness (mm)	0.2

Structure 1

Phase name	Copper
R-Bragg	0.510
Space group	Fm-3m
Scale	0.001188(11)
Cell Mass	254.185
Cell Volume (Å^3)	47.1688(70)
Crystallite Size	
k: 0.89 LVol-FWHM (nm)	93.2(24)
Crystal Density (g/cm^3)	8.9484(13)
Preferred Orientation Spherical Harmonics	
Order	6
k00	1
k41	-0.0495(76)
k61	0.0236(98)
Lattice parameters	
a (Å)	3.61314(18)

Site	Np	x	y	z	Atom	Occ	Beq
Cu1	4	0.00000	0.00000	0.00000	Cu	1	1



20-91
File 1 : " Copper.raw"

R-Values

Rexp : 8.71 Rwp : 9.23 Rp : 7.30 GOF : 1.06
Rexp`: 26.25  Rwp`: 27.81 Rp` : 37.56 DW : 1.85

Quantitative Analysis - Rietveld

Phase 1 : Copper	100.000 %

Background

Chebychev polynomial, Coefficient	0	111.83(26)
	1	3.31(43)
	2	-1.11(42)
	3	1.46(38)
	4	-0.36(37)
	5	-0.60(32)
	6	0.14(32)

Instrument

Primary radius (mm)	217.5
Secondary radius (mm)	217.5
Receiving slit width (mm)	0.2
Divergence angle (°)	1
Full Axial Convolution	
Filament Length (mm)	12
Sample Length (mm)	15
Receiving Slit Length (mm)	12
Primary Sollers (°)	2.3
Secondary Sollers (°)	2.3

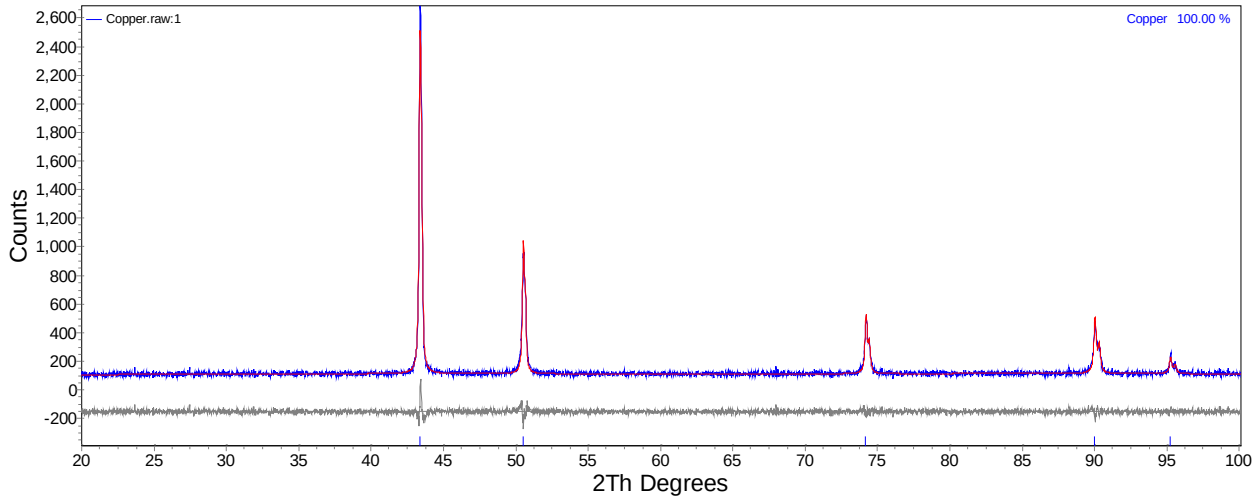
Corrections

Specimen displacement	-0.1410(80)
LP Factor	26.4
Absorption (1/cm)	40.6(97)
Sample Thickness (mm)	0.2

Structure 1

Phase name	Copper
R-Bragg	0.564
Space group	Fm-3m
Scale	0.001195(27)
Cell Mass	254.185
Cell Volume (Å^3)	47.1601(39)
Crystallite Size	
k: 0.89 LVol-FWHM (nm)	87.5(21)
Crystal Density (g/cm^3)	8.95003(74)
Preferred Orientation Spherical Harmonics	
Order	6
k00	1
k41	-0.0469(75)
k61	0.020(15)
Lattice parameters	
a (Å)	3.61292(10)

Site	Np	x	y	z	Atom	Occ	Beq
Cu1	4	0.00000	0.00000	0.00000	Cu	1	0.563(86)



20-100
File 1 : Copper.raw

R-Values

Rexp : 8.75	Rwp : 9.24	Rp : 7.33	GOF : 1.06
Rexp` : 27.45	Rwp` : 28.99	Rp` : 39.36	DW : 1.87

Quantitative Analysis - Rietveld

Phase 1 : Copper		100.000 %

Background

Chebychev polynomial, Coefficient	0	111.57(23)
	1	2.40(38)
	2	-1.96(36)
	3	0.59(33)
	4	-1.15(33)
	5	-0.65(30)
	6	0.42(30)

Instrument

Primary radius (mm)	217.5
Secondary radius (mm)	217.5
Receiving slit width (mm)	0.2
Divergence angle (°)	1
Full Axial Convolution	
Filament Length (mm)	12
Sample Length (mm)	15
Receiving Slit Length (mm)	12
Primary Sollers (°)	2.3
Secondary Sollers (°)	2.3

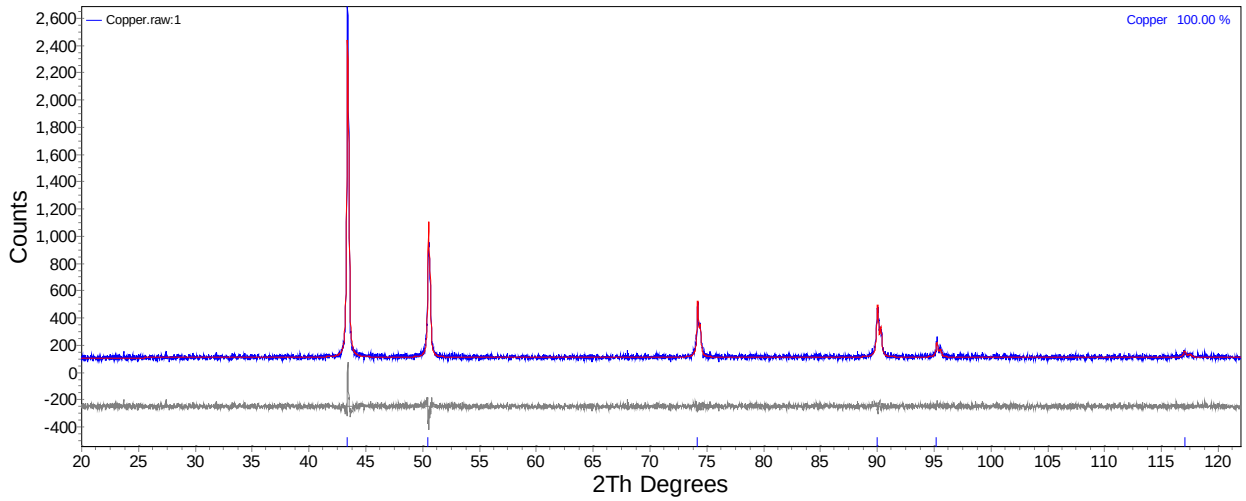
Corrections

Specimen displacement	-0.1406(79)
LP Factor	26.4
Absorption (1/cm)	38.3(90)
Sample Thickness (mm)	0.2

Structure 1

Phase name	Copper
R-Bragg	0.577
Space group	Fm-3m
Scale	0.001189(22)
Cell Mass	254.185
Cell Volume (Å^3)	47.1567(37)
Crystallite Size	
k: 0.89 LVol-FWHM (nm)	87.9(21)
Crystal Density (g/cm^3)	8.95069(69)
Preferred Orientation Spherical Harmonics	
Order	6
k00	1
k41	-0.0468(75)
k61	0.022(13)
Lattice parameters	
a (Å)	3.612832(93)

Site	Np	x	y	z	Atom	Occ	Beq
Cu1	4	0.00000	0.00000	0.00000	Cu	1	0.549(68)



20-120
File 1 : Copper.raw

R-Values

Rexp : 8.88 Rwp : 9.31 Rp : 7.41 GOF : 1.05
Rexp`: 30.57  Rwp`: 32.05 Rp` : 44.48 DW : 1.87

Quantitative Analysis - Rietveld

Phase 1 : Copper	100.000 %

Background

Chebychev polynomial, Coefficient	0	111.44(20)
	1	2.00(33)
	2	-2.01(32)
	3	1.33(29)
	4	-0.39(29)
	5	0.99(26)
	6	0.36(26)

Instrument

Primary radius (mm)	217.5
Secondary radius (mm)	217.5
Receiving slit width (mm)	0.2
Divergence angle (°)	1
Full Axial Convolution	

Filament Length (mm)	12
Sample Length (mm)	15
Receiving Slit Length (mm)	12
Primary Sollers (°)	2.3
Secondary Sollers (°)	2.3

Corrections

Specimen displacement	-0.1400(78)
LP Factor	26.4
Absorption (1/cm)	39.9(93)
Sample Thickness (mm)	0.2

Structure 1

Phase name	Copper
R-Bragg	0.592
Space group	Fm-3m
Scale	0.001197(21)
Cell Mass	254.185
Cell Volume (Å^3)	47.1578(35)
Crystallite Size	
k: 0.89 LVol-FWHM (nm)	87.1(20)
Crystal Density (g/cm^3)	8.95047(67)
Preferred Orientation Spherical Harmonics	
Order	6
k00	1
k41	-0.04673799
k61	0.01977366
Lattice parameters	
a (Å)	3.612861(90)

Site	Np	x	y	z	Atom	Occ	Beq
Cu1	4	0.00000	0.00000	0.00000	Cu	1	0.562(62)