Sheffield Hallam University

APPENDICES

Processing-composition-structure effects on the optical band gap of $KNbO_3$-based ceramics

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Contents

Volume II

APPENDIX A

Chapter 3: Processing and Characterisation of $KNbO_3$ ceramics

A.1. Rietveld Refinements plots

A.1.1. $KNbO_3$

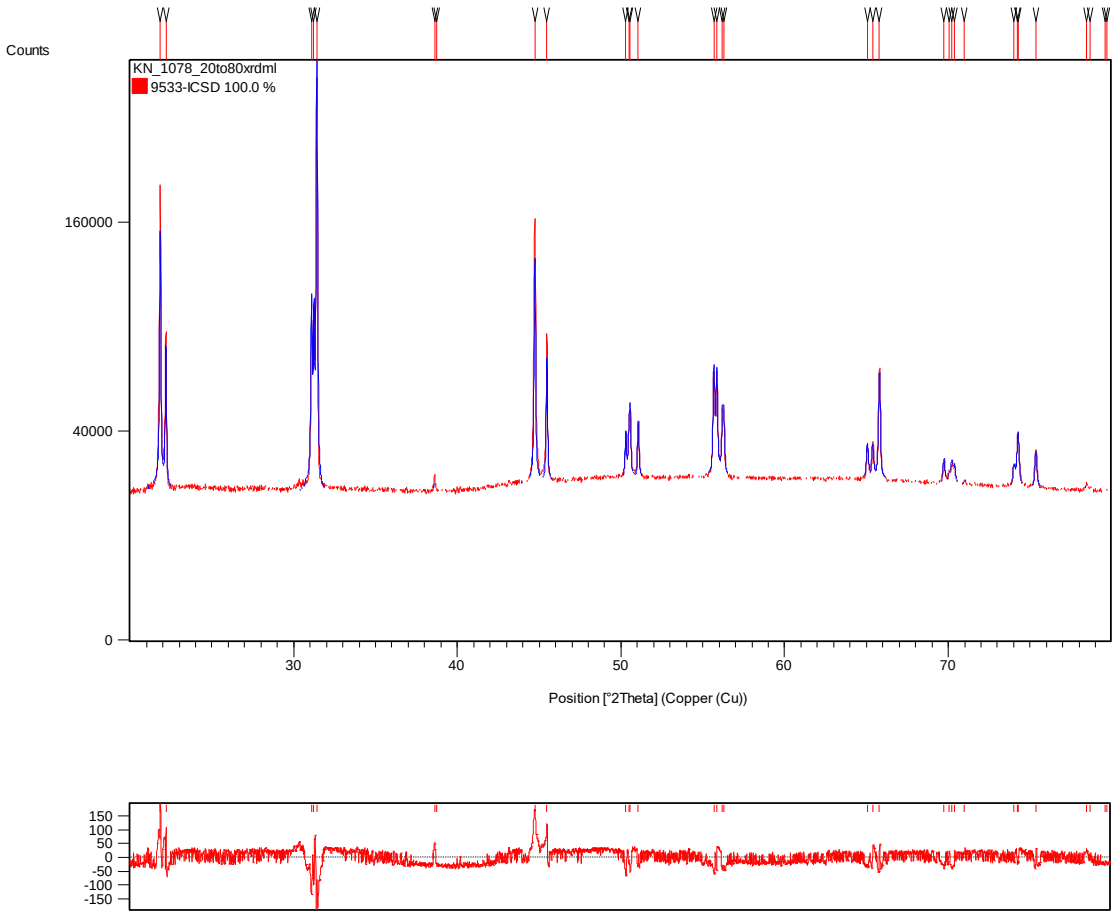


Figure A. 1.: Experimental X-ray diffraction data (red), calculated fitting profile (blue) and difference plot for $KNbO_3$.

Atom	Wyck.	s.o.f.	x	y	z	Biso/ 10^4 pm^2
K1	2b	1.000000	0.500000	0.000000	0.528924	0.000000
Nb1	2a	1.000000	0.000000	0.000000	0.000000	0.000000
O1	2b	1.000000	0.500000	0.000000	-0.007275	0.000000
O2	4d	1.000000	0.000000	0.252400	0.335(5)	0.000000

Table A. 1 Occupancy, atomic fract. coordinates and Biso for KN

A.1.2. $K_{0.95}NbO_{2.975}$

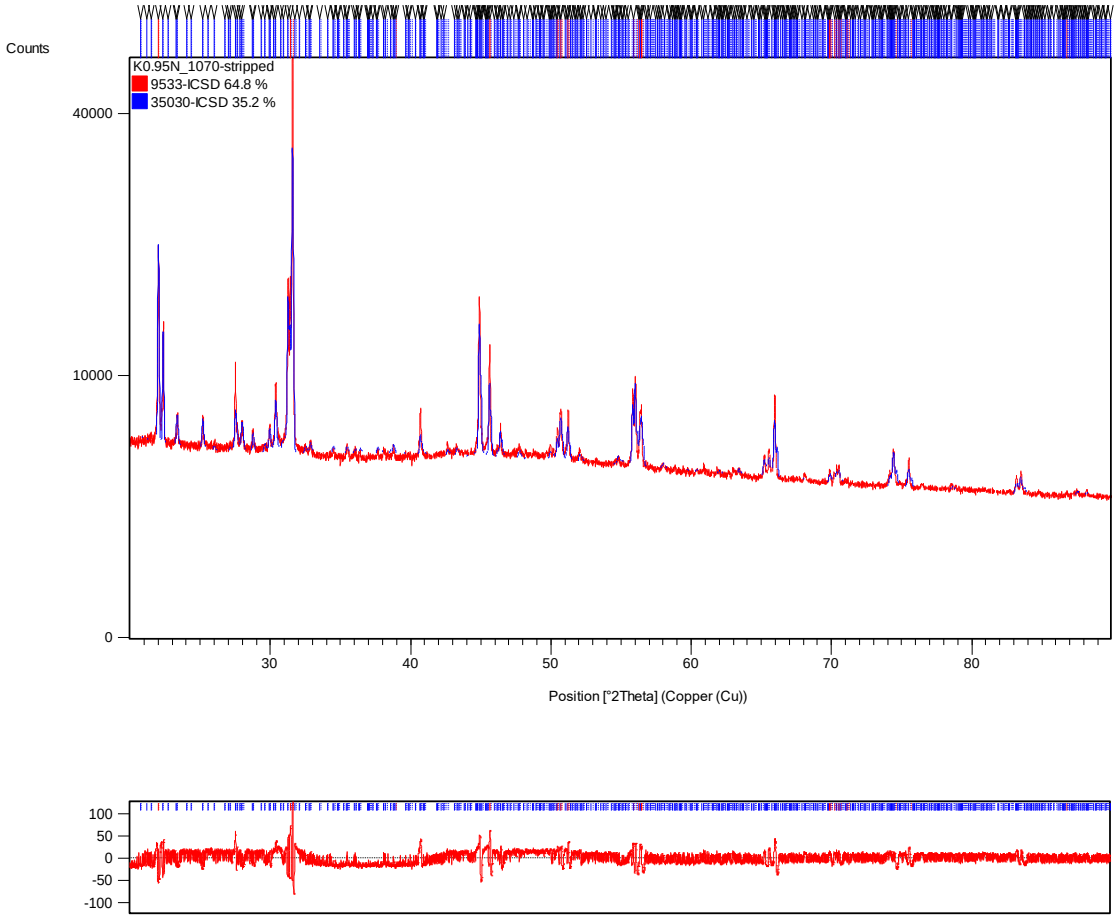


Figure A. 2: Experimental X-ray diffraction data (red), calculated fitting profile (blue) and difference plot for $K_{0.95}NbO_{2.975}$ and $K_4Nb_6O_{17}$.

Atom	Wyck.	s.o.f.	x	y	z	Biso/ 10^4 pm^2
K1	2b	0.950000	0.500000	0.000000	0.513800	0.000000
Nb1	2a	1.000000	0.000000	0.000000	0.000000	0.000000
O1	2b	1.000000	0.500000	0.000000	0.036400	0.000000
O2	4d	1.000000	0.000000	0.252400	0.284200	0.000000

Table A. 2: Occupancy, atomic fraction. coordinates and Biso for $K_{0.95}NbO_{2.975}$

Atom	Wyck.	s.o.f.	x	y	z	Biso/ 10^4 pm^2
Nb1	4a	1.000000	0.325900	0.298300	0.264600	2.100000
Nb2	4a	1.000000	0.174100	0.794100	0.272400	0.700000
Nb3	4a	1.000000	0.125200	0.244200	0.763500	1.100000
Nb4	4a	1.000000	0.127200	0.232500	0.279300	1.700000
Nb5	4a	1.000000	0.404600	0.363100	0.526300	1.300000
Nb6	4a	1.000000	0.049900	0.319800	0.026000	1.600000
K1	4a	1.000000	0.220900	0.348900	0.013000	0.700000
K2	4a	1.000000	0.217700	0.354700	0.515500	1.600000
K3	4a	1.000000	0.418100	0.166100	0.014500	1.400000
K4	4a	1.000000	0.021400	0.205200	0.518800	1.900000
O1	4a	1.000000	0.278100	0.222000	0.307700	3.200000
O2	4a	1.000000	0.227900	0.721400	0.250800	1.700000
O3	4a	1.000000	0.355500	0.002400	0.277700	0.100000
O4	4a	1.000000	0.153600	0.483800	0.283500	0.500000
O5	4a	1.000000	0.068000	0.328900	0.787400	0.100000
O6	4a	1.000000	0.068300	0.290000	0.278800	3.000000
O7	4a	1.000000	0.321700	0.595200	0.269900	0.400000

O8	4a	1.000000	0.190200	0.084000	0.273700	3.600000
O9	4a	1.000000	0.390100	0.408200	0.283500	0.100000
O10	4a	1.000000	0.602600	0.572900	0.253100	2.800000
O11	4a	1.000000	0.120900	0.188800	0.024500	0.400000
O12	4a	1.000000	0.116900	0.218600	0.521300	2.400000
O13	4a	1.000000	0.042600	0.017000	0.000000	2.400000
O14	4a	1.000000	0.332400	0.267300	0.014600	1.900000
O15	4a	1.000000	0.343900	0.277000	0.503600	0.900000
O16	4a	1.000000	0.496000	0.125200	0.040400	2.400000
O17	4a	1.000000	0.073700	0.612600	0.042600	0.100000

Table A. 3: Occupancy, atomic fraction. coordinates and Biso for $K_4Nb_6O_{17}$.

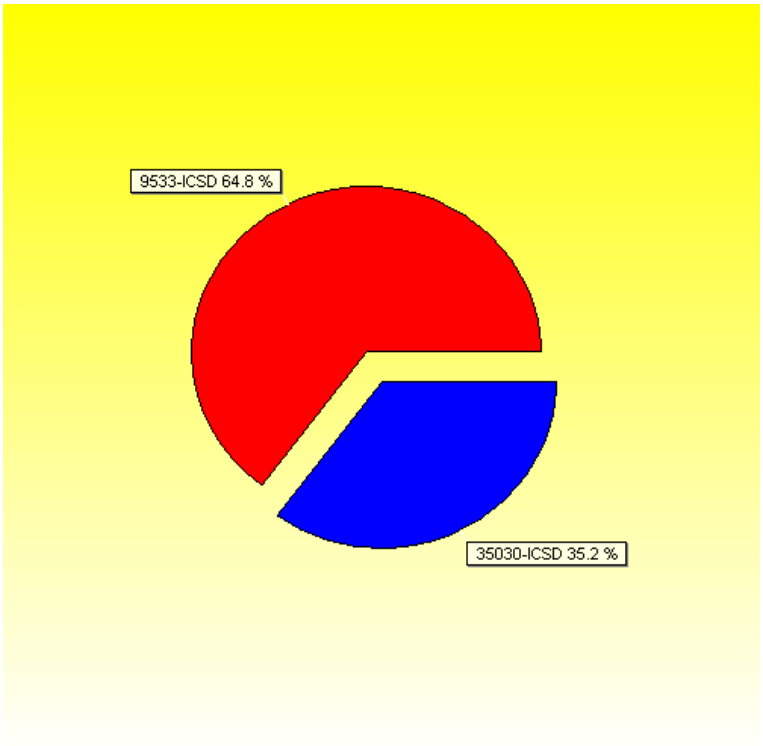


Figure A. 3.: The pie chart represents the percent quantity of $K_{0.95}NbO_{2.975}$ and $K_4Nb_6O_{17}$.

A.1.3. $KNb_{0.95}O_{3-\delta}$

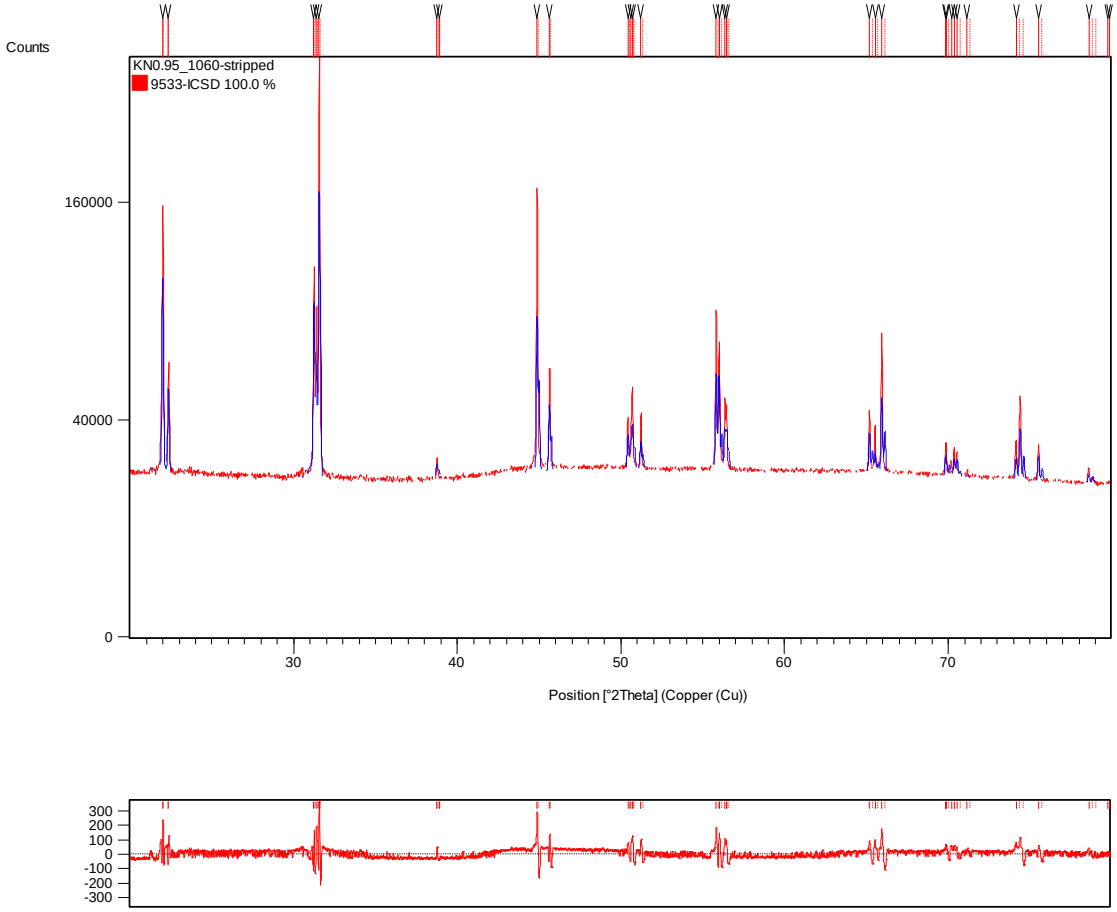


Figure A. 4.: Experimental X-ray diffraction data (red), calculated fitting profile (blue) and difference plot for $KNb_{0.95}O_{2.875}$

Atom	Wyck.	s.o.f.	x	y	z	Biso/ 10^4 pm^2
K1	2b	1.000000	0.500000	0.000000	0.526955	0.000000
Nb1	2a	0.950000	0.000000	0.000000	0.000000	0.000000
O1	2b	1.000000	0.500000	0.000000	0.036871	0.000000
O2	4d	1.000000	0.000000	0.222768	0.267(6)	0.000000

Table A. 4.: Occupancy, atomic fraction. coordinates and Biso for $KNb_{0.95}O_{2.875}$

A.2. EDX measurements

A.2.1. $KNbO_3$

K (%)	Nb (%)	K/Nb
50	50	1

Table A. 5: Theoretical K and Nb atomic percent for nominal $KNbO_3$

Measurements	K (%)	Nb (%)	K/Nb
1	52	48	1.073
2	52	48	1.063
3	51	49	1.058
4	51	49	1.053
5	51	49	1.048
6	51	49	1.043
7	51	49	1.033
8	51	49	1.023
9	50	50	1.018
10	50	50	1.009
11	49	51	0.963

Table A. 6.: K and Nb atomic percent for $KNbO_3$.

A.2.2. $K_{0.95}NbO_{2.975}$

K (%)	Nb (%)	K/Nb
48	50	0.95

Table A. 7.: Atomic percent of K and Nb, for the nominal $K_{0.95}NbO_{2.975}$ composition.

Measurements	K (%)	Nb (%)	K/Nb
1	54	46	1.170
2	54	46	1.155
3	53	47	1.134
4	52	48	1.103
5	52	48	1.063
6	51	49	1.038
7	47	53	0.901
8	47	53	0.901
9	47	53	0.901
10	46	54	0.861
11	42	58	0.713
12	40	60	0.655

Table A. 8: Experimental atomic percent of K and Nb by EDX spectra for $K_{0.95}NbO_{2.975}$.

A.2.3. $KNb_{0.95}O_{2.875}$

K (%)	Nb (%)	K/Nb
50	~48	~1.05

Table A. 9: Atomic percent of K and Nb, for the nominal $KNb_{0.95}O_{2.875}$ composition.

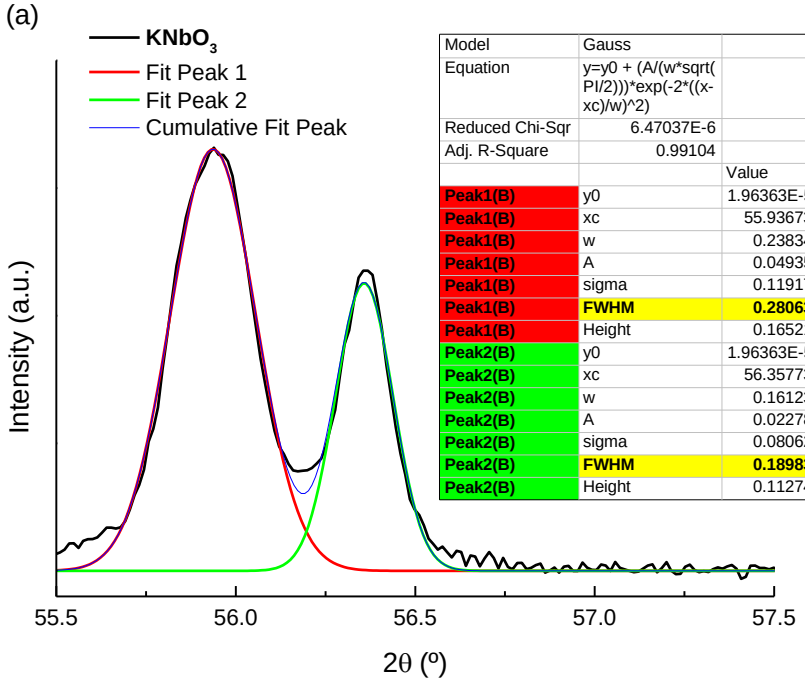
Measurements	K (%)	Nb (%)	K/Nb
1	53	47	1.113
2	53	47	1.108
3	52	48	1.098
4	52	48	1.093
5	52	48	1.068
6	52	48	1.063
7	51	49	1.058
8	51	49	1.044
9	51	49	1.028
10	51	49	1.023
11	44	56	0.801

Table A. 10: Experimental atomic percent of K and Nb by EDX spectra for $KNb_{0.95}O_{2.875}$.

A.3. FWHM values for XRD peaks from 55º to 57º

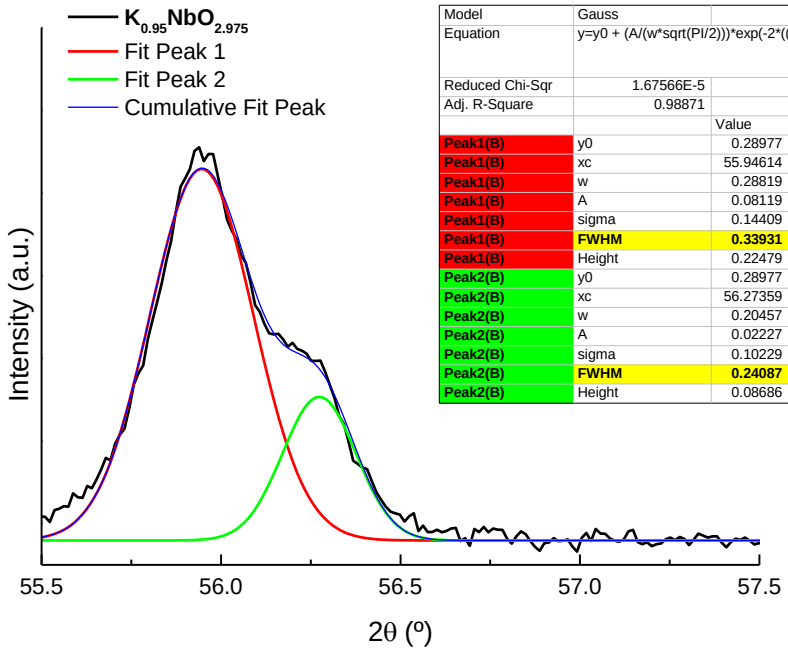
Gaussian fitting permits to compare the FWHM values of the peaks from 55º to 57º (Figure A. 5) even if the entire quadruplet could not be fitted for the patterns. The FWHM values for K-excess compound (0.130º, 0.129º and 0.191º) are much lower than pure (0.280º and 0.189º) and K-deficiency (0.339º and 0.241º) values.

(a)

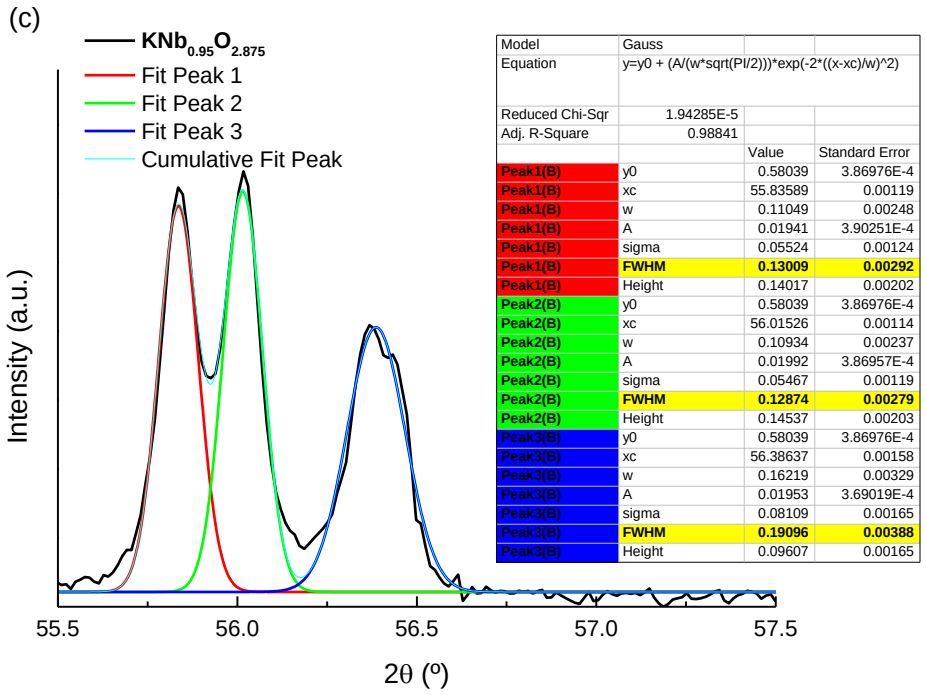


Model	Gauss		
Equation	y=y0 + (A/(w*sqrt(PI/2)))*exp(-2*((x-xc)/w)^2)		
Reduced Chi-Sqr	6.47037E-6		
Adj. R-Square	0.99104		
		Value	Standard Error
Peak1(B)	y0	1.96363E-5	9.63481E-5
Peak1(B)	xc	55.93673	6.55707E-4
Peak1(B)	w	0.23834	0.00138
Peak1(B)	A	0.04935	2.45034E-4
Peak1(B)	sigma	0.11917	6.88065E-4
Peak1(B)	**FWHM**	**0.28063**	**0.00162**
Peak1(B)	Height	0.16521	7.8575E-4
Peak2(B)	y0	1.96363E-5	9.63481E-5
Peak2(B)	xc	56.35773	7.96406E-4
Peak2(B)	w	0.16123	0.00163
Peak2(B)	A	0.02278	2.00584E-4
Peak2(B)	sigma	0.08062	8.17065E-4
Peak2(B)	**FWHM**	**0.18983**	**0.00192**
Peak2(B)	Height	0.11274	9.46077E-4

(b)



Model	Gauss		
Equation	y=y0 + (A/(w*sqrt(PI/2)))*exp(-2*((x-xc)/w)^2)		
Reduced Chi-Sqr	1.67566E-5		
Adj. R-Square	0.98871		
		Value	Standard Error
Peak1(B)	y0	0.28977	1.551E-4
Peak1(B)	xc	55.94614	0.00182
Peak1(B)	w	0.28819	0.0033
Peak1(B)	A	0.08119	9.16014E-4
Peak1(B)	sigma	0.14409	0.00165
Peak1(B)	**FWHM**	**0.33931**	**0.00388**
Peak1(B)	Height	0.22479	0.00119
Peak2(B)	y0	0.28977	1.551E-4
Peak2(B)	xc	56.27359	0.00359
Peak2(B)	w	0.20457	0.00587
Peak2(B)	A	0.02227	8.57425E-4
Peak2(B)	sigma	0.10229	0.00294
Peak2(B)	**FWHM**	**0.24087**	**0.00691**
Peak2(B)	Height	0.08686	0.00182



Model	Gauss		
Equation	y=y0 + (A/(w*sqrt(PI/2)))*exp(-2*((x-xc)/w)^2)		
Reduced Chi-Sqr	1.94285E-5		
Adj. R-Square	0.98841		
		Value	Standard Error
Peak1(B)	y0	0.58039	3.86976E-4
Peak1(B)	xc	55.83589	0.00119
Peak1(B)	w	0.11049	0.00248
Peak1(B)	A	0.01941	3.90251E-4
Peak1(B)	sigma	0.05524	0.00124
Peak1(B)	**FWHM**	**0.13009**	**0.00292**
Peak1(B)	Height	0.14017	0.00202
Peak2(B)	y0	0.58039	3.86976E-4
Peak2(B)	xc	56.01526	0.00114
Peak2(B)	w	0.10934	0.00237
Peak2(B)	A	0.01992	3.86957E-4
Peak2(B)	sigma	0.05467	0.00119
Peak2(B)	**FWHM**	**0.12874**	**0.00279**
Peak2(B)	Height	0.14537	0.00203
Peak3(B)	y0	0.58039	3.86976E-4
Peak3(B)	xc	56.38637	0.00158
Peak3(B)	w	0.16219	0.00329
Peak3(B)	A	0.01953	3.69019E-4
Peak3(B)	sigma	0.08109	0.00165
Peak3(B)	**FWHM**	**0.19096**	**0.00388**
Peak3(B)	Height	0.09607	0.00165

Figure A. 5: Gaussian fitting for estimation of the FWHM of peaks from 55º to 57º for (a) $KNbO_3$, (b) $K_{0.95}NbO_{2.975}$ and (c) $KNb_{0.95}O_{2.875}$, suggesting a large degree of crystallisation in powders prepared with an excess of potassium.

APPENDIX B

Chapter 3:

System (1−*x*) $KNbO_3$-*x*$(Ba_{0.5}Bi_{0.5})(Zn_{0.5}Nb_{0.5})O_3$

B.1. Rietveld Refinements plots

B.1.1. (1-x) $KNbO_3$-x $BaBiNbZnO_3$ (KBNN)

B.1.1.1. x=0.05

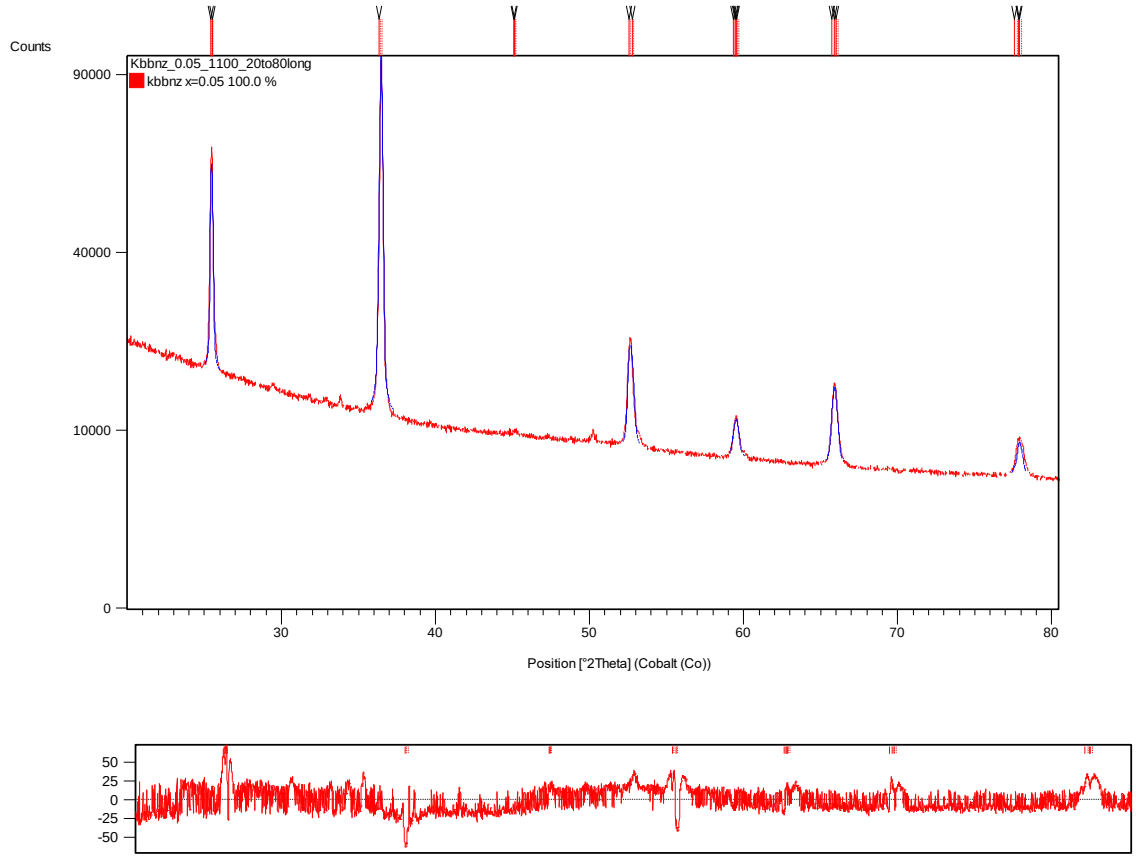


Figure B. 1.: Experimental X-ray diffraction data (red), calculated fitting profile (blue) and difference plot for KBNNZ x=0.05.

Atom	Wyck.	s.o.f.	x	y	z	Biso/ 10^4 pm^2
K	2a	0.950000	0.000000	0.000000	0.000000	0.500000
Be	2a	0.025000	0.000000	0.000000	0.000000	0.500000
Bi	2a	0.025000	0.000000	0.000000	0.000000	0.500000
Nb	2b	0.925000	0.500000	0.000000	0.460680	0.500000
Zn	2b	0.025000	0.500000	0.000000	0.217439	0.500000
O	2a	1.000000	0.000000	0.000000	0.425334	0.500000
O	4e	1.000000	0.500000	0.215555	0.194157	0.500000

Table B. 1.: Occupancy, atomic fract. coordinates and Biso for orthorhombic KBBNZ x=0.05

B.1.1.2. x=0.10

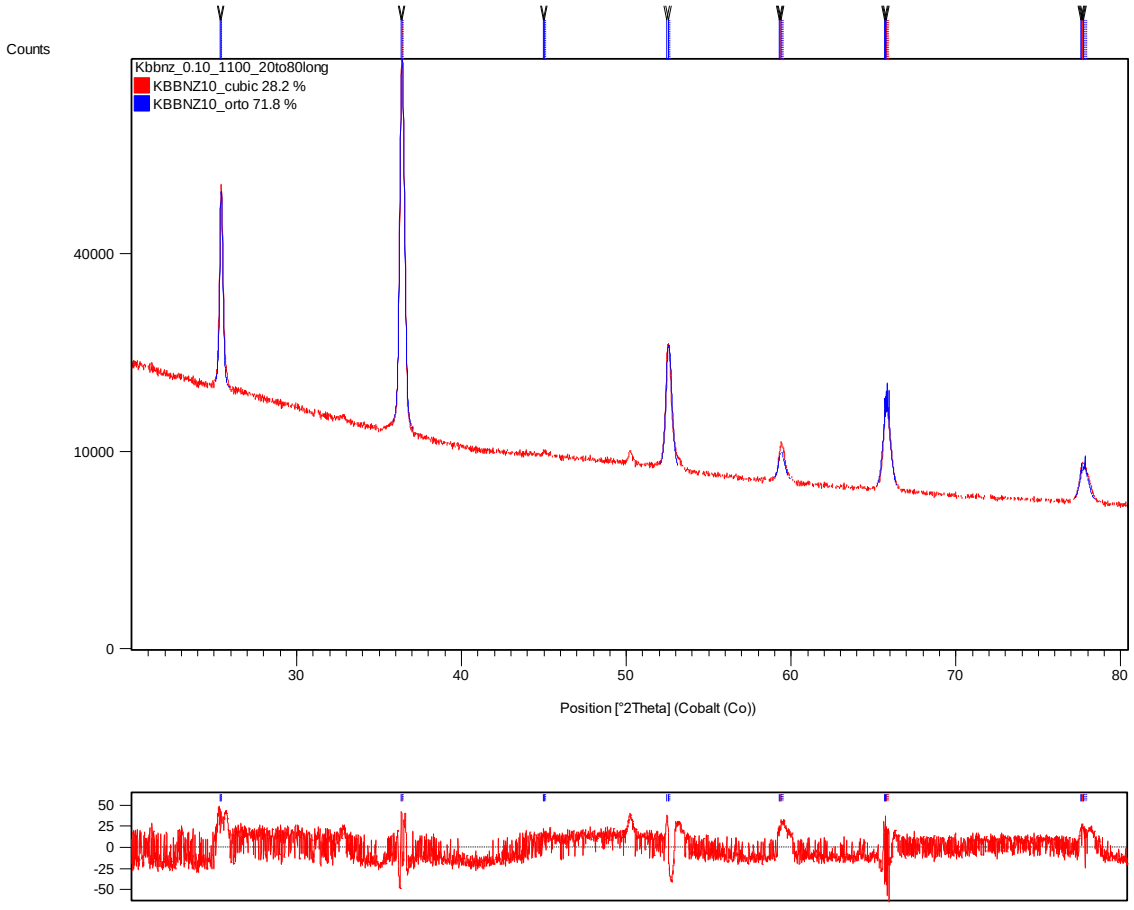


Figure B. 2.: Experimental X-ray diffraction data (red), calculated fitting profile (blue) and difference plot for KBNNZ x=0.10.

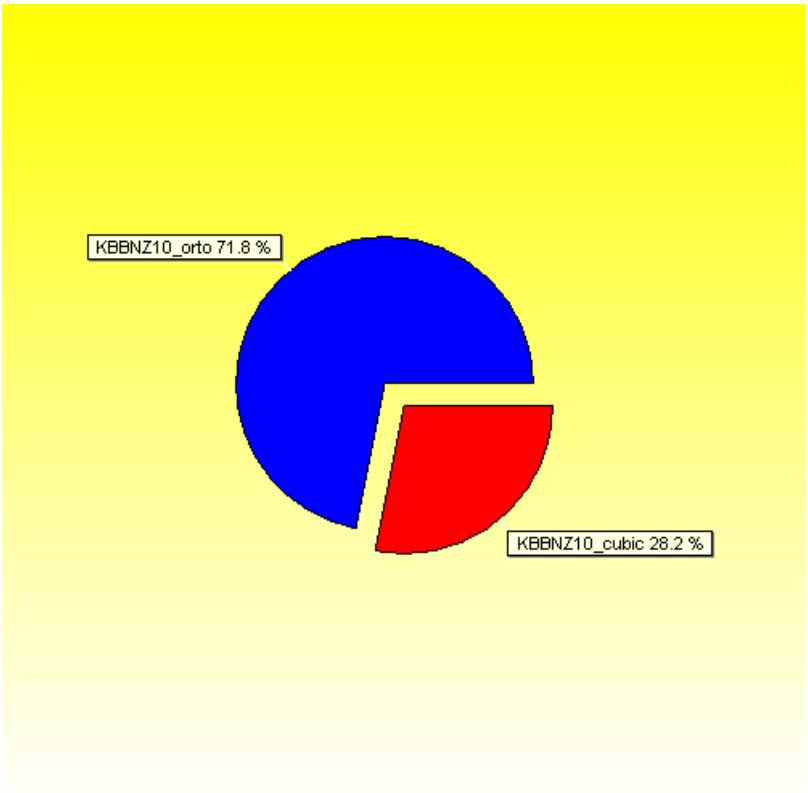


Figure B. 3.: The pie chart represents the percent quantity of the two polymorphs (orthorhombic and cubic) for KBBNZ x=0.10.

Atom	Wyck.	s.o.f.	x	y	z	Biso/ 10^4 pm^2
K1	1a	0.900000	0.000000	0.000000	0.000000	0.020500
Nb1	1b	0.950000	0.500000	0.500000	0.500000	0.015490
O1	3c	1.000000	0.000000	0.500000	0.500000	1.339634
Bi	1a	0.050000	0.000000	0.000000	0.000000	0.020500
Ba	1a	0.050000	0.000000	0.000000	0.000000	0.020500
Zn	1b	0.050000	0.500000	0.500000	0.500000	0.015490

Table B. 2.: Occupancy, atomic fract. coordinates and Biso for cubic KBBNZ x=0.10

Atom	Wyck.	s.o.f.	x	y	z	Biso/ 10^4 pm^2
K1	2a	0.900000	0.000000	0.000000	0.000000	10.000000

Nb1	2b	0.950000	0.500000	0.000000	0.514000	10.000000
O1	2a	1.000000	0.000000	0.000000	0.477600	10.000000
O2	4e	1.000000	0.500000	0.252400	0.229800	10.000000
Bi	2a	0.050000	0.000000	0.000000	0.000000	10.000000
Ba	2a	0.050000	0.000000	0.000000	0.000000	10.000000
Zn	2b	0.050000	0.500000	0.000000	0.514000	10.000000

Table B. 3.: Occupancy, atomic fract. coordinates and Biso for orthorhombic KBBNZ x=0.10

B.1.1.3. x=0.15

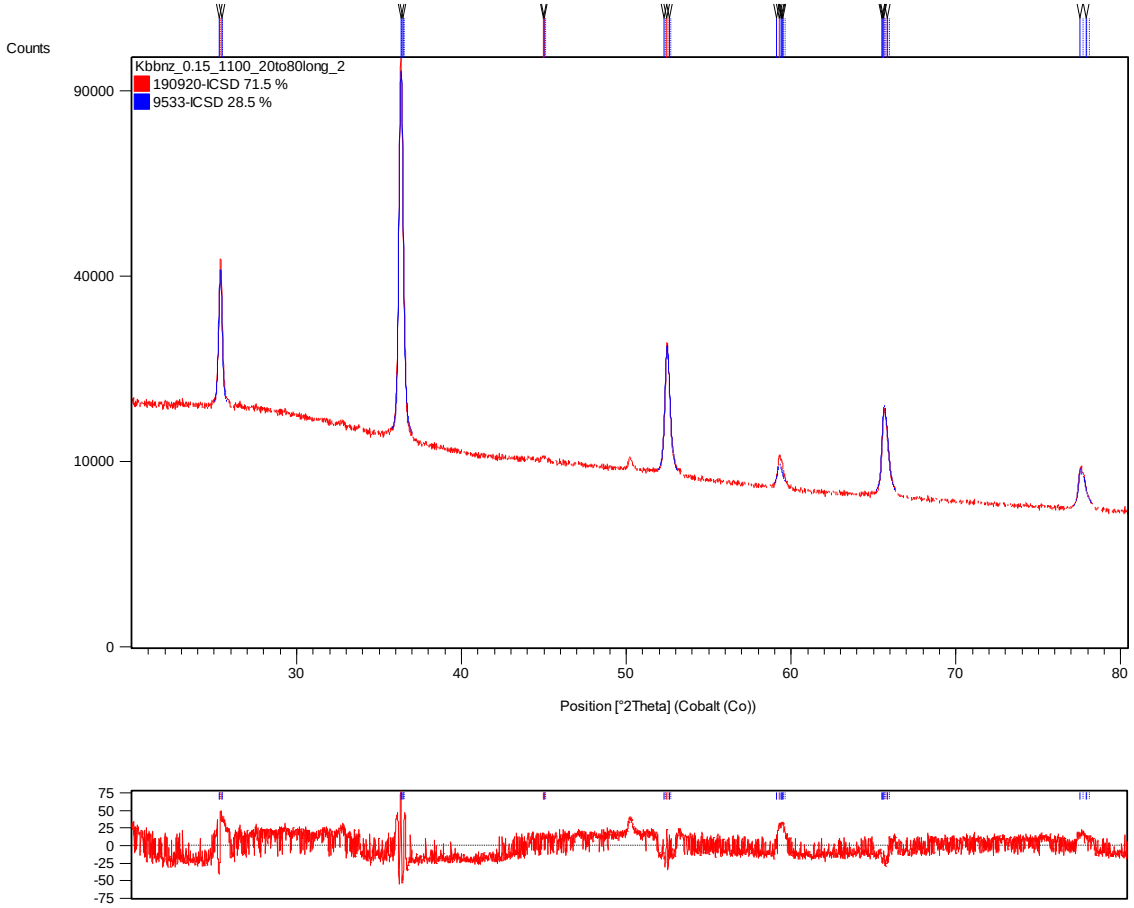


Figure B. 4.: Experimental X-ray diffraction data (red), calculated fitting profile (blue) and difference plot for KBNNZ x=0.15

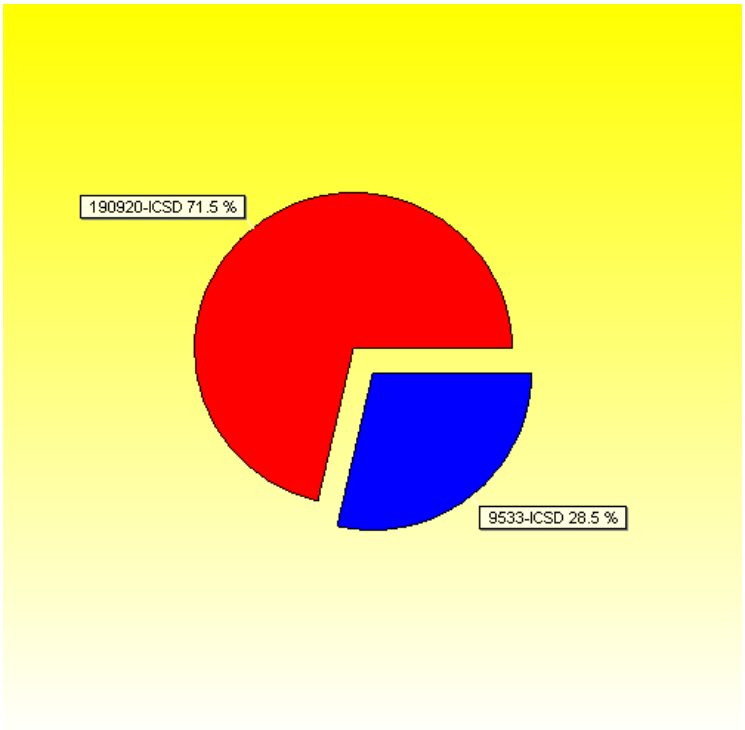


Figure B. 5.: The pie chart represents the percent quantity of the two polymorphs (orthorhombic and cubic) for KBBNZ x=0.15.

Atom	Wyck.	s.o.f.	x	y	z	Biso/ 10^4 pm^2
K1	1b	0.850000	0.500000	0.500000	0.500000	0.020500
Nb1	1a	0.925000	0.000000	0.000000	0.000000	0.015490
O1	3d	1.000000	0.500000	0.000000	0.000000	0.000000
Ba	1b	0.075000	0.500000	0.500000	0.500000	0.020500
Bi	1b	0.075000	0.500000	0.500000	0.500000	0.020500
Zn	1a	0.075000	0.000000	0.000000	0.000000	0.015490

Table B. 4.: Occupancy, atomic fract. coordinates and Biso for cubic KBBNZ x=0.15

Atom	Wyck.	s.o.f.	x	y	z	Biso/ 10^4 pm^2
K1	2b	0.850000	0.500000	0.000000	0.513800	0.000000
Nb1	2a	0.925000	0.000000	0.000000	0.000000	0.000000

O1	2b	1.000000	0.500000	0.000000	0.036400	0.000000
O2	4d	1.000000	0.000000	0.252400	0.284200	0.000000
Ba	2b	0.075000	0.500000	0.000000	0.513800	0.000000
Bi	2b	0.075000	0.500000	0.000000	0.513800	0.000000
zn	2a	0.075000	0.000000	0.000000	0.000000	0.000000

Table B. 5.: Occupancy, atomic fract. coordinates and Biso for orthorhombic KBBNZ x=0.15

B.1.1.4. x=0.20

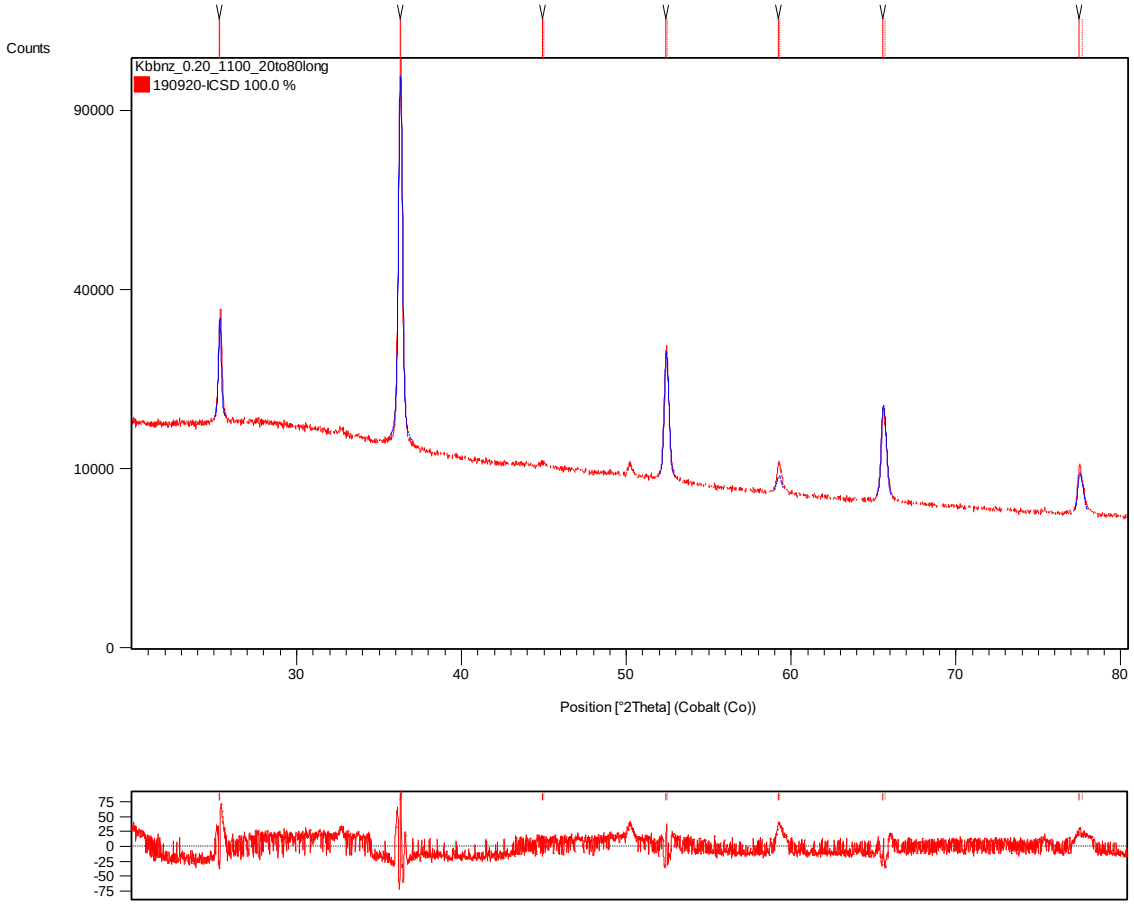


Figure B. 6: Experimental X-ray diffraction data (red), calculated fitting profile (blue) and difference plot for KBNNZ x=0.20

Atom	Wyck.	s.o.f.	x	y	z	Biso/ 10^4 pm^2
K1	1b	0.800000	0.500000	0.500000	0.500000	0.020500

Nb1	1a	0.900000	0.000000	0.000000	0.000000	0.015490
O1	3d	1.000000	0.500000	0.000000	0.000000	0.000000
Ba	1b	0.100000	0.500000	0.500000	0.500000	0.020500
bi	1b	0.100000	0.500000	0.500000	0.500000	0.020500
zn	1a	0.100000	0.000000	0.000000	0.000000	0.015490

Table B. 6.: Occupancy, atomic fract. coordinates and Biso for cubic KBBNZ x=0.05

B.1.1.5 x=0.25

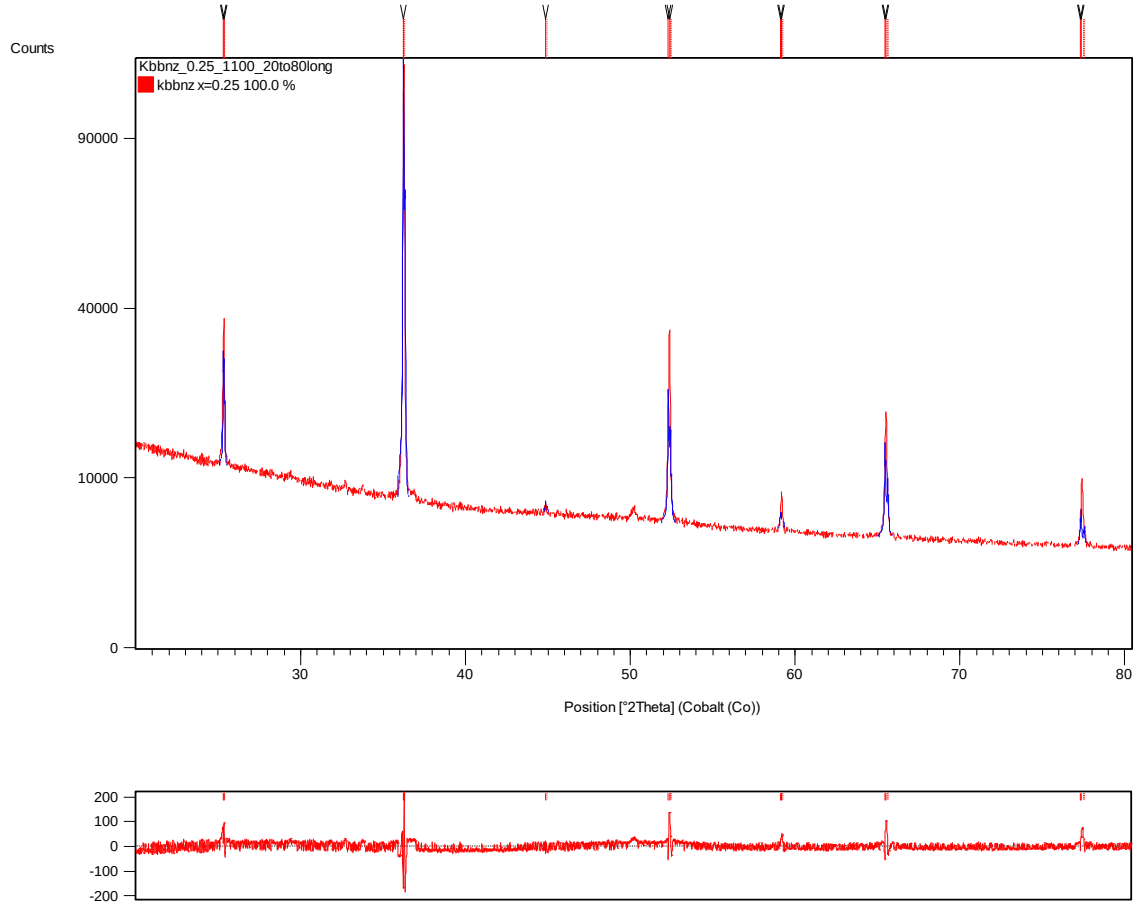


Figure B. 7 Experimental X-ray diffraction data (red), calculated fitting profile (blue) and difference plot for KBNNZ x=0.25.

Atom	Wyck.	s.o.f.	x	y	z	Biso/ 10^4 pm^2
K	1a	0.750000	0.000000	0.000000	0.000000	0.500000
Ba	1a	0.125000	0.000000	0.000000	0.000000	0.500000

Bi	1a	0.125000	0.000000	0.000000	0.000000	0.500000
Nb	1b	0.875000	0.500000	0.500000	0.450222	0.500000
Zn	1b	0.125000	0.500000	0.500000	0.517100	0.500000
O	1b	1.000000	0.500000	0.500000	-0.026000	0.500000
O	2c	1.000000	0.000000	0.500000	0.406751	0.500000

Table B. 7.: Occupancy, atomic fract. coordinates and Biso for cubic KBBNZ x=0.25

B.2. EDX measurements

B.2.1. (1-x) $KNbO_3$-x $BaBiNbZnO_3$ (KNBBZ)

B.2.1.1 x=0.05

K (%)	Nb (%)	Ba (%)	Bi (%)	Zn (%)	K/Nb	K/Ba	K/Bi	K/Zn
47.5	48.75	1.25	1.25	1.25	0.974	38	38	38

Table B. 8.: Atomic percent of K, Nb, Ba, Bi, Zn and molar relations for the nominal KNBBZ x=0.05composition.

	K (%)	Nb (%)	Ba (%)	Bi (%)	Zn (%)	K/Nb	K/Ba	K/Bi	K/Zn
1	51.82	46.82	0.54	0.56	0.26	1.107	96	84	199
2	50.68	46.59	1.11	1.28	0.34	1.088	46	36	149
3	49.73	47.03	1.29	1.47	0.47	1.057	39	32	106
4	50.75	46.64	1.06	1.05	0.50	1.088	48	44	102
5	49.35	46.97	1.78	1.38	0.52	1.051	28	34	95
6	49.75	47.32	1.30	1.07	0.56	1.051	38	44	89
7	49.94	47.66	1.00	0.84	0.57	1.048	50	57	88
8	50.35	46.66	1.21	1.20	0.58	1.079	42	39	87

9	47.33	49.22	1.95	0.95	0.56	0.962	24	52	85
10	49.75	46.83	1.53	1.29	0.60	1.062	33	36	83
11	50.34	46.98	0.95	1.07	0.67	1.072	53	44	75
12	44.11	49.72	3.57	1.97	0.64	0.887	12	25	69
13	48.49	47.26	1.73	1.61	0.90	1.026	28	29	54
14	49.55	46.69	1.19	1.12	1.46	1.061	42	42	34

Table B. 9.: Experimental atomic percent of K, Nb, Ba, Bi, Zn and molar relations for KNBBZ x=0.05 composition by EDX spectra.

B.2.1.2. x=0.10

K (%)	Nb (%)	Ba (%)	Bi (%)	Zn (%)	K/Nb	K/Ba	K/Bi	K/Zn
45	47.5	2.5	2.5	2.5	0.947	18	18	18

Table B. 10.: Atomic percent of K, Nb, Ba, Bi, Zn and molar relations for the nominal KNBBZ x=0.10 composition.

	K (%)	Nb (%)	Ba (%)	Bi (%)	Zn (%)	K/Nb	K/Ba	K/Bi	K/Zn
1	30.37	55.72	9.61	4.29	0.00	0.545	3	7	-
2	51.84	45.84	0.64	1.53	0.16	1.131	81	34	324
3	29.99	55.54	10.20	4.06	0.21	0.540	3	7	143
4	39.43	50.62	6.17	3.27	0.50	0.779	6	12	79
5	50.63	45.93	1.45	1.22	0.77	1.102	35	42	66
6	50.58	46.07	1.57	0.75	1.02	1.098	32	67	50
7	28.74	55.09	10.88	4.65	0.64	0.522	3	6	45
8	47.47	47.65	2.52	1.25	1.10	0.996	19	38	43

9	34.92	52.83	8.01	3.31	0.94	0.661	4	11	37
10	49.39	45.74	1.60	1.76	1.51	1.080	31	28	33
11	49.77	45.00	1.87	1.81	1.56	1.106	27	27	32
12	23.99	57.30	13.16	4.79	0.76	0.419	2	5	32
13	49.77	46.02	1.00	1.29	1.93	1.081	50	39	26
14	48.59	45.21	1.79	2.19	2.23	1.075	27	22	22
15	46.86	44.88	3.38	2.43	2.46	1.044	14	19	19
16	32.69	53.33	7.58	4.52	1.88	0.613	4	7	17
17	38.29	50.87	5.53	3.11	2.21	0.753	7	12	17

Table B. 11.: Experimental atomic percent of K, Nb, Ba, Bi, Zn and molar relations for the nominal KNBBZ x=0.10 composition by EDX spectra.

B.2.1.3. x=0.15

K (%)	Nb (%)	Ba (%)	Bi (%)	Zn (%)	K/Nb	K/Ba	K/Bi	K/Zn
42.5	46.25	3.75	3.75	3.75	0.919	11.333	11.333	11.333

Table B. 12.: Atomic percent of K, Nb, Ba, Bi, Zn and molar relations for the nominal KNBBZ x=0.15composition.

	K (%)	Nb (%)	Ba (%)	Bi (%)	Zn (%)	K/Nb	K/Ba	K/Bi	K/Zn
1	46.73	45.58	2.78	2.71	2.21	1.025	17	17	21
2	47.06	45.04	2.7	2.8	2.41	1.045	17	17	20
3	45.78	45.24	3.14	3.27	2.57	1.012	15	14	18
4	45.78	45.24	3.14	3.27	2.57	1.012	15	14	18
5	45.52	45.06	3.13	3.56	2.72	1.010	15	13	17
6	45.19	45.31	3.73	3.04	2.73	0.997	12	15	17

7	39.6	47.16	5.45	4.65	3.13	0.840	7	9	13
8	43.49	45.28	4.29	3.4	3.53	0.960	10	13	12
9	34.64	50.62	7.14	4.75	2.86	0.684	5	7	12
10	44.17	44.55	3.92	3.71	3.65	0.991	11	12	12
11	46.33	44.95	2.2	2.61	3.91	1.031	21	18	12
12	41.65	45.46	4.82	4.5	3.56	0.916	9	9	12
13	42	45.26	5.09	3.33	4.31	0.928	8	13	10
14	42.15	44.08	5.41	3.82	4.54	0.956	8	11	9

Table B. 13.: Experimental atomic weight of K, Nb, Ba, Bi, Zn and molar relations for the nominal KNBBZ x=0.15 composition by EDX spectra.

B.2.1.4 x=0.20

K (%)	Nb (%)	Ba (%)	Bi (%)	Zn (%)	K/Nb	K/Ba	K/Bi	K/Zn
40	45	5	5	5	0.889	8	8	8

Table B. 14.: Atomic percent of K, Nb, Ba, Bi, Zn and molar relations for the nominal KNBBZ x=0.20 composition.

	K (%)	Nb (%)	Ba (%)	Bi (%)	Zn (%)	K/Nb	K/Ba	K/Bi	K/Zn
1	43.46	44.12	4.34	4.74	3.34	0.985	10	9	13
2	42.93	43.54	4.73	4.9	3.90	0.986	9	9	11
3	43.10	43.58	3.89	5.43	4.00	0.989	11	8	11
4	42.24	43.71	5.00	4.99	4.06	0.966	8	8	10
5	42.16	43.82	4.66	5.2	4.15	0.962	9	8	10
6	41.76	43.76	5.13	5.13	4.22	0.954	8	8	10
7	42.83	43.58	3.99	5.26	4.33	0.983	11	8	10

8	41.31	43.63	5.73	4.95	4.39	0.947	7	8	9
9	40.62	44.09	5.38	5.36	4.55	0.921	8	8	9
10	39.93	43.78	5.7	5.6	4.98	0.912	7	7	8

Table B. 15.: Experimental atomic percent of K, Nb, Ba, Bi, Zn and molar relations for the nominal KNBBZ x=0.20 composition by EDX spectra.

B.2.1.5. x=0.25

K (%)	Nb (%)	Ba (%)	Bi (%)	Zn (%)	K/Nb	K/Ba	K/Bi	K/Zn
37.5	43.75	6.25	6.25	6.25	0.857	6	6	6

Table B. 16.: Atomic percent of K, Nb, Ba, Bi, Zn and molar relations for the nominal KNBBZ x=0.25 composition.

	K (%)	Nb (%)	Ba (%)	Bi (%)	Zn (%)	K/Nb	K/Ba	K/Bi	K/Zn
1	39.68	43.54	5.04	6.40	5.34	0.911	8	6	7
2	37.57	43.38	6.73	6.33	5.99	0.866	6	6	6
3	39.20	43.02	4.59	6.85	6.34	0.911	9	6	6
4	36.52	43.46	8.61	5.48	5.92	0.840	4	7	6
5	39.74	43.05	3.92	6.61	6.67	0.923	10	6	6
6	36.52	43.04	8.30	6.00	6.13	0.849	4	6	6
7	36.28	43.03	9.27	5.24	6.18	0.843	4	7	6
8	37.40	43.17	6.35	6.61	6.47	0.866	6	6	6
9	37.23	43.53	6.08	6.35	6.80	0.855	6	6	5
10	37.13	43.04	6.56	6.36	6.92	0.863	6	6	5
11	36.78	42.36	8.12	5.82	6.92	0.868	5	6	5
12	36.42	42.62	6.96	6.50	7.49	0.855	5	6	5

13	35.68	42.57	9.30	5.06	7.40	0.838	4	7	5
14	36.08	42.46	7.87	5.73	7.86	0.850	5	6	5
15	35.48	42.39	7.82	6.00	8.31	0.837	5	6	4

Table B. 17.: Experimental atomic percent of K, Nb, Ba, Bi, Zn and molar relations for the nominal KNBBZ x=0.25 composition by EDX spectra.

B.3. P-E and S-E loops

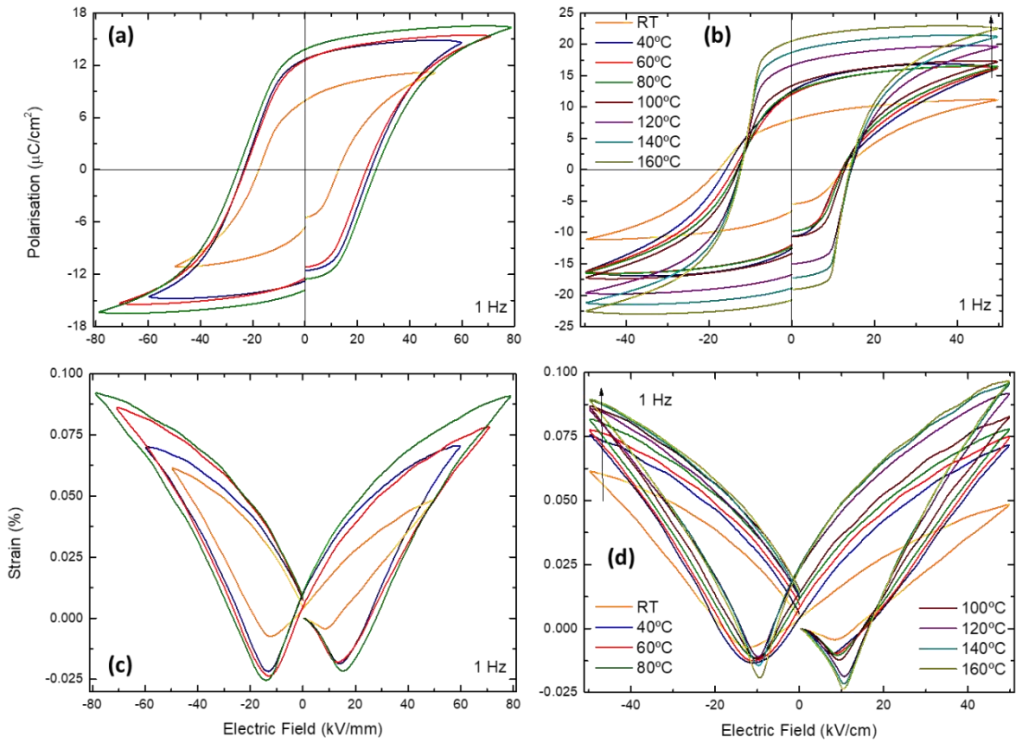


Figure B. 8: (a) P-E and (c) S-E loops up to 80 kV/cm at RT. (b) P-E and (d) S-E loops from RT up to 200º under electric field of 50 kV/cm for KN at 1 Hz.

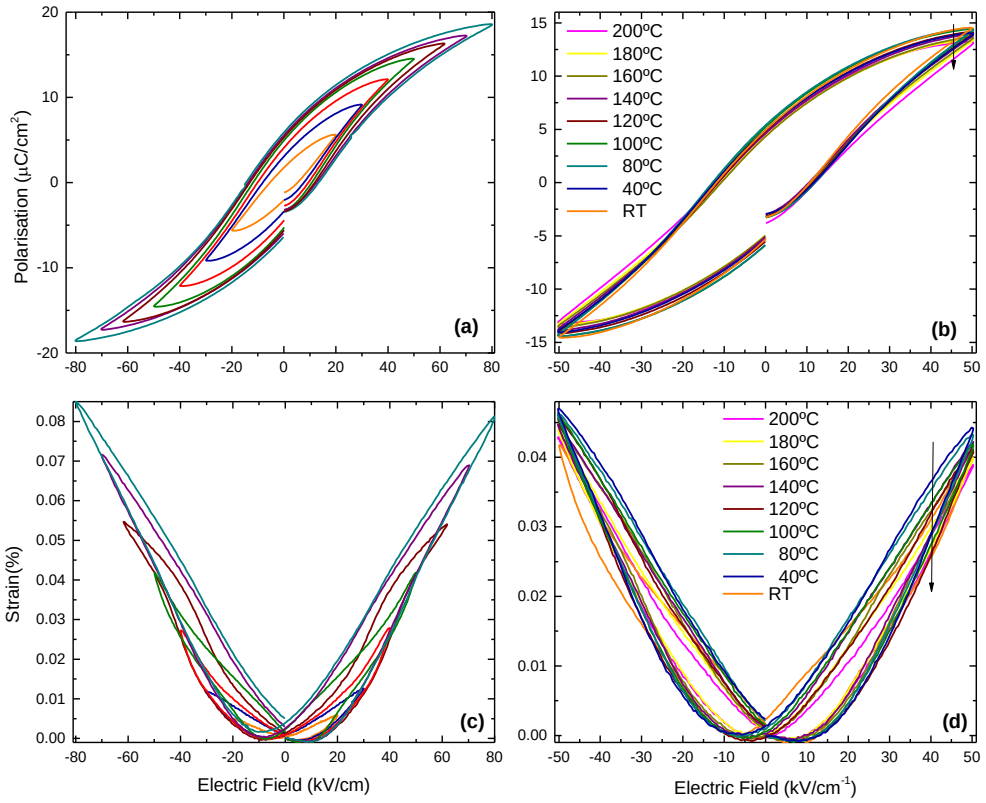


Figure B. 9: (a) P-E and (c) S-E loops up to 80 kV/cm at RT. (b) P-E and (d) S-E loops from RT up to 200º under electric field of 50 kV/cm for KBBNZ x=0.05 at 1 Hz.

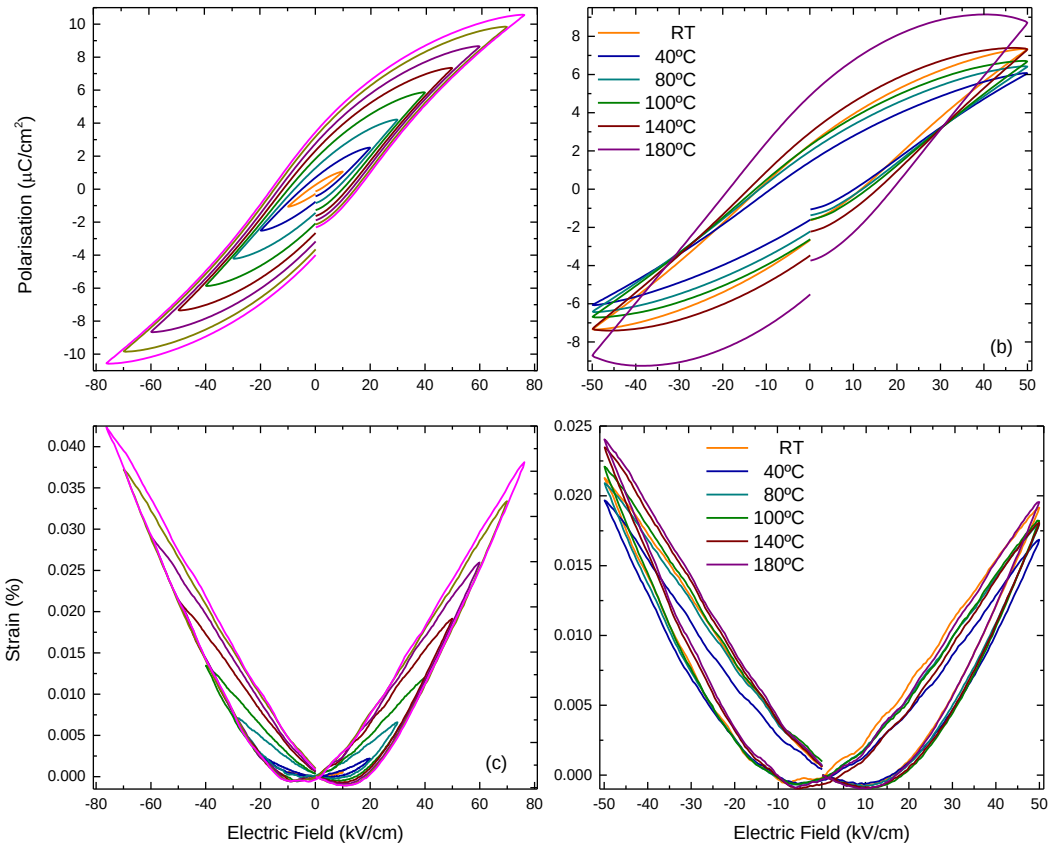


Figure B. 10: (a) P-E and (c) S-E loops up to 80 kV/cm at RT. (b) P-E and (d) S-E loops from RT up to 200º under electric field of 50 kV/cm for KBBNZ x=0.05 at 1 Hz.

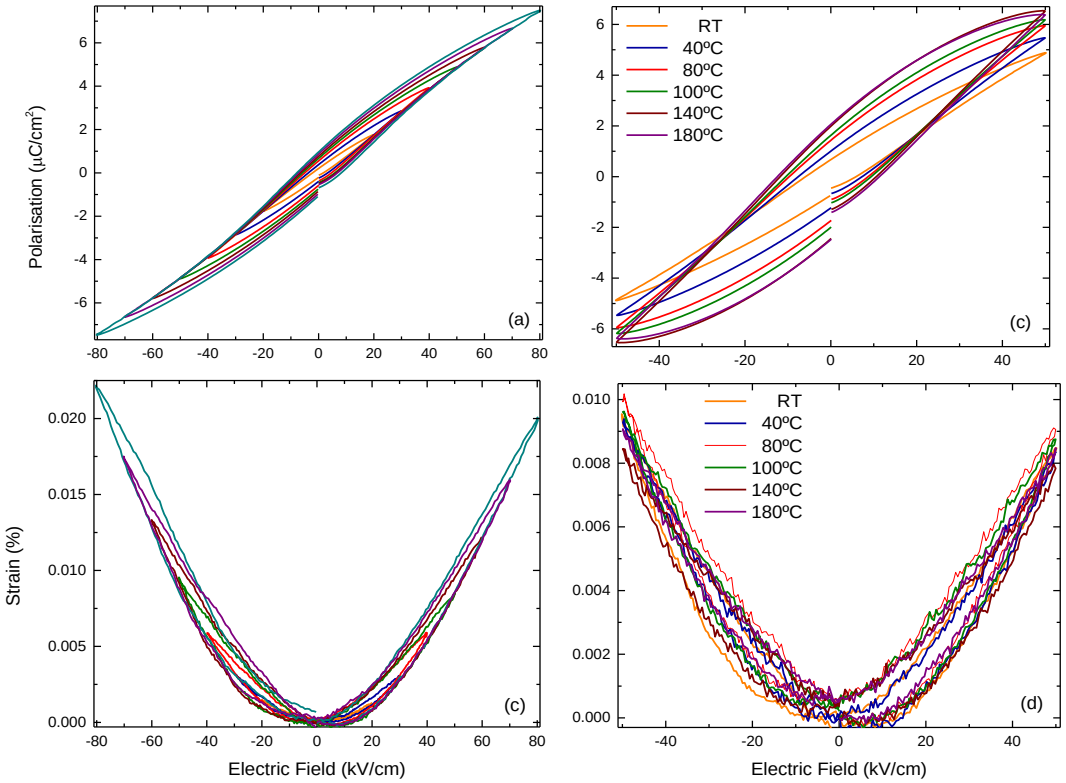


Figure B. 11.:(a) P-E and (c) S-E loops up to 80 kV/cm at RT. (b) P-E and (d) S-E loops from RT up to 180ºC under electric field of 50 kV/cm for KBBNZ x=0.15 at 1 Hz.

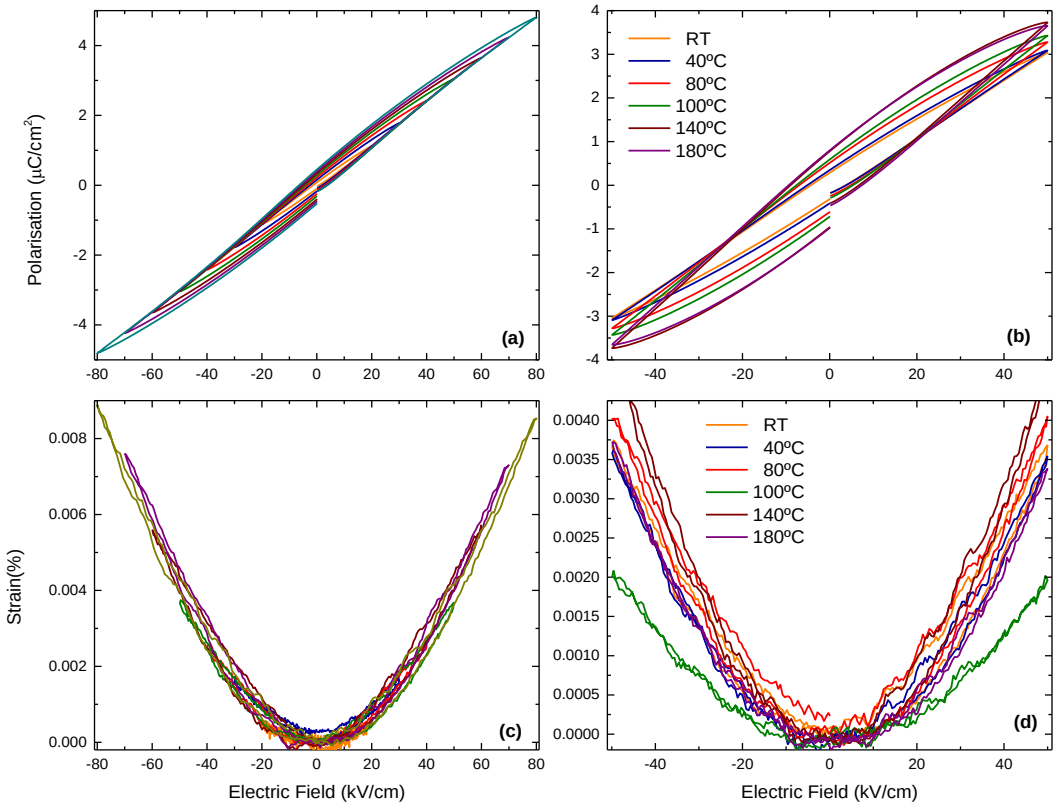


Figure B.12.: (a) P-E and (c) S-E loops up to 80 kV/cm at RT. (b) P-E and (d) S-E loops from RT up to 180ºC under electric field of 50 kV/cm for KBBNZ x=0.20 at 1 Hz.

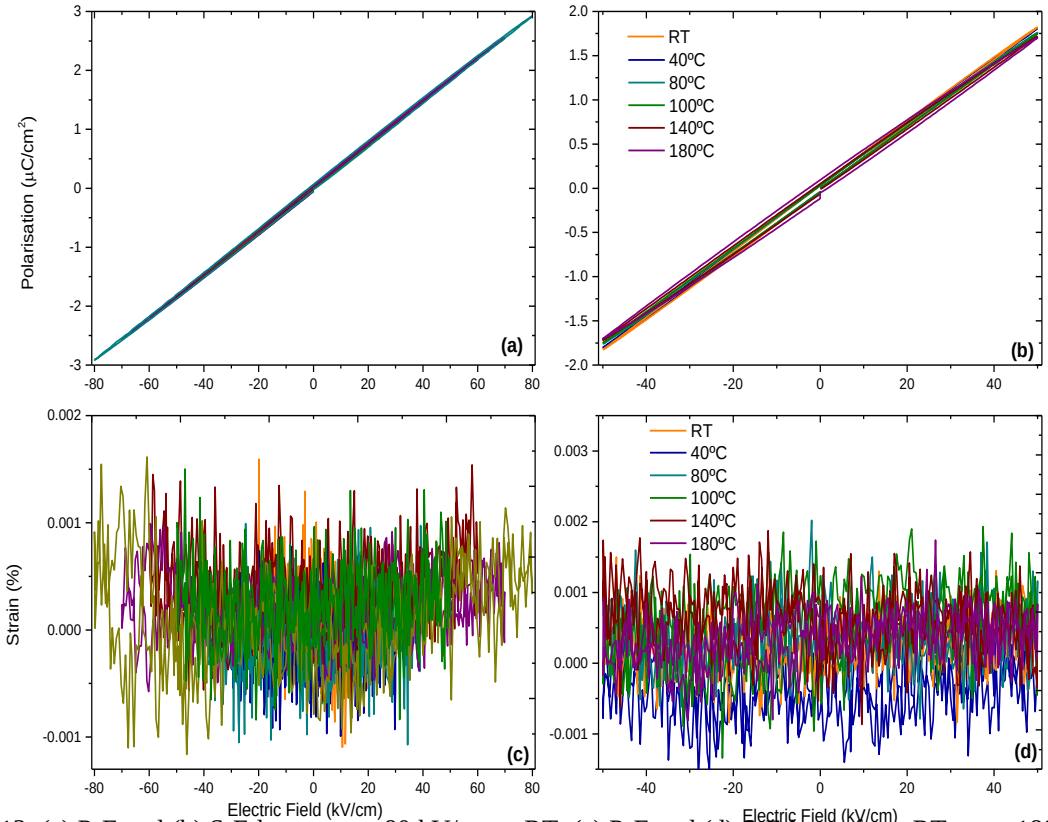


Figure B. 13: (a) P-E and (b) S-E loops up to 80 kV/cm at RT. (c) P-E and (d) S-E loops from RT up to 180ºC under electric field of 50 kV/cm for KBBNZ x=0.25 at 1 Hz.

APPENDIX C

Chapter 5: System (1-x) $KNbO_3$- x $BiFeO_3$

C.1. Rietveld Refinements plots

C.1.1. (1-x) $KNbO_3$- x $BiFeO_3$

C.1.1.1. x=0.05

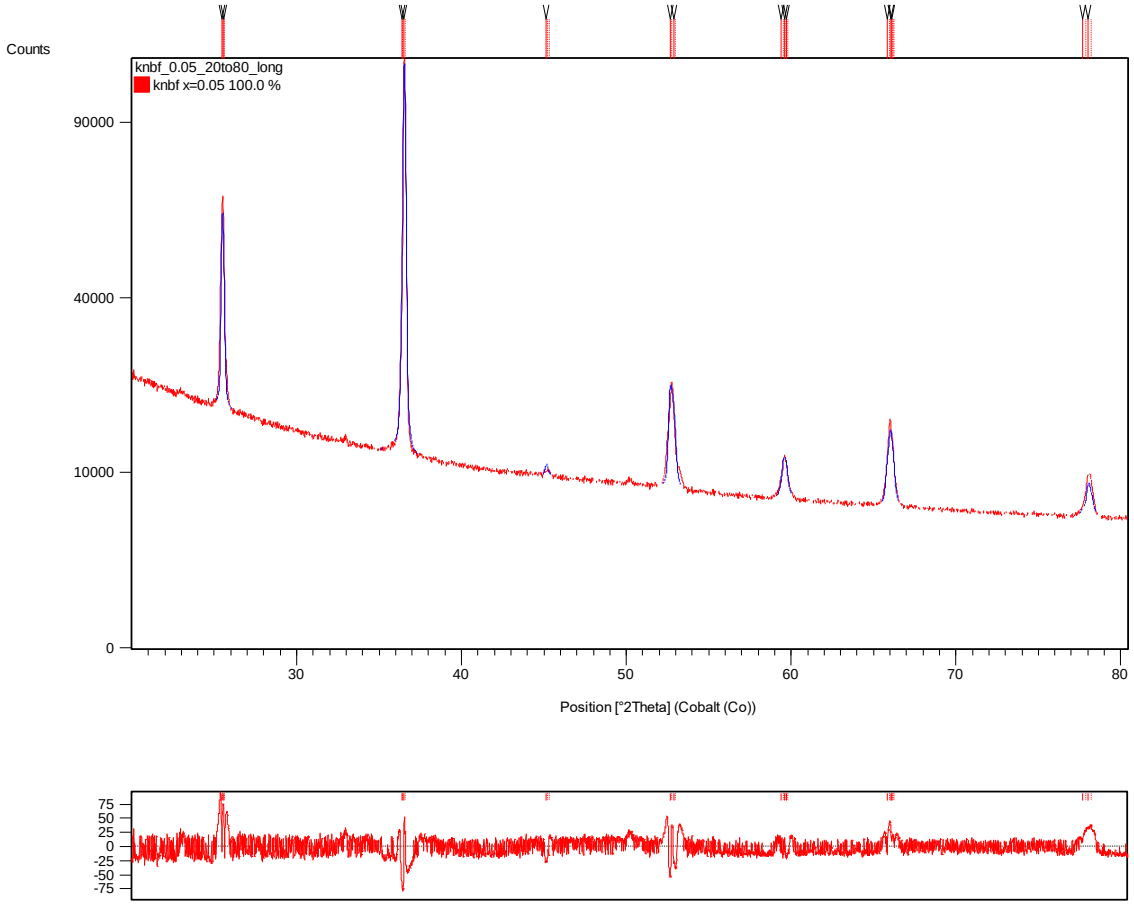


Figure C. 1.: Experimental X-ray diffraction data (red), calculated fitting profile (blue) and difference plot for KNBF x=0.05.

Atom	Wyck.	s.o.f.	x	y	z	Biso/ 10^4 pm^2
K	2a	0.950000	0.000000	0.000000	0.000000	0.500000
Bi	2a	0.050000	0.000000	0.000000	0.000000	0.500000
Nb	2b	0.950000	0.500000	0.000000	0.5435(9)	0.500000
Fe	2b	0.050000	0.500000	0.000000	0.515500	0.500000
O	2a	1.000000	0.000000	0.000000	0.481000	0.500000
O	4e	1.000000	0.500000	0.284807	0.288864	0.500000

Table C. 1.: Occupancy, atomic fract. coordinates and Biso for orthorhombic KNBF x=0.05

C.1.1.2. x=0.10

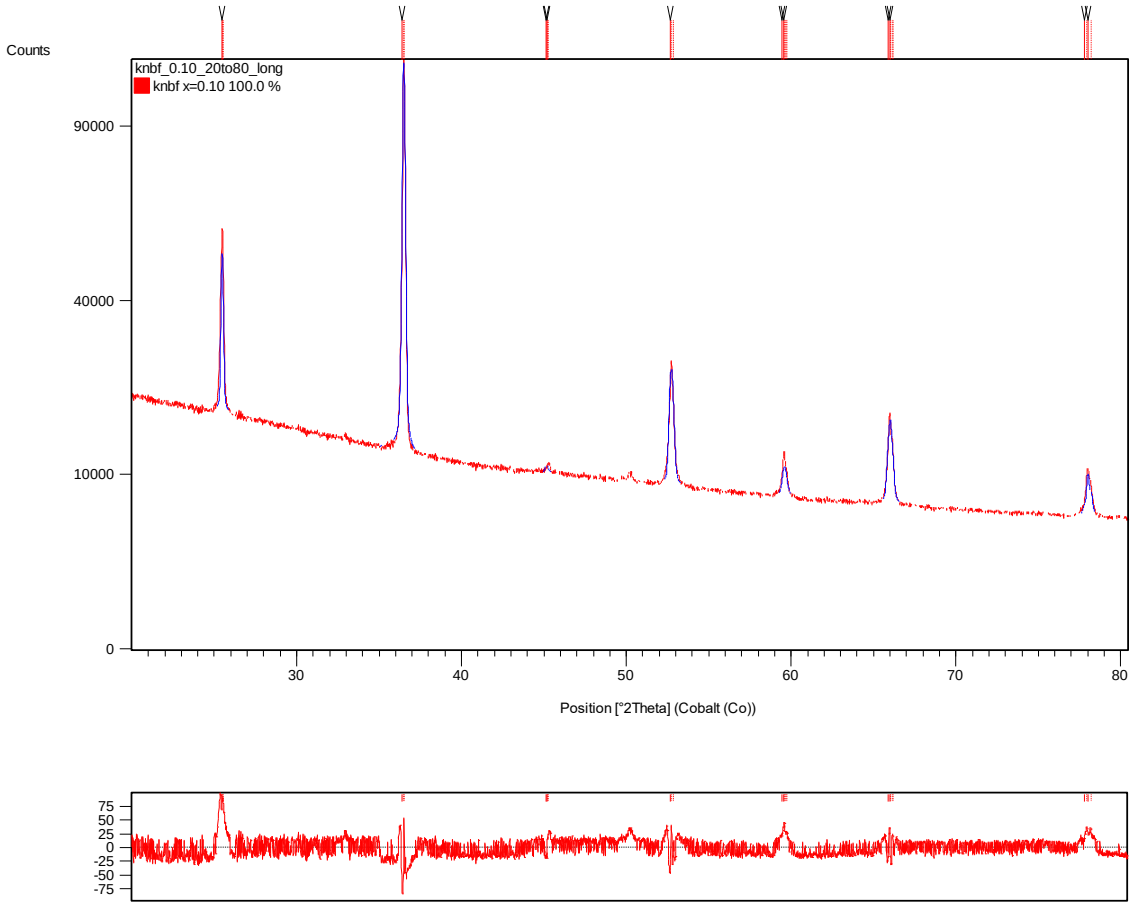


Figure C. 2.: Experimental X-ray diffraction data (red), calculated fitting profile (blue) and difference plot for KNBF x=0.10.

Atom	Wyck.	s.o.f.	x	y	z	Biso/ 10^4 pm^2
K	2a	0.900000	0.000000	0.000000	0.000000	0.500000
Bi	2a	0.100000	0.000000	0.000000	0.000000	0.500000
Nb	2b	0.900000	0.500000	0.000000	0.529697	0.500000
Fe	2b	0.100000	0.500000	0.000000	0.515500	0.500000
O	2a	1.000000	0.000000	0.000000	0.481000	0.500000
o	4e	1.000000	0.500000	0.717720	0.272945	0.500000

Table C. 2.: Occupancy, atomic fract. coordinates and Biso for orthorhombic KNBF x=0.10

C.1.1.3. X=0.15

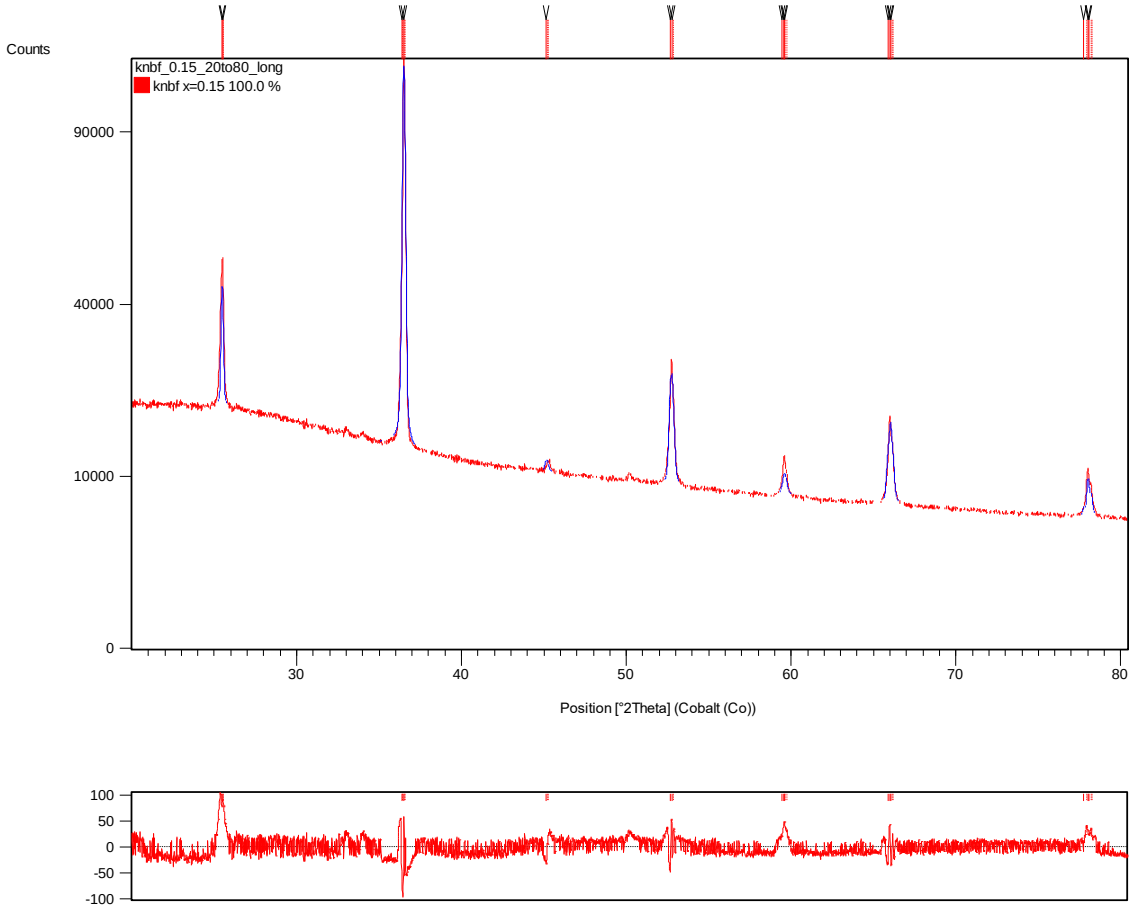


Figure C. 3.: Experimental X-ray diffraction data (red), calculated fitting profile (blue) and difference plot for KNBF x=0.15.

Atom	Wyck.	s.o.f.	x	y	z	Biso/ 10^4 pm^2

K	2a	0.850000	0.000000	0.000000	0.000000	0.500000
Bi	2a	0.150000	0.000000	0.000000	0.000000	0.500000
Nb	2b	0.850000	0.500000	0.000000	0.537619	0.500000
Fe	2b	0.150000	0.500000	0.000000	0.515500	0.500000
0	2a	1.000000	0.000000	0.000000	0.481000	0.500000
o	4e	1.000000	0.500000	0.296350	0.279225	0.500000

Table C. 3.: Occupancy, atomic fract. coordinates and Biso for orthorhombic KNBF x=0.15.

C.1.1.4. X=0.20

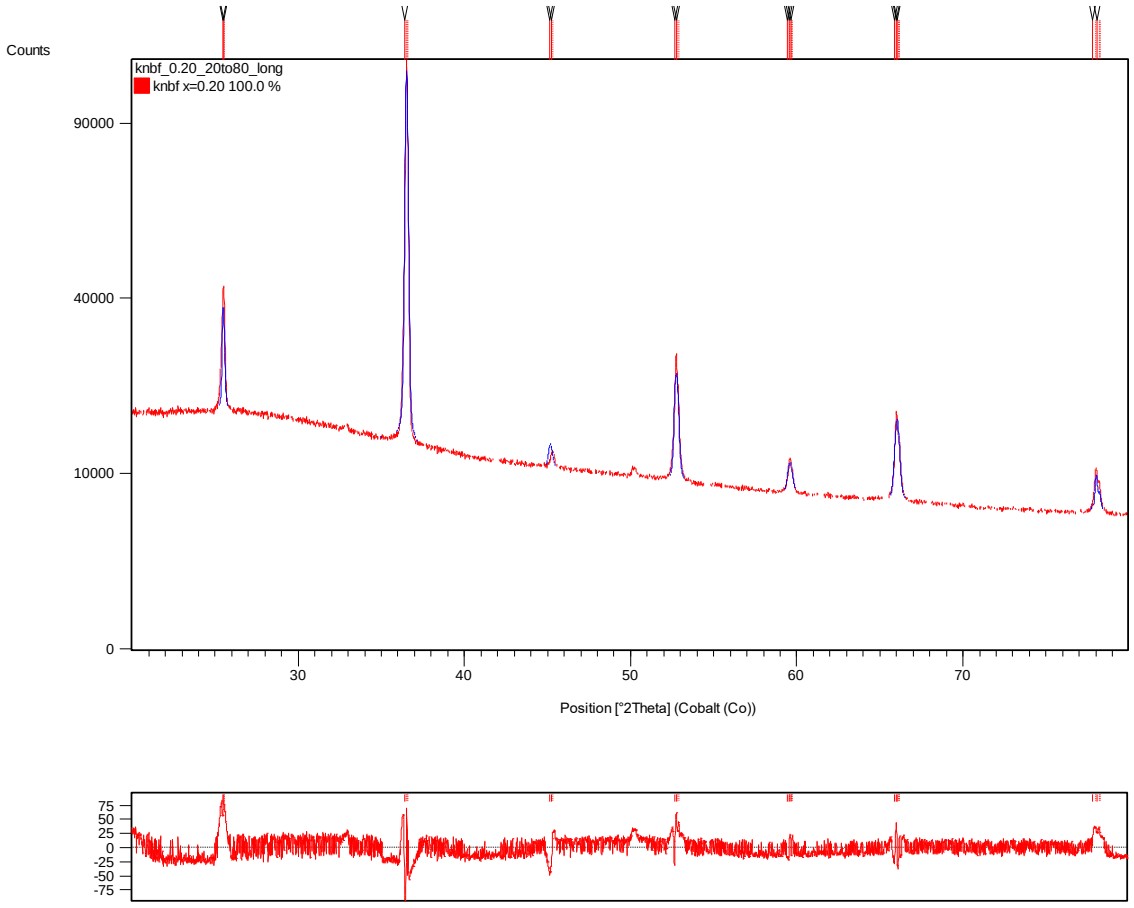


Figure C. 4.: Experimental X-ray diffraction data (red), calculated fitting profile (blue) and difference plot for KNBF x=0.20.

Atom	Wyck.	s.o.f.	x	y	z	Biso/ 10^4 pm^2

K	2a	0.800000	0.000000	0.000000	0.000000	0.500000
Bi	2a	0.200000	0.000000	0.000000	0.000000	0.500000
Nb	2b	0.800000	0.500000	0.000000	0.566504	0.500000
Fe	2b	0.200000	0.500000	0.000000	0.515500	0.500000
O	2a	1.000000	0.000000	0.000000	0.481000	0.500000
o	4e	1.000000	0.500000	0.305515	0.313098	0.500000

Table C. 4.: Occupancy, atomic fract. coordinates and Biso for orthorhombic KNBF x=0.20

C.1.1.5 X=0.25

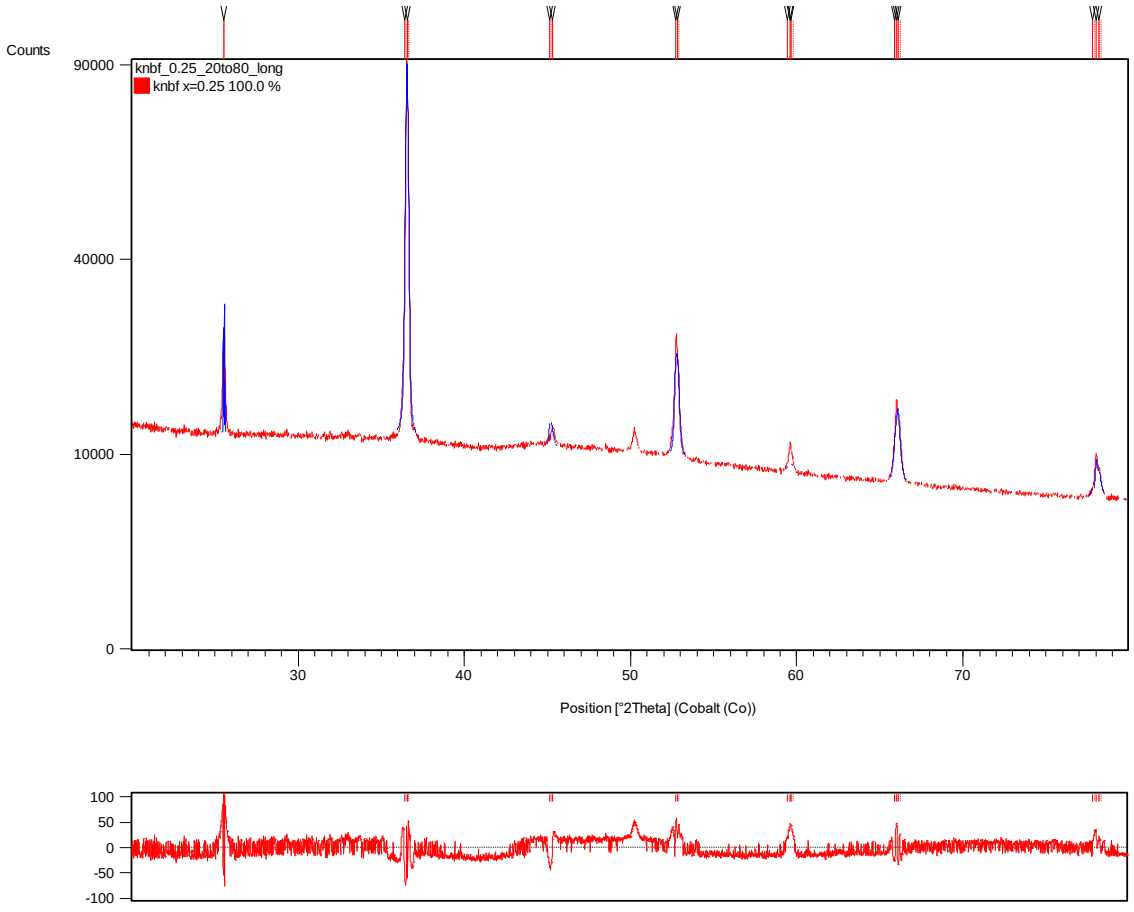


Figure C. 5.: Experimental X-ray diffraction data (red), calculated fitting profile (blue) and difference plot for KNBF x=0.25.

Atom	Wyck.	s.o.f.	x	y	z	Biso/ 10^4 pm^2

k	2a	0.750000	0.000000	0.000000	0.000000	0.500000
Bi	2a	0.250000	0.000000	0.000000	0.000000	0.500000
Nb	2b	0.750000	0.500000	0.000000	0.538650	0.500000
Fe	2b	0.250000	0.500000	0.000000	0.515500	0.500000
O	2a	1.000000	0.000000	0.000000	0.481000	0.500000
O	4e	1.000000	0.500000	0.252700	0.229800	0.500000

Table C. 5.: Occupancy, atomic fract. coordinates and Biso for orthorhombic KNBF x=0.25.

C.2. EDX measurements

C.2.1. (1-x) $KNbO_3$- x $BiFeO_3$

C.2.1.1. x=0.05

K(%)	Nb(%)	Bi(%)	Fe(%)	K/Nb	K/Bi	K/Fe
47.5	47.5	2.5	2.5	1	19	19

Table C. 6.: Atomic weight of K, Nb, Bi, Fe and molar relations for the nominal KNBF x=0.05composition.

	K(%)	Nb(%)	Bi(%)	Fe(%)	K/Nb	K/Bi	K/Fe
1	48.90	49.90	4.70	0.50	0.980	10	98
2	44.90	48.00	1.30	0.80	0.935	35	56
3	47.50	48.60	1.50	1.10	0.977	32	43
4	38.10	50.80	1.40	1.10	0.750	27	35
5	46.60	50.80	1.40	1.10	0.917	33	42
6	44.80	48.60	1.50	1.10	0.922	30	41
7	47.20	48.40	3.00	1.10	0.975	16	43
8	46.60	49.30	3.00	1.50	0.945	16	31
9	44.80	46.40	3.80	1.70	0.966	12	26

10	47.20	48.60	2.40	1.80	0.971	20	26
11	38.80	48.60	2.40	1.80	0.798	16	22
12	44.90	48.00	2.80	2.10	0.935	16	21
13	47.10	48.00	2.90	2.30	0.981	16	20
14	48.90	47.00	4.40	2.40	1.040	11	20
15	50.00	45.90	3.70	3.00	1.089	14	17
16	46.20	44.20	5.60	3.20	1.045	8	14
17	47.00	47.30	4.50	3.40	0.994	10	14
18	47.40	47.30	4.50	3.40	1.002	11	14
19	48.10	45.80	5.60	3.70	1.050	9	13
20	46.20	45.50	10.80	5.60	1.015	4	8

Table C. 7.: Experimental atomic weight of K, Nb, Bi, Fe and molar relations for KNBF x=0.05 composition by EDX spectra.

C.2.1.2. x=0.10

K(%)	Nb(%)	Bi(%)	Fe(%)	K/Nb	K/Bi	K/Fe
45	45	5	5	1	9	9

Table C. 8.: Atomic weight of K, Nb, Bi, Fe and molar relations for the nominal KNBF x=0.10 composition

	K(%)	Nb(%)	Bi(%)	Fe(%)	K/Nb	K/Bi	K/Fe
1	48.4	47.4	3.4	0.8	1.021	14	61
2	47.8	49.1	1.7	1.5	0.974	28	32
3	46	48.9	3.6	1.5	0.941	13	31
4	46.7	47.1	4.3	1.9	0.992	11	25
5	47.5	47.6	2.8	2.1	0.998	17	23
6	46.7	48.9	2.2	2.2	0.955	21	21

7	45.6	49.1	2.7	2.7	0.929	17	17
8	46.1	45.9	5.1	3	1.004	9	15
9	45.1	46.1	5.5	3.2	0.978	8	14
10	50.5	36.5	9.3	3.7	1.384	5	14
11	43.9	47.9	4.2	4	0.916	10	11
12	43.4	47.8	4.4	4.4	0.908	10	10
13	43.1	45.8	6.4	4.6	0.941	7	9
14	45	44.4	5.6	5.1	1.014	8	9
15	39.2	41.5	10	9.3	0.945	4	4
16	37.2	34.6	15.5	12.8	1.075	2	3
17	38.5	35.7	12.1	13.6	1.078	3	3

Table C. 9.: Experimental atomic weight of K, Nb, Bi, Fe and molar relations for KNBF x=0.10 composition by EDX spectra.

C.2.1.3. x=0.15

K(%)	Nb(%)	Bi(%)	Fe(%)	K/Nb	K/Bi	K/Fe
42.5	42.5	7.5	7.5	1	5.67	5.67

Table C. 10.: Atomic weight of K, Nb, Bi, Fe and molar relations for the nominal KNBF x=0.15 composition.

	K(%)	Nb(%)	Bi(%)	Fe(%)	K/Nb	K/Bi	K/Fe
1	45.8	46.8	5	2.3	0.979	9	20
2	44.4	47.2	5.6	2.7	0.941	8	16
3	47.5	46.3	3.3	3	1.026	14	16
4	47	45.4	4.6	3.1	1.035	10	15
5	47	44.2	5.6	3.2	1.063	8	15

6	43.2	47.8	5.6	3.5	0.904	8	12
7	43.3	45.1	6.8	4.8	0.960	6	9
8	43.4	43.3	8	5.3	1.002	5	8
9	42.4	43	6.8	7.7	0.986	6	6
10	42.4	43	6.8	7.7	0.986	6	6
11	38.8	42.3	10.2	8.7	0.917	4	4
12	39.7	38.5	11.1	10.7	1.031	4	4
13	37.9	37.7	12.5	11.9	1.005	3	3
14	37.2	36.4	13.2	13.1	1.022	3	3
15	35.9	32.5	16.5	15.1	1.105	2	2
16	20.8	24.8	30.6	23.8	0.839	1	1

Table C. 11.: Experimental atomic weight of K, Nb, Bi, Fe and molar relations for KNBF x=0.15 composition by EDX spectra.

C.2.1.4. x=0.20

K(%)	Nb(%)	Bi(%)	Fe(%)	K/Nb	K/Bi	K/Fe
40	40	10	10	1	4	4

Table C. 12.: Atomic weight of K, Nb, Bi, Fe and molar relations for the nominal KNBF x=0.20 composition.

	K(%)	Nb(%)	Bi(%)	Fe(%)	K/Nb	K/Bi	K/Fe
1	44.90	46.90	5.00	3.20	0.957	9	14
2	46.10	43.70	5.80	4.40	1.055	8	10
3	44.50	44.60	6.30	4.70	0.998	7	9
4	44.50	44.60	6.30	4.70	0.998	7	9
5	42.30	46.90	6.00	4.80	0.902	7	9
6	43.10	43.50	7.80	5.60	0.991	6	8

7	44.30	41.60	7.50	6.50	1.065	6	7
8	41.60	44.30	7.50	6.50	0.939	6	6
9	40.40	41.50	11.40	6.70	0.973	4	6
10	42.30	41.80	8.70	7.20	1.012	5	6
11	41.40	41.20	10.00	7.40	1.005	4	6
12	39.20	40.10	13.30	7.40	0.978	3	5
13	39.30	40.40	11.90	8.50	0.973	3	5
14	40.60	38.70	11.40	9.30	1.049	4	4
15	40.60	38.70	11.40	9.30	1.049	4	4
16	39.70	38.50	11.10	10.70	1.031	4	4
17	32.40	36.10	18.50	12.90	0.898	2	3
18	32.60	31.30	20.50	15.50	1.042	2	2

Table C. 13.: Experimental atomic weight of K, Nb, Bi, Fe and molar relations for KNBF x=0.20 composition by EDX spectra.

C.2.1.5. x=0.25

K(%)	Nb(%)	Bi(%)	Fe(%)	K/Nb	K/Bi	K/Fe
37.5	37.5	12.5	12.5	1	3	3

Table C. 14.: Atomic weight of K, Nb, Bi, Fe and molar relations for the nominal KNBF x=0.25 composition

	K(%)	Nb(%)	Bi(%)	Fe(%)	K/Nb	K/Bi	K/Fe
1	44.4	45.3	6.8	3.6	0.980	7	12
2	42	39.5	12.4	6.1	1.063	3	7
3	39.7	41.6	11.8	6.8	0.954	3	6

4	41.4	41.2	10	7.4	1.005	4	6
5	36.2	42.9	13.9	7.1	0.844	3	5
6	40.5	40.4	10.5	8.5	1.002	4	5
7	39.3	40.4	11.9	8.5	0.973	3	5
8	39.7	38.5	11.1	10.7	1.031	4	4
9	39.7	36.7	12	11.7	1.082	3	3
10	33.3	41.7	14.4	10.6	0.799	2	3
11	34.6	37	15.9	12.6	0.935	2	3
12	33.7	37.2	16.5	12.7	0.906	2	3
13	34	34.7	17.4	13.9	0.980	2	2
14	33.8	35.4	15.5	15.2	0.955	2	2
15	32.9	36.1	15.9	15.1	0.911	2	2
16	32.6	31.3	20.5	15.5	1.042	2	2
17	30	38.4	17	14.6	0.781	2	2
18	30.4	32.7	19.4	17.5	0.930	2	2
19	29.5	29.6	21.4	19.5	0.997	1	2
20	27.5	27	23.5	22.1	1.019	1	1
21	26.3	23.8	27.3	22.6	1.105	1	1

Table C. 15.: Experimental atomic weight of K, Nb, Bi, Fe and molar relations for KNBF x=0.25 composition by EDX spectra.

APPENDIX D

Chapter 6: System (1-x) $KNbO_3$- x $BiMnO_3$

D.1. Rietveld Refinements plots

D.1.1. (1-x) $KNbO_3$- x $BiMnO_3$

D.1.1.1. x=0.05

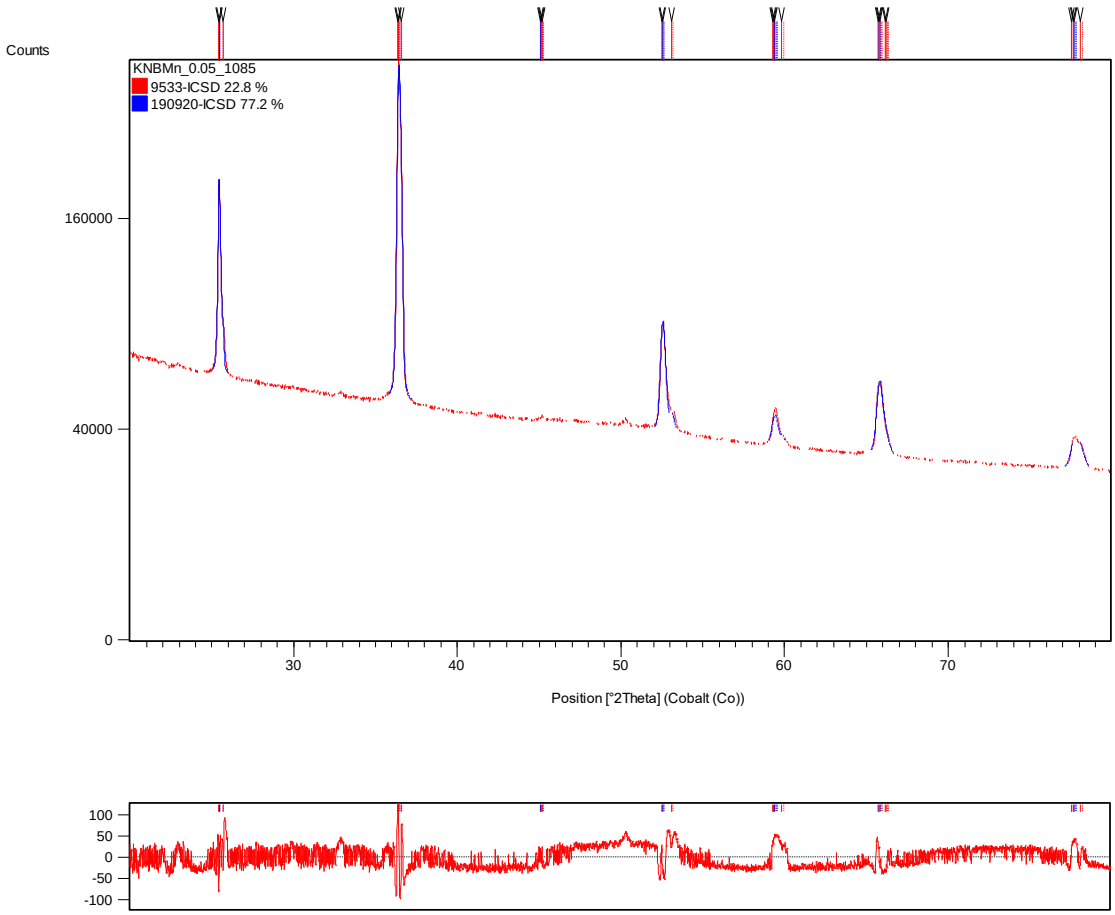


Figure D. 1.: Experimental X-ray diffraction data (red), calculated fitting profile (blue) and difference plot for KNBM x=0.05.

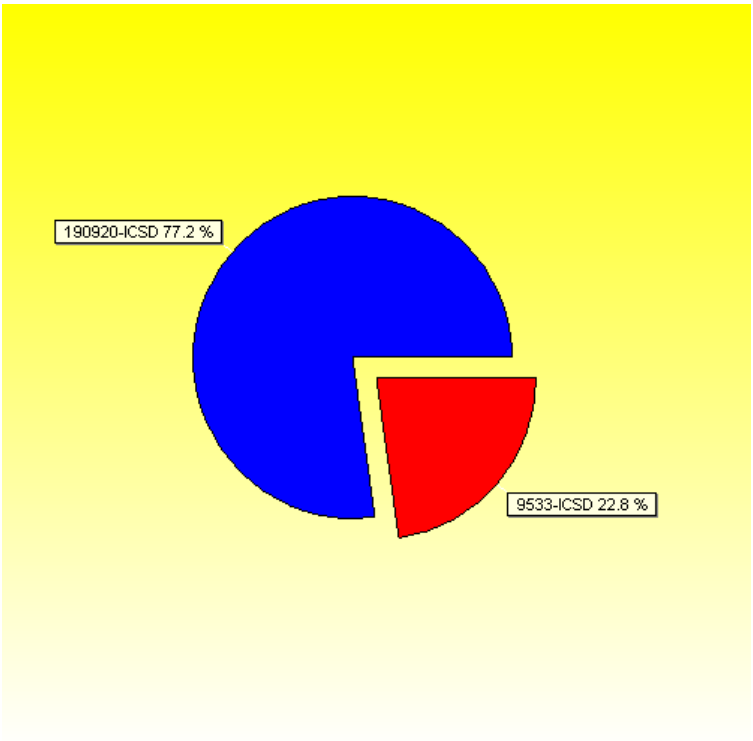


Figure D. 2.: The pie chart represents the percent quantity of the two polymorphs (orthorhombic and cubic) for KNBM x=0.05.

Atom	Wyck.	s.o.f.	x	y	z	Biso/ 10^4 pm^2
K1	2b	0.950000	0.500000	0.000000	0.513800	0.000000
Nb1	2a	0.950000	0.000000	0.000000	0.000000	0.000000
O1	2b	1.000000	0.500000	0.000000	0.036400	0.000000
O2	4d	1.000000	0.000000	0.252400	0.284200	0.000000
Bi	2b	0.050000	0.500000	0.000000	0.513800	0.000000
Mn	2a	0.050000	0.000000	0.000000	0.000000	0.000000

Table D. 1.: Occupancy, atomic fraction coordinates and Biso for orthorhombic KNBF x=0.05.

Atom	Wyck.	s.o.f.	x	y	z	Biso/ 10^4 pm^2
K1	1b	0.950000	0.500000	0.500000	0.500000	0.020500
Nb1	1a	0.950000	0.000000	0.000000	0.000000	0.015490
O1	3d	1.000000	0.500000	0.000000	0.000000	0.000000
Bi	1b	0.050000	0.500000	0.500000	0.500000	0.020500
Mn	1a	0.050000	0.000000	0.000000	0.000000	0.015490

Table D. 2.: Occupancy, atomic fraction coordinates and Biso for cubic KNBF x=0.05.

D.1.1.2. x=0. 10

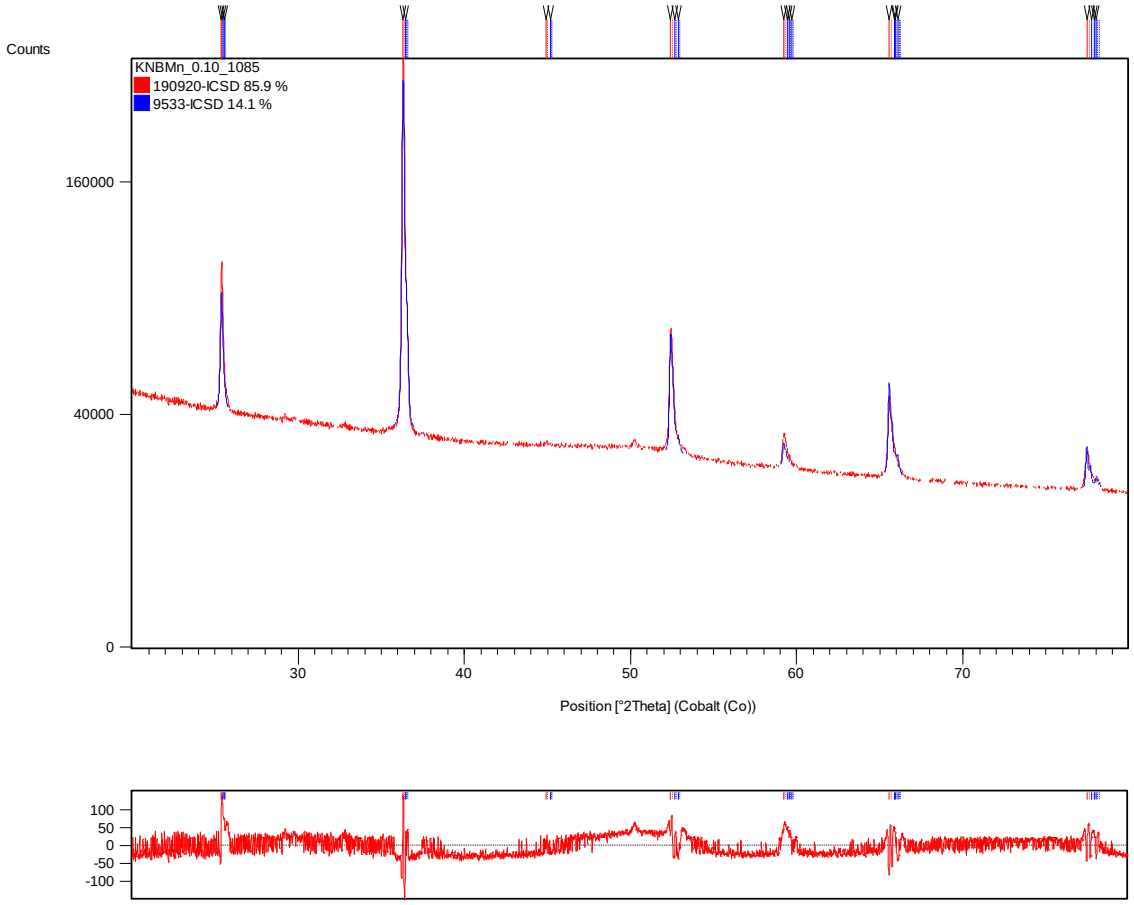


Figure D. 3.: Experimental X-ray diffraction data (red), calculated fitting profile (blue) and difference plot for KNBM x=0.10.

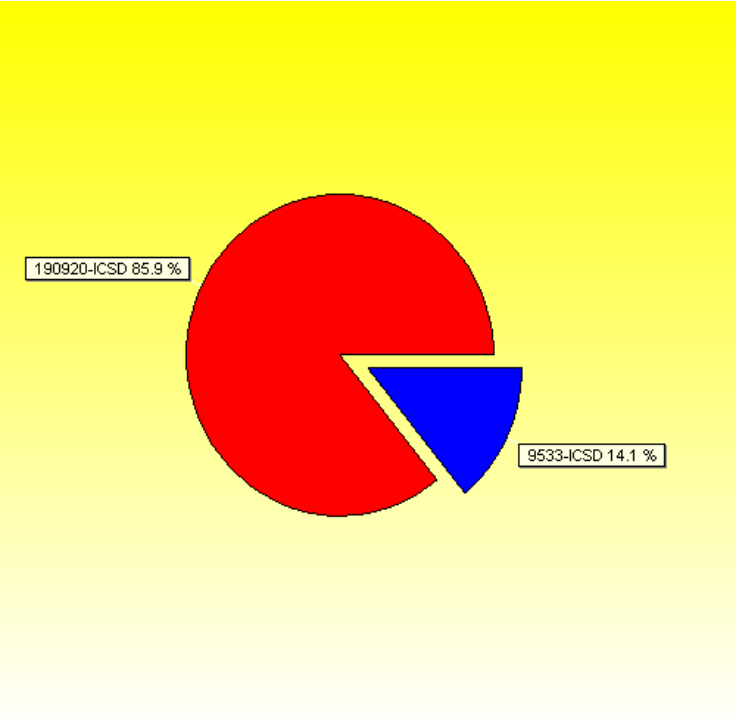


Figure D. 4.: The pie chart represents the percent quantity of the two polymorphs (orthorhombic and cubic) for KNBM x=0.10.

Atom	Wyck.	s.o.f.	x	y	z	Biso/ 10^4 pm^2
K1	1b	0.900000	0.500000	0.500000	0.500000	0.020500
Nb1	1a	0.900000	0.000000	0.000000	0.000000	0.015490
O1	3d	1.000000	0.500000	0.000000	0.000000	0.000000
bi	1b	0.100000	0.500000	0.500000	0.500000	0.020500
Mn	1a	0.100000	0.000000	0.000000	0.000000	0.015490

Table D. 3.: Occupancy, atomic fraction coordinates and Biso for cubic. KNBF x=0.10.

Atom	Wyck.	s.o.f.	x	y	z	Biso/ 10^4 pm^2
K1	2b	0.900000	0.500000	0.000000	0.513800	0.000000
Nb1	2a	0.900000	0.000000	0.000000	0.000000	0.000000
O1	2b	1.000000	0.500000	0.000000	0.036400	0.000000

O2	4d	1.000000	0.000000	0.252400	0.284200	0.000000
Bi	2b	0.100000	0.500000	0.000000	0.513800	0.000000
Mn	2a	0.100000	0.000000	0.000000	0.000000	0.000000

Table D. 4.: Occupancy, atomic fraction coordinates and Biso for orthorhombic KNBF x=0.10.

D.1.1.3. x=0.15

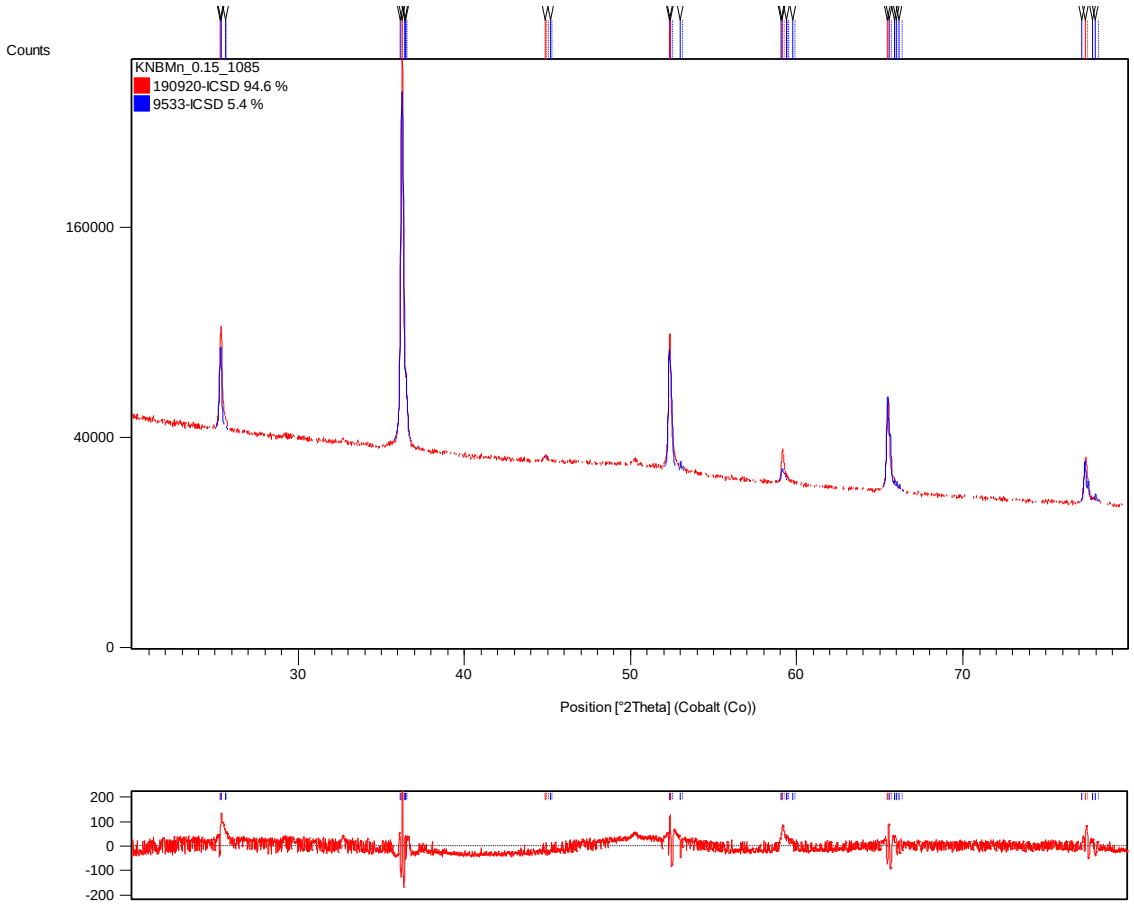


Figure D. 5.: Experimental X-ray diffraction data (red), calculated fitting profile (blue) and difference plot for KNBM x=0.15.

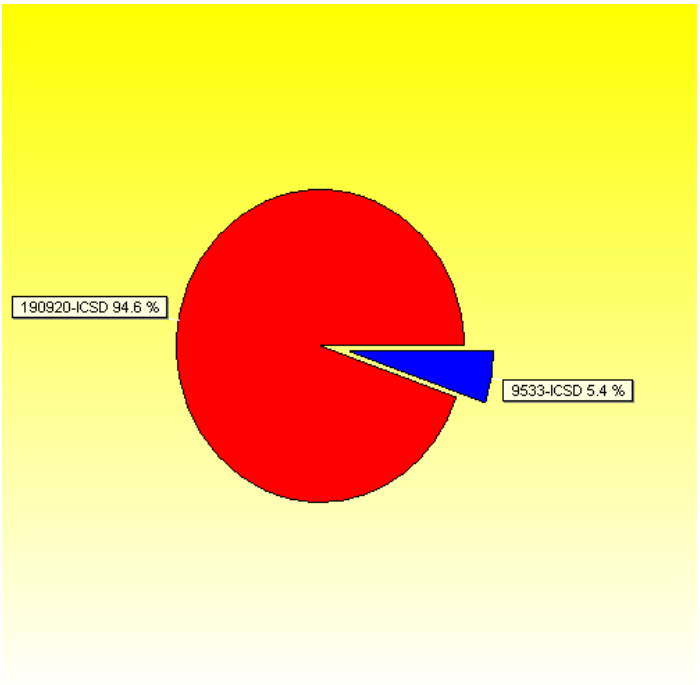


Figure D. 6.: The pie chart represents the percent quantity of the two polymorphs (orthorhombic and cubic) for KNBM x=0.15.

Atom	Wyck.	s.o.f.	x	y	z	Biso/ 10^4 pm^2
K1	1b	0.850000	0.500000	0.500000	0.500000	0.020500
Nb1	1a	0.850000	0.000000	0.000000	0.000000	0.015490
O1	3d	1.000000	0.500000	0.000000	0.000000	0.000000
Bi	1b	0.150000	0.500000	0.500000	0.500000	0.020500
Mn	1a	0.150000	0.000000	0.000000	0.000000	0.015490

Table D. 5.: Occupancy, atomic fraction coordinates and Biso for cubic KNBF x=0.15.

Atom	Wyck.	s.o.f.	x	y	z	Biso/ 10^4 pm^2
K1	2b	0.850000	0.500000	0.000000	0.513800	0.000000
Nb1	2a	0.850000	0.000000	0.000000	0.000000	0.000000
O1	2b	1.000000	0.500000	0.000000	0.036400	0.000000
O2	4d	1.000000	0.000000	0.252400	0.284200	0.000000
Bi	2b	0.150000	0.500000	0.000000	0.513800	0.000000
Mn	2a	0.150000	0.000000	0.000000	0.000000	0.000000

Table D. 6.: Occupancy, atomic fraction coordinates and Biso for orthorhombic KNBF x=0.15.

D.1.1.4. x=0.20

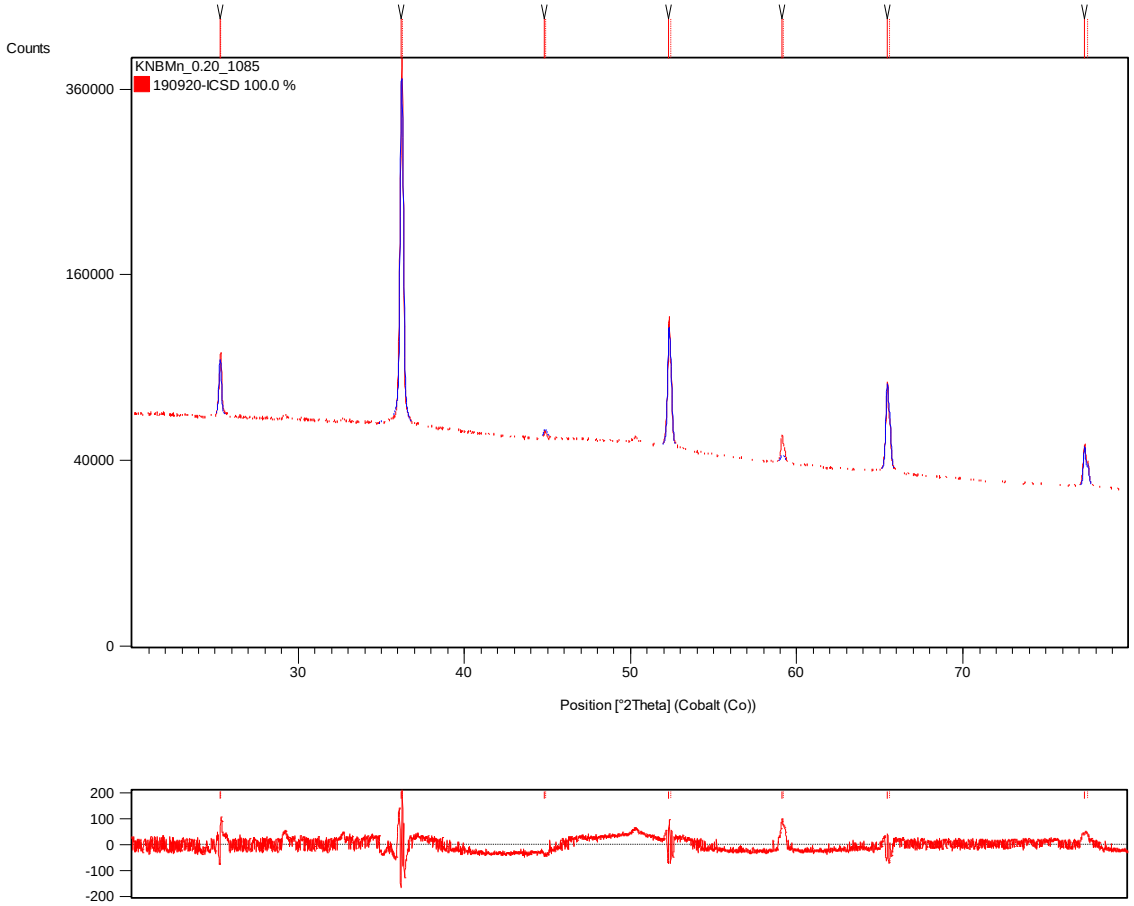


Figure D. 7.: Experimental X-ray diffraction data (red), calculated fitting profile (blue) and difference plot for KNBM x=0.20.

Atom	Wyck.	s.o.f.	x	y	z	Biso/ 10^4 pm^2
K1	1b	0.800000	0.500000	0.500000	0.500000	0.020500
Nb1	1a	0.800000	0.000000	0.000000	0.000000	0.015490
O1	3d	1.000000	0.500000	0.000000	0.000000	0.000000
Bi	1b	0.200000	0.500000	0.500000	0.500000	0.020500
Mn	1a	0.200000	0.000000	0.000000	0.000000	0.015490

Table D. 7.: Occupancy, atomic fraction coordinates and Biso for cubic KNBF x=0.20.

D.1.1.5. x=0.25

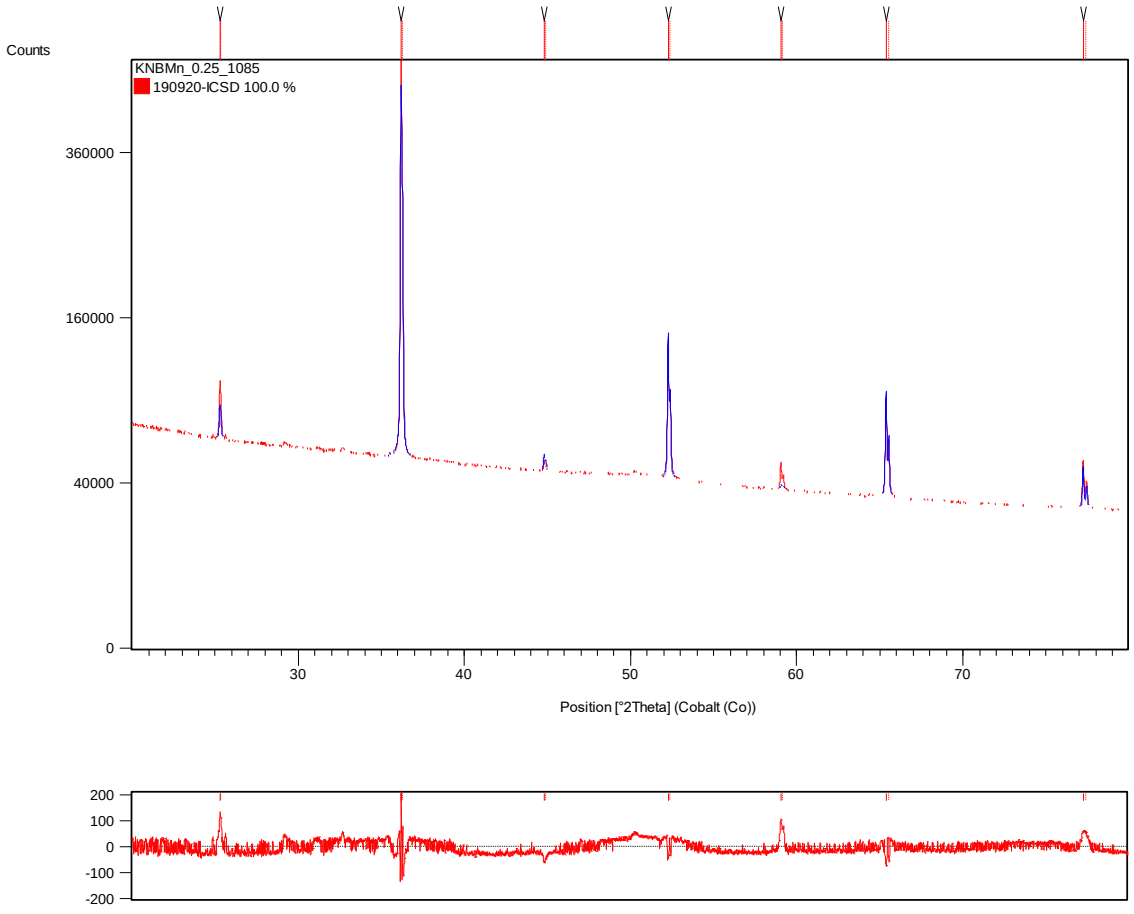


Figure D. 8.: Experimental X-ray diffraction data (red), calculated fitting profile (blue) and difference plot for KNBM x=0.25.

Atom	Wyck.	s.o.f.	x	y	z	Biso/ 10^4 pm^2
K1	1b	0.750000	0.500000	0.500000	0.500000	0.020500
Nb1	1a	0.750000	0.000000	0.000000	0.000000	0.015490
O1	3d	1.000000	0.500000	0.000000	0.000000	0.000000
Bi	1b	0.250000	0.500000	0.500000	0.500000	0.020500
Mn	1a	0.250000	0.000000	0.000000	0.000000	0.015490

Table D. 8.: Occupancy, atomic fraction coordinates and Biso for cubic KNBF x=0.25.

D.2. EDX measurements

D.2.1. (1-x) $KNbO_3$- x $BiMnO_3$

D.2.1.1. x=0.05

K (%)	Nb (%)	Bi (%)	Mn (%)	K/Nb	K/Bi	K/Mn
47.5	47.5	2.5	2.5	1	19	19

Table D. 9: Atomic weight of K, Nb, Bi, Mn and molar relations for the nominal KNBM x=0.05composition

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	K (%)	Nb (%)	Bi (%)	Mn (%)	K/Nb	K/Bi	K/Mn
1	48.32	42.78	8.36	0.55	1.129	6	88
2	48.96	47.16	3.05	0.83	1.038	16	59
3	43.78	45.69	9.46	1.07	0.958	5	41
4	41.44	48.51	7.5	2.54	0.854	6	16
5	48.84	44.27	3.83	3.06	1.103	13	16
6	45.88	46.49	4.26	3.37	0.987	11	14
7	43.97	47.25	5.4	3.38	0.931	8	13
8	43.69	44.99	7.24	4.08	0.971	6	11

9	44.61	43.67	7.17	4.55	1.022	6	10
10	40.67	45.17	9.63	4.53	0.900	4	9
11	46.01	43.71	4.8	5.48	1.053	10	8
12	43.52	42.11	9.13	5.24	1.033	5	8
13	44.4	43.96	5.9	5.74	1.010	8	8
14	44.88	40.15	8.92	6.05	1.118	5	7
15	40.19	44.16	9.78	5.87	0.910	4	7

Table D. 10 Experimental atomic weight of K, Nb, Bi, n and molar relations for KNBM x=0.05 composition by EDX spectra.

D.2.1.2. x=0.10

K (%)	Nb (%)	Bi (%)	Mn (%)	K/Nb	K/Bi	K/Mn
45	45	5	5	1	9	9

Table D. 11: Atomic weight of K, Nb, Bi, Mn and molar relations for the nominal KNBM x=0.10 composition.

	K (%)	Nb (%)	Bi (%)	Mn (%)	K/Nb	K/Bi	K/Mn
1	57.04	34.3	5.14	3.53	1.663	11	16
2	56.72	32.89	6.13	4.26	1.725	9	13
3	41.2	45.69	9.51	3.6	0.902	4	11
4	43.09	44.03	8.31	4.58	0.979	5	9
5	43.1	43.1	8.26	5.54	1.000	5	8
6	45.5	39.7	8.88	5.92	1.146	5	8
7	43.07	42.31	8.81	5.81	1.018	5	7
8	40.7	41.04	12.16	6.11	0.992	3	7

9	41.93	43.23	7.69	7.16	0.970	5	6
10	38.84	33.14	6.56	21.47	1.172	6	2

Table D. 12: Experimental atomic weight of K, Nb, Bi, Mn and molar relations for KNBM x=0.10 composition by EDX spectra.

D.2.1.3. x=0.15

K (%)	Nb (%)	Bi (%)	Mn (%)	K/Nb	K/Bi	K/Mn
42.5	42.5	7.5	7.5	1	5.67	5.67

Table D. 13: Atomic weight of K, Nb, Bi, Mn and molar relations for the nominal KNBM x=0.15 composition.

	K (%)	Nb (%)	Bi (%)	Mn (%)	K/Nb	K/Bi	K/Mn
1	1	62.3	28.48	4.63	4.6	2.188	13
2	2	56.23	31.69	5.9	6.19	1.774	10
3	3	48.86	39.68	6.08	5.38	1.231	8
4	4	43.57	41.85	8.66	5.92	1.041	5
5	5	41.79	40.43	11.32	6.46	1.034	4
6	6	41.38	42.94	9.19	6.48	0.964	5
7	7	41.5	41.17	10.3	7.03	1.008	4
8	8	41.9	40.99	9.54	7.56	1.022	4
9	9	40.17	41.76	10.65	7.41	0.962	4
10	10	40.51	40.38	11.58	7.54	1.003	3
11	11	52.56	22.58	4.44	20.41	2.328	12

Table D. 14: Experimental atomic weight of K, Nb, Bi, Mn and molar relations for KNBM x=0.15 composition by EDX spectra.

D.2.1.4. x=0.20

K (%)	Nb (%)	Bi (%)	Mn (%)	K/Nb	K/Bi	K/Mn
40	40	10	10	1	4	4

Table D. 15.: Atomic weight of K, Nb, Bi, Mn and molar relations for the nominal KNBM x=0.20 composition.

	K (%)	Nb (%)	Bi (%)	Mn (%)	K/Nb	K/Bi	K/Mn
1	41.54	40.67	10.98	6.82	1.021	4	6
2	40.16	42.01	11.22	6.62	0.956	4	6
3	40.47	41.46	10.72	7.34	0.976	4	6
4	40.52	41.17	10.89	7.42	0.984	4	5
5	40.44	40.23	11.92	7.41	1.005	3	5
6	40.21	42.73	9.44	7.62	0.941	4	5
7	41.66	38.87	11.55	7.92	1.072	4	5
8	40.11	40.59	11.62	7.68	0.988	3	5
9	39.79	40.78	11.72	7.72	0.976	3	5
10	40.25	40.49	11.23	8.03	0.994	4	5
11	39.89	40.26	11.64	8.21	0.991	3	5
12	39.91	39.88	11.97	8.24	1.001	3	5
13	38.72	43	9.99	8.28	0.900	4	5
14	38.61	39.12	13.42	8.85	0.987	3	4
15	38.8	39.98	12.18	9.04	0.970	3	4

Table D. 16.: Experimental atomic weight of K, Nb, Bi, Mn and molar relations for KNBM x=0.20 composition by EDX spectra.

D.2.1.5. x=0.25

K (%)	Nb (%)	Bi (%)	Mn (%)	K/Nb	K/Bi	K/Mn
37.5	37.5	12.5	12.5	1	3	3

Table D. 17.: Atomic weight of K, Nb, Bi, Mn and molar relations for the nominal KNBM x=0.25 composition.

	K (%)	Nb (%)	Bi (%)	Mn (%)	K/Nb	K/Bi	K/Mn
1	35.84	37.97	15.16	11.04	0.944	2	3
2	36.07	37.46	15.05	11.43	0.963	2	3
3	35.47	37.72	15.24	11.57	0.940	2	3
4	35.12	36.96	16.21	11.71	0.950	2	3
5	34.99	36.24	15.86	12.92	0.966	2	3
6	33.86	37.89	15.61	12.63	0.894	2	3
7	34.45	35.66	16.31	13.59	0.966	2	3
8	34.23	35.82	16.37	13.58	0.956	2	3
9	33.91	35.93	16.4	13.76	0.944	2	2

Table D. 18.: Experimental atomic weight of K, Nb, Bi, Mn and molar relations for KNBM x=0.25 composition by EDX spectra.

APPENDIX E

Chapter 7: System (1−x) $KNbO_3$-x $BiCoO_3$

E.1. Rietveld Refinements plots

E.1.1. (1-x) $KNbO_3$-x $BiCoO_3$ (KNBC)

E.1.1.1. x=0.05

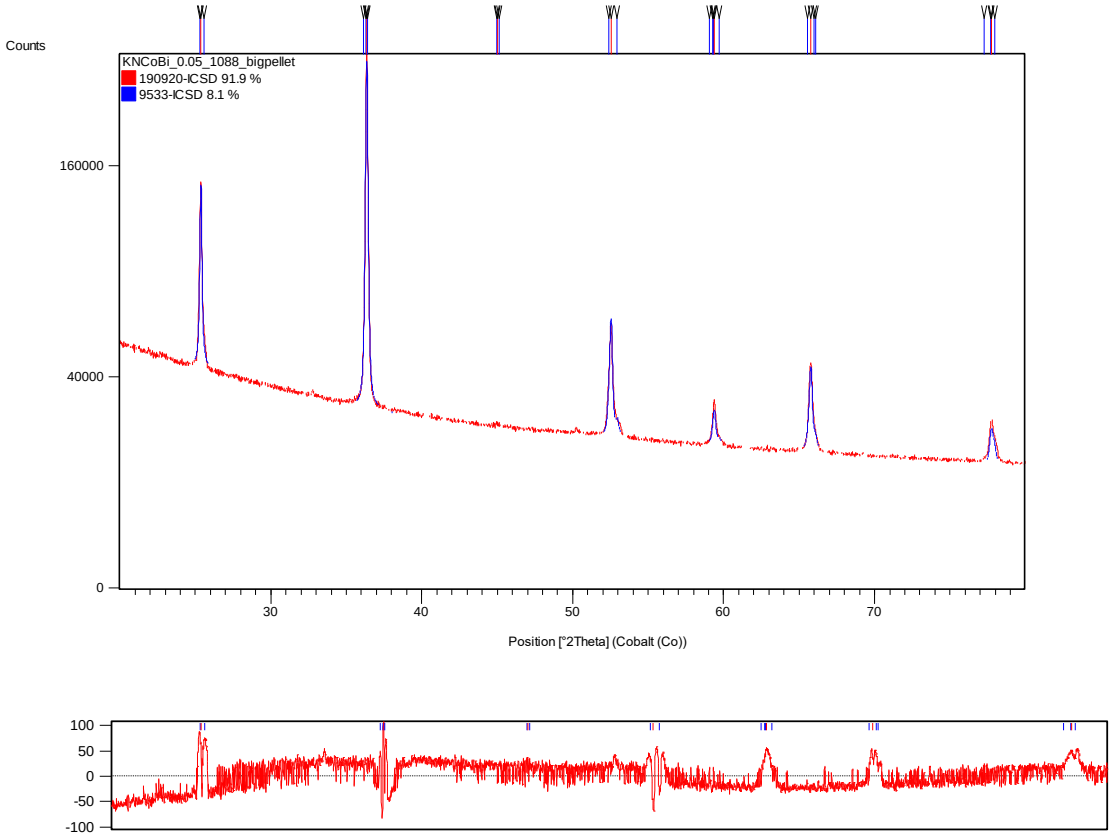

Figure E. 1: Experimental X-ray diffraction data (red), calculated fitting profile (blue) and difference plot for KNBC x=0.05.

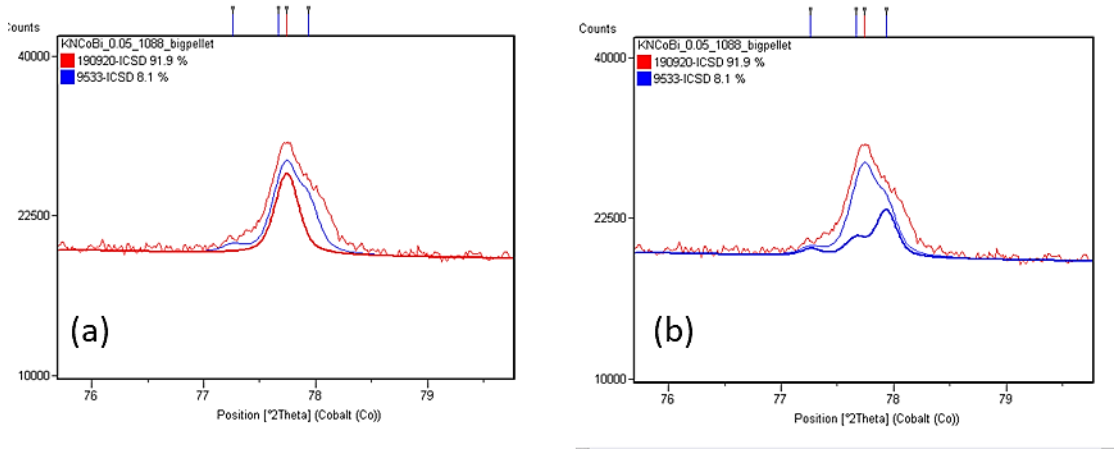

Figure E. 2: Coexistence of two phases, (a) cubic and (b) orthorhombic, refined by Rietveld method for KNBC x=0.05

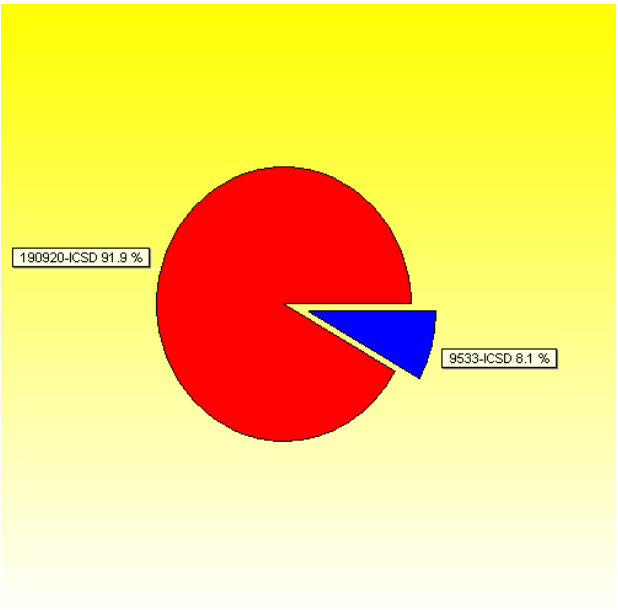

Figure E. 3.: The pie chart represents the percent quantity of the two polymorphs (orthorhombic and cubic) for KNBC x=0.05.

Atom	Wyck.	s.o.f.	x	y	z	Biso/ 10^4 pm^2
K1	2b	0.950000	0.500000	0.000000	0.513800	0.000000
Nb1	2a	0.950000	0.000000	0.000000	0.000000	0.000000
O1	2b	1.000000	0.500000	0.000000	0.036400	0.000000
O2	4d	1.000000	0.000000	0.252400	0.284200	0.000000
Bi	2b	0.050000	0.500000	0.000000	0.513800	0.000000

Co	2a	0.050000	0.000000	0.000000	0.000000	0.000000

Table E. 1: Occupancy, atomic fract. coordinates and Biso for orthorhombic KNBC x=0.05

Atom	Wyck.	s.o.f.	x	y	z	Biso/ 10^4 pm^2
K1	1b	0.950000	0.500000	0.500000	0.500000	0.020500
Nb1	1a	0.950000	0.000000	0.000000	0.000000	0.015490
O1	3d	1.000000	0.500000	0.000000	0.000000	0.000000
Bi	1b	0.050000	0.500000	0.500000	0.500000	0.000000
Co	1a	0.050000	0.000000	0.000000	0.000000	0.000000

Table E. 2: Occupancy, atomic fract. coordinates and Biso for cubic KNBC x=0.05

E.1.1.2. x=0.10

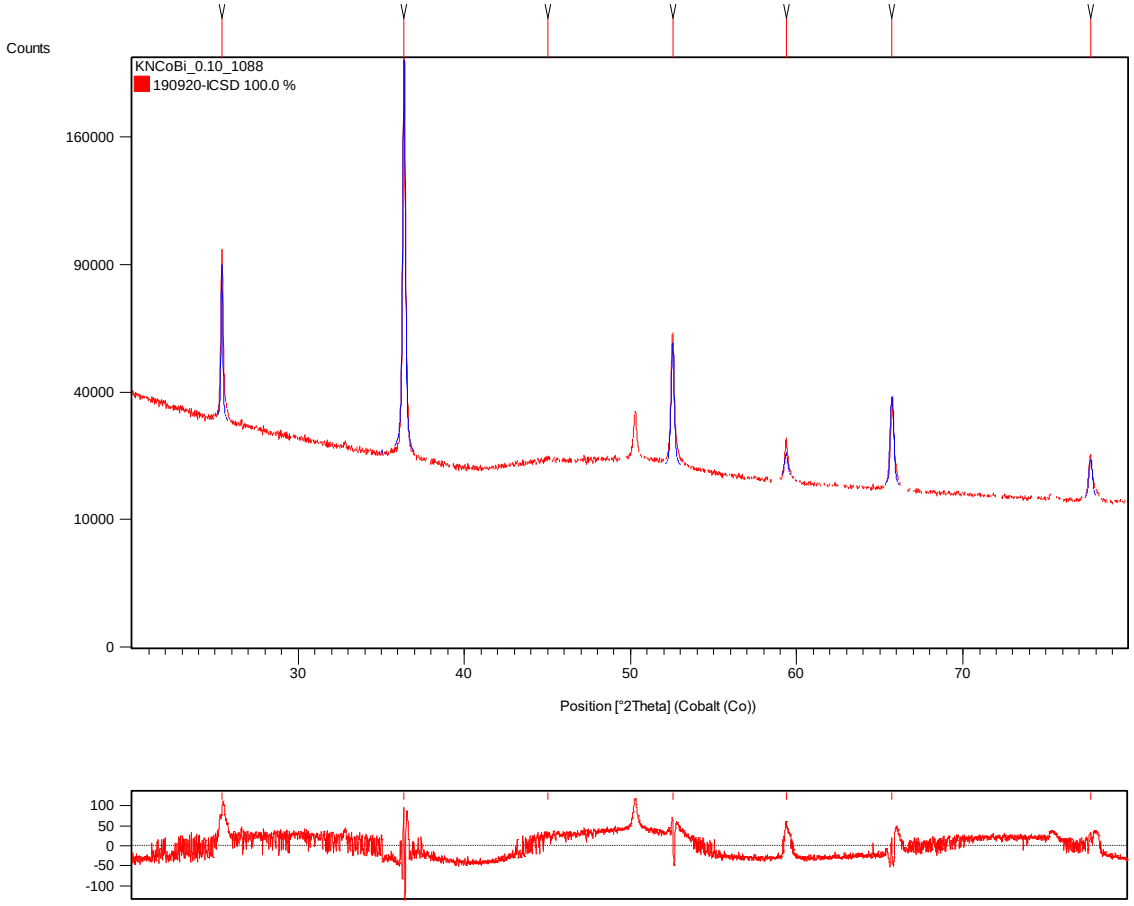

Figure E. 4: Experimental X-ray diffraction data (red), calculated fitting profile (blue) and difference plot for KNBC x=0.10.

Atom	Wyck.	s.o.f.	x	y	z	Biso/ 10^4 pm^2
K1	1b	0.900000	0.500000	0.500000	0.500000	0.020500
Nb1	1a	0.900000	0.000000	0.000000	0.000000	0.015490
O1	3d	1.000000	0.500000	0.000000	0.000000	0.000000
Bi	1b	0.100000	0.500000	0.500000	0.500000	0.000000
Co	1a	0.100000	0.000000	0.000000	0.000000	0.000000

Table E. 3: Occupancy, atomic fract. coordinates and Biso for cubic KNBC x=0.10

E.1.1.3. x=0.15

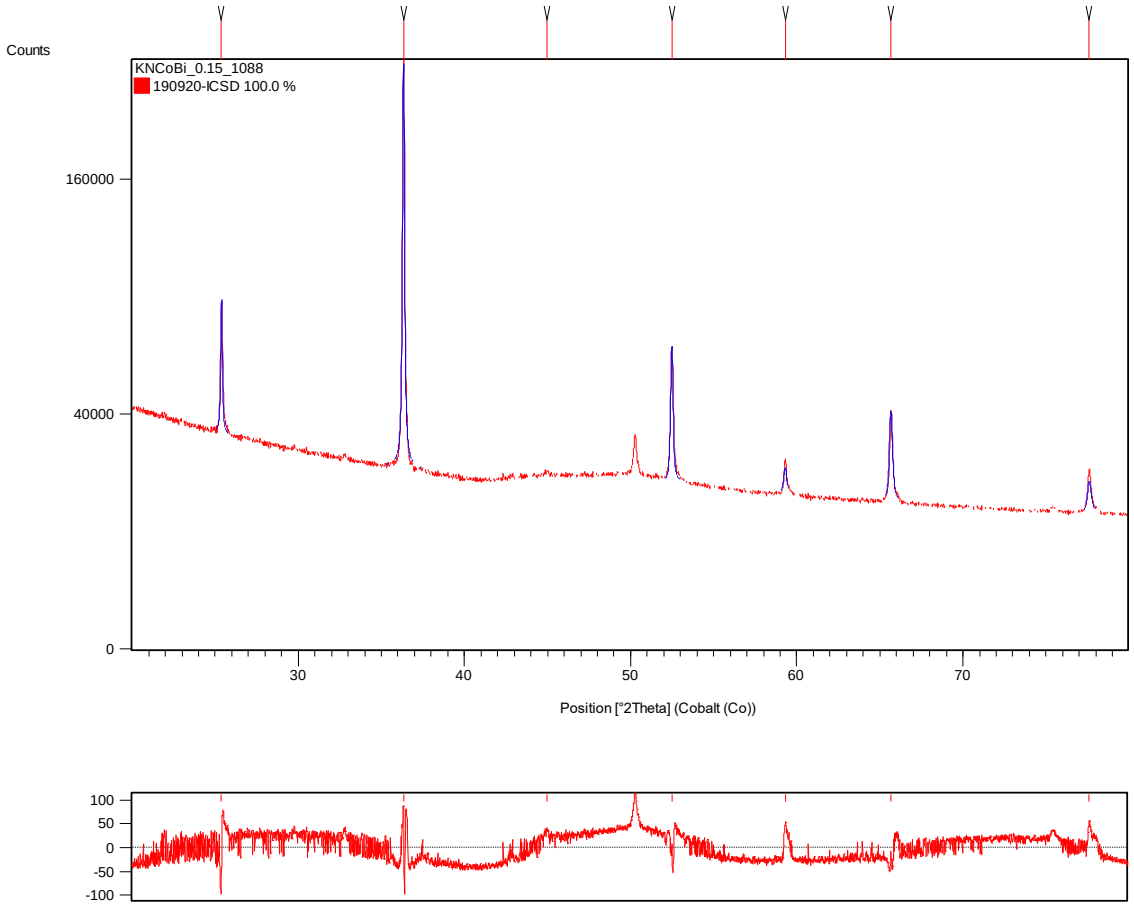

Figure E. 5: Experimental X-ray diffraction data (red), calculated fitting profile (blue) and difference plot for KNBC x=0.15.

Atom	Wyck.	s.o.f.	x	y	z	Biso/ 10^4 pm^2
K1	1b	0.850000	0.500000	0.500000	0.500000	0.020500
Nb1	1a	1.000000	0.000000	0.000000	0.000000	0.015490
O1	3d	1.000000	0.500000	0.000000	0.000000	0.000000
Bi	1b	0.150000	0.500000	0.500000	0.500000	0.000000
Co	1a	0.150000	0.000000	0.000000	0.000000	0.000000

Table E. 4: Occupancy, atomic fract. coordinates and Biso for cubic KNBC x=0.15

E.1.1.4. x=0.20

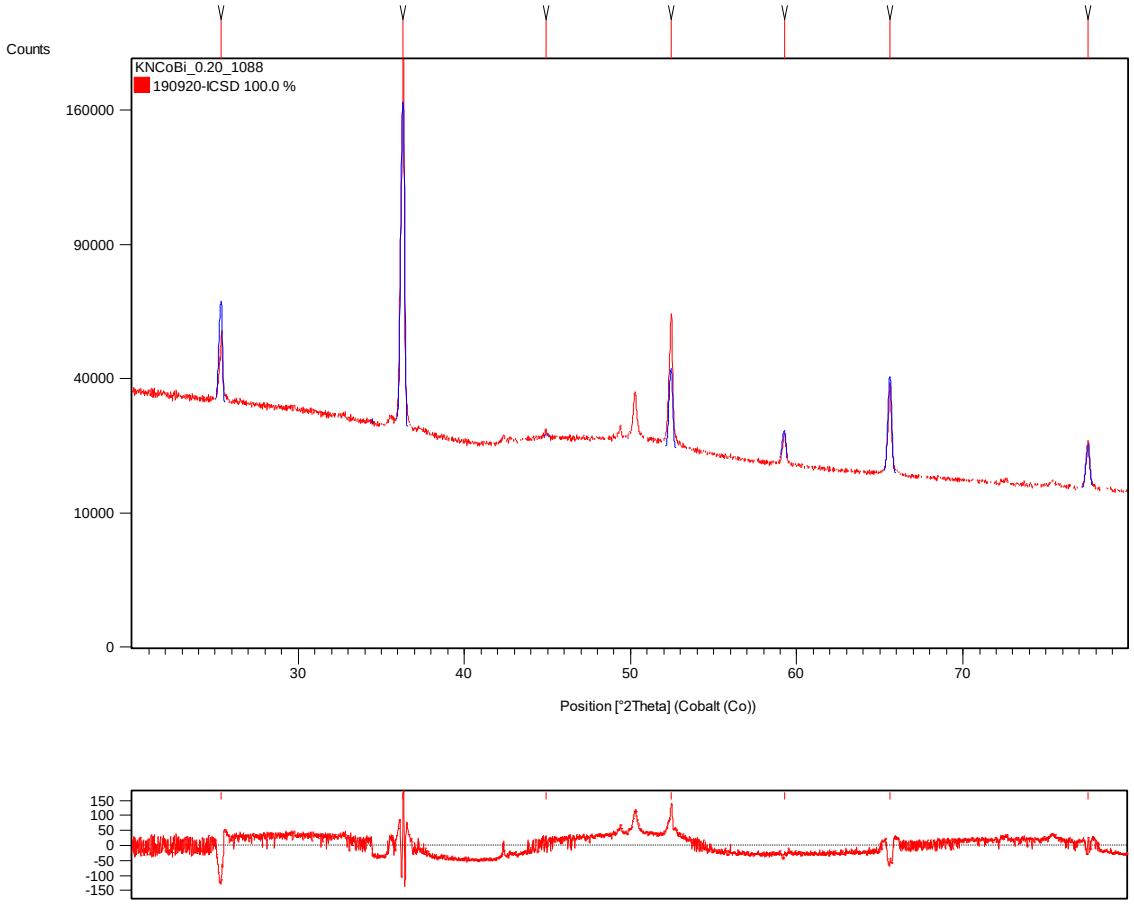

Figure E. 6: Experimental X-ray diffraction data (red), calculated fitting profile (blue) and difference plot for KNBC x=0.20

Atom	Wyck.	s.o.f.	x	y	z	Biso/ 10^4 pm^2
K1	1b	0.800000	0.500000	0.500000	0.500000	0.020500
Nb1	1a	1.000000	0.000000	0.000000	0.000000	0.015490
O1	3d	1.000000	0.500000	0.000000	0.000000	0.000000
Bi	1b	0.200000	0.500000	0.500000	0.500000	0.020500
Co	1a	1.000000	0.000000	0.000000	0.000000	0.015490

Table E. 5: Occupancy, atomic fract. coordinates and Biso for cubic KNBC x=0.20

E.1.1.5 x=0.25

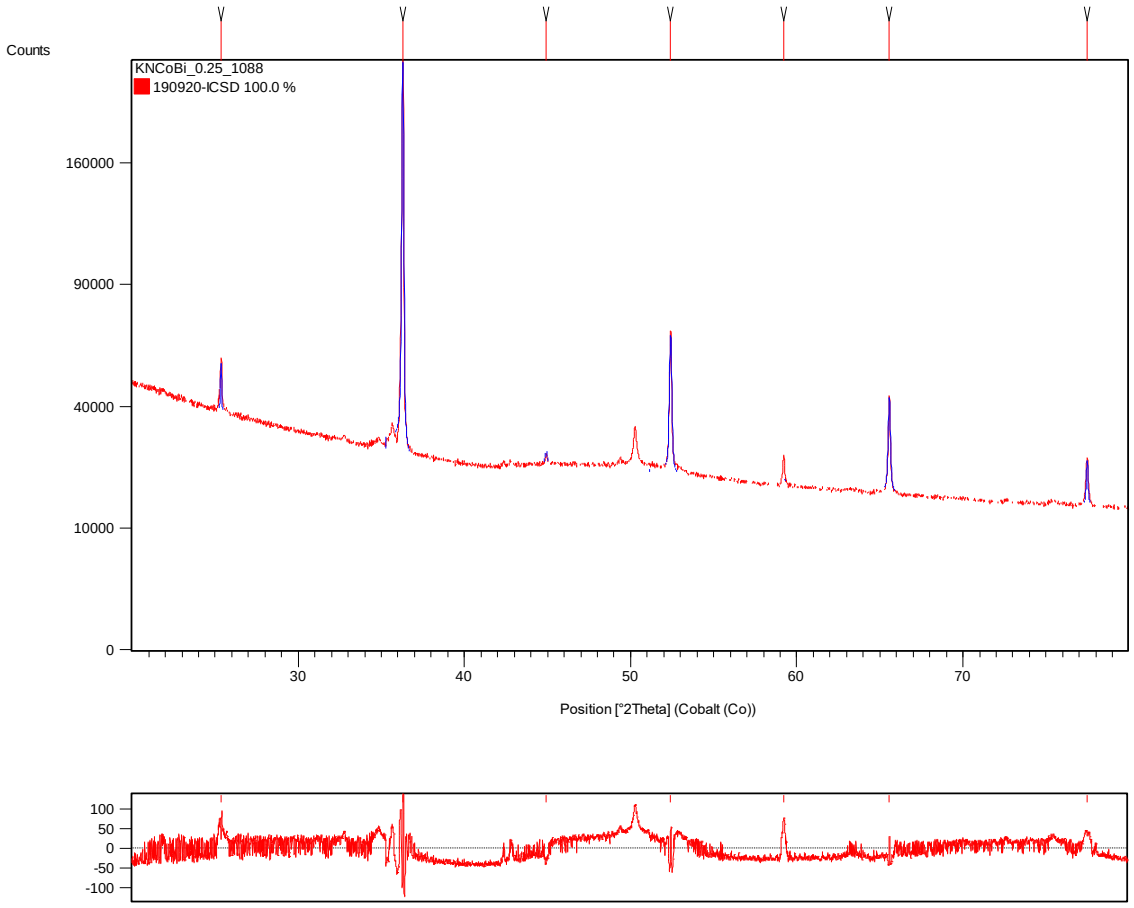

Figure E. 7: Experimental X-ray diffraction data (red), calculated fitting profile (blue) and difference plot for KNBC x=0.25.

Atom	Wyck.	s.o.f.	x	y	z	Biso/ 10^4 pm^2
K1	1b	0.750000	0.500000	0.500000	0.500000	0.020500
Nb1	1a	0.750000	0.000000	0.000000	0.000000	0.015490
O1	3d	1.000000	0.500000	0.000000	0.000000	0.000000
Bi	1b	0.250000	0.500000	0.500000	0.500000	0.000000
Co	1a	0.250000	0.000000	0.000000	0.000000	0.000000

Table E. 6: Occupancy, atomic fract. coordinates and Biso for cubic KBBNZ x=0.25

E.2. EDX measurements

E.2.1. (1-x) $KNbO_3$- x $BiCoO_3$

E.2.1.1. x=0.05

K (%)	Nb (%)	Bi (%)	Co (%)	K/Nb	K/Bi	K/Co
47.5	47.5	2.5	2.5	1	19	19

Table E. 7: Atomic percent of K, Nb, Bi, Co and molar relations for the nominal KNBC x=0.05composition.

	K (%)	Nb (%)	Bi (%)	Co (%)	K/Nb	K/Bi	K/Fe
1	47.3	47.4	2.9	2.5	0.997	16	19
2	45.5	50.1	2.1	2.3	0.908	22	20
3	46.3	47.8	3.7	2.2	0.968	13	21
4	47.6	47.1	3.3	2.0	1.009	15	23
5	48.1	46.8	3.1	1.9	1.028	15	25
6	46.9	48.3	3.0	1.8	0.970	16	26
7	47.5	48.4	2.3	1.8	0.981	21	27
8	47.8	48.3	2.2	1.8	0.989	22	27

9	48.6	47.5	2.2	1.8	1.022	22	28
10	47.5	47.1	3.7	1.7	1.007	13	28
11	48.3	47.4	2.7	1.6	1.019	18	29
12	46.9	47.6	4.1	1.5	0.985	12	32
13	48.2	47.2	3.1	1.4	1.021	15	34
14	49.0	47.3	2.3	1.4	1.036	22	35
15	47.2	48.7	2.7	1.3	0.969	17	36
16	47.6	48.3	2.7	1.3	0.985	17	36
17	48.6	47.4	2.7	1.3	1.025	18	37
18	47.8	48.7	2.2	1.3	0.981	22	37
19	46.5	49.3	3.0	1.2	0.943	15	39
20	46.6	49.6	2.6	1.2	0.940	18	39
21	47.5	49.3	2.0	1.2	0.963	23	40
22	49.3	47.0	2.5	1.2	1.047	19	42
23	47.4	49.8	1.7	1.1	0.952	28	44
24	48.2	48.9	2.1	0.8	0.986	23	59
25	48.9	48.3	2.1	0.7	1.013	23	70
26	48.2	49.5	1.7	0.6	0.975	28	83
27	49.5	49.1	0.9	0.6	1.008	55	87

Table E. 8: Experimental atomic percent of K, Nb, Bi, Co and molar relations for KNBC x=0.05 composition by EDX spectra.

E.2.1.2. x=0.10

K (%)	Nb (%)	Bi (%)	Co (%)	K/Nb	K/Bi	K/Co
45	45	5	5	1	9	9

Table E. 9: Atomic percent of K, Nb, Bi, Co and molar relations for the nominal KNBC x=0.10 composition

	K (%)	Nb (%)	Bi (%)	Co (%)	K/Nb	K/Bi	K/Co
1	34.6	36.7	16.4	12.4	0.942	2	3
2	37.7	39.5	13.0	9.8	0.955	3	4
3	41.1	38.8	11.7	8.5	1.060	4	5
4	40.9	40.5	10.5	8.1	1.011	4	5
5	40.3	39.6	12.3	7.8	1.017	3	5
6	42.5	39.2	10.9	7.4	1.086	4	6
7	44.8	36.7	11.4	7.2	1.221	4	6
8	42.7	42.0	8.2	7.1	1.016	5	6
9	42.4	41.2	9.6	6.8	1.031	4	6
10	44.3	38.6	10.6	6.5	1.146	4	7
11	43.2	39.4	11.3	6.2	1.097	4	7
12	43.5	41.6	9.3	5.7	1.045	5	8
13	47.5	37.1	10.1	5.2	1.280	5	9
14	62.8	26.4	6.0	4.8	2.384	10	13
15	47.5	39.1	9.8	3.6	1.215	5	13

Table E. 10: Experimental atomic percent of K, Nb, Bi, Co and molar relations for KNBC x=0.10 composition by EDX spectra.

E.2.1.3. x=0.15

K (%)	Nb (%)	Bi (%)	Co (%)	K/Nb	K/Bi	K/Co
42.5	42.5	7.5	7.5	1	5.67	5.67

Table E. 11: Atomic percent of K, Nb, Bi, Fe and molar relations for the nominal KNBC x=0.15 composition

	K (%)	Nb (%)	Bi (%)	Co (%)	K/Nb	K/Bi	K/Co
1	35.2	48.3	5.6	10.9	0.729	6	3
2	38.3	39.2	12.7	9.9	0.977	3	4
3	38.6	40.0	12.8	8.6	0.964	3	4
4	40.7	43.1	9.5	6.8	0.944	4	6
5	42.0	42.8	9.0	6.2	0.981	5	7
6	43.4	42.8	7.9	6.0	1.015	6	7
7	42.3	41.7	10.1	5.9	1.014	4	7
8	41.1	45.3	7.8	5.8	0.906	5	7
9	41.6	42.7	10.4	5.3	0.975	4	8
10	41.6	42.7	10.4	5.3	0.975	4	8
11	42.7	42.3	9.8	5.1	1.009	4	8
12	44.1	42.7	8.2	5.1	1.032	5	9
13	43.2	45.3	7.3	4.2	0.953	6	10
14	44.1	44.4	7.9	3.6	0.992	6	12

Table E. 12: Experimental atomic percent of K, Nb, Bi, Co and molar relations for KNBC x=0.15 composition by EDX spectra.

E.2.1.4. x=0.20

K (%)	Nb (%)	Bi (%)	Co (%)	K/Nb	K/Bi	K/Co
40	40	10	10	1	4	4

Table E. 13: Atomic percent of K, Nb, Bi, Co and molar relations for the nominal KNBC x=0.20 composition.

	K (%)	Nb (%)	Bi (%)	Co (%)	K/Nb	K/Bi	K/Co
1	30.7	47.8	6.6	14.9	0.643	5	2
2	32.4	43.3	10.0	14.4	0.748	3	2
3	35.6	39.5	14.8	10.1	0.902	2	4
4	38.5	41.9	11.1	8.5	0.917	3	5
5	38.2	43.9	9.9	8.0	0.871	4	5
6	38.8	40.4	13.2	7.6	0.960	3	5
7	39.1	43.0	10.3	7.6	0.910	4	5
8	40.4	41.7	10.6	7.3	0.969	4	6
9	39.8	42.5	10.7	6.9	0.938	4	6
10	38.4	41.3	13.5	6.8	0.928	3	6
11	40.0	41.6	11.8	6.6	0.962	3	6
12	40.7	41.8	11.0	6.5	0.973	4	6
13	40.4	42.9	10.3	6.5	0.940	4	6
14	40.4	41.6	11.5	6.4	0.971	4	6
15	40.8	42.7	10.1	6.4	0.956	4	6
16	40.3	41.2	12.2	6.4	0.976	3	6
17	41.2	41.9	10.7	6.2	0.985	4	7

Table E. 14: Experimental atomic percent of K, Nb, Bi, Co and molar relations for KNBC x=0.20 composition by EDX spectra.

E.2.1.5. x=0.25

K (%)	Nb (%)	Bi (%)	Co (%)	K/Nb	K/Bi	K/Co
37.5	37.5	12.5	12.5	1	3	3

Table E. 15: Atomic percent of K, Nb, Bi, Co and molar relations for the nominal KNBC x=0.25 composition

	K (%)	Nb (%)	Bi (%)	Co (%)	K/Nb	K/Bi	K/Fe
1	33.4	40.7	12.4	13.6	0.821	3	2
2	34.1	40.8	12.4	12.7	0.834	3	3
3	35.7	39.6	13.2	11.5	0.903	3	3
4	35.0	41.2	12.5	11.4	0.850	3	3
5	35.6	40.6	13.2	10.6	0.876	3	3
6	37.1	39.4	13.4	10.1	0.940	3	4
7	38.3	39.2	12.7	9.9	0.977	3	4
8	37.1	39.3	13.8	9.8	0.946	3	4
9	38.0	38.7	13.8	9.5	0.983	3	4
10	37.1	39.0	14.6	9.3	0.953	3	4
11	36.2	39.2	15.3	9.3	0.925	2	4
12	36.9	39.9	14.1	9.1	0.927	3	4
13	36.9	39.9	14.3	8.9	0.926	3	4
14	38.0	40.3	13.1	8.6	0.944	3	4
15	38.1	39.5	14.0	8.4	0.963	3	5

Table E. 16: Experimental atomic percent of K, Nb, Bi, Co and molar relations for KNBC x=0.25 composition by EDX spectra.

APPENDIX F

Chapter 8: System (1-x) $KNbO_3$- x $BiNiO_3$

F.1. Rietveld Refinements plots

F.1.1. (1-x) $KNbO_3$- x $BiNiO_3$

F.1.1.1. x=0.05

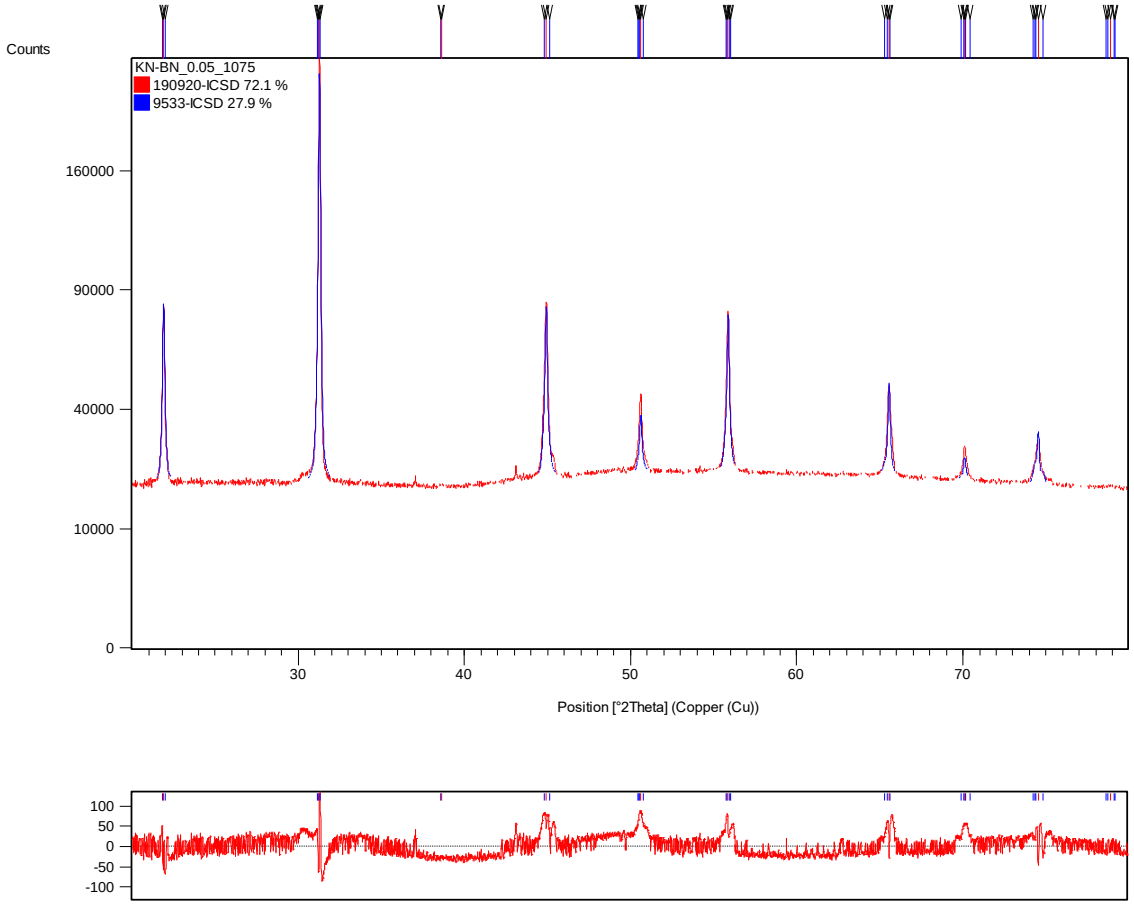

Figure F. 1: Experimental X-ray diffraction data (red), calculated fitting profile (blue) and difference plot for KNBN x=0.05.

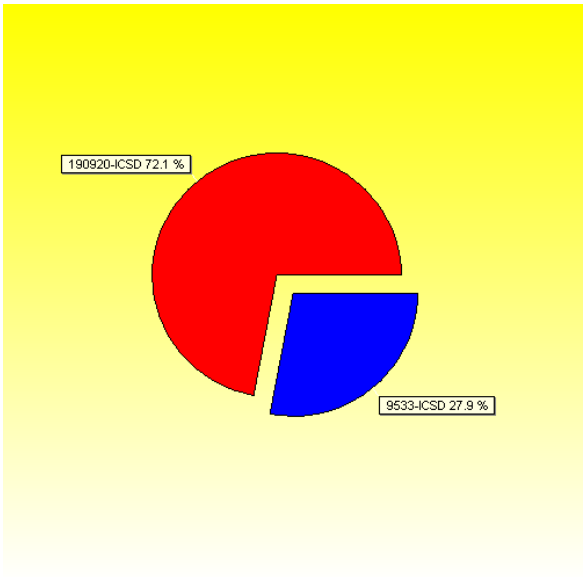

Figure F. 2: The pie chart represents the percent quantity of the two polymorphs (orthorhombic and cubic) for KNBN x=0.05.

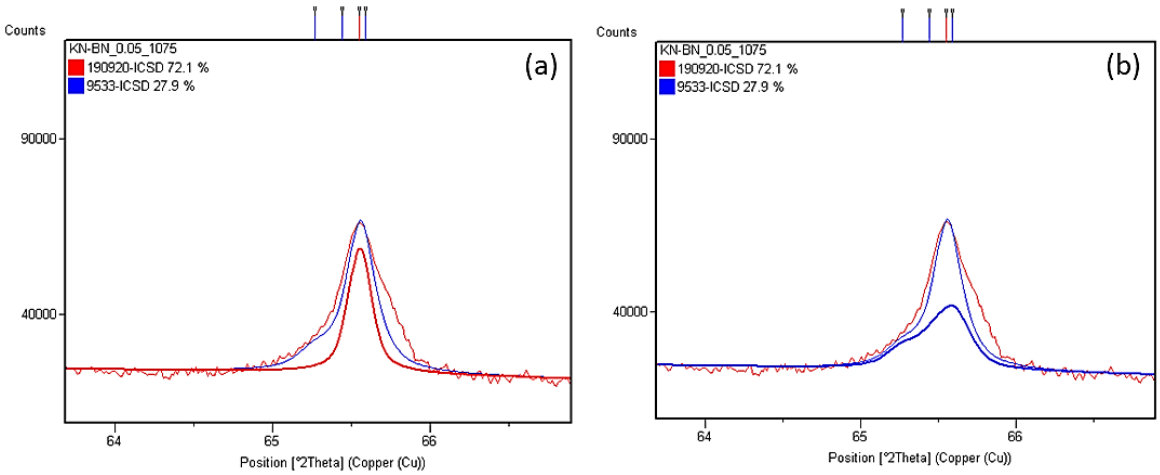

Figure F. 3: Coexistence of two phases, (a) cubic and (b) orthorhombic, refined by Rietveld method for KNBC x=0.05

Atom	Wyck.	s.o.f.	x	y	z	Biso/ 10^4 pm^2
K1	2b	0.950000	0.500000	0.000000	0.513800	0.000000
Nb1	2a	0.950000	0.000000	0.000000	0.000000	0.000000
O1	2b	1.000000	0.500000	0.000000	0.036400	0.000000
O2	4d	1.000000	0.000000	0.252400	0.284200	0.000000
Bi	2b	0.050000	0.500000	0.000000	0.513800	0.000000
Ni	2a	0.050000	0.000000	0.000000	0.000000	0.000000

Table F. 1: Occupancy, atomic fract. coordinates and Biso for orthorhombic KNBN x=0.05

Atom	Wyck.	s.o.f.	x	y	z	Biso/ 10^4 pm^2
K1	1b	0.950000	0.500000	0.500000	0.500000	0.020500
Nb1	1a	0.950000	0.000000	0.000000	0.000000	0.015490
O1	3d	1.000000	0.500000	0.000000	0.000000	0.000000
Bi	1b	0.050000	0.500000	0.500000	0.500000	0.020500
Ni	1a	0.050000	0.000000	0.000000	0.000000	0.015490

Table F. 2: Occupancy, atomic fract. coordinates and Biso for cubic KNBN x=0.05

F.1.1.2. x=0.10

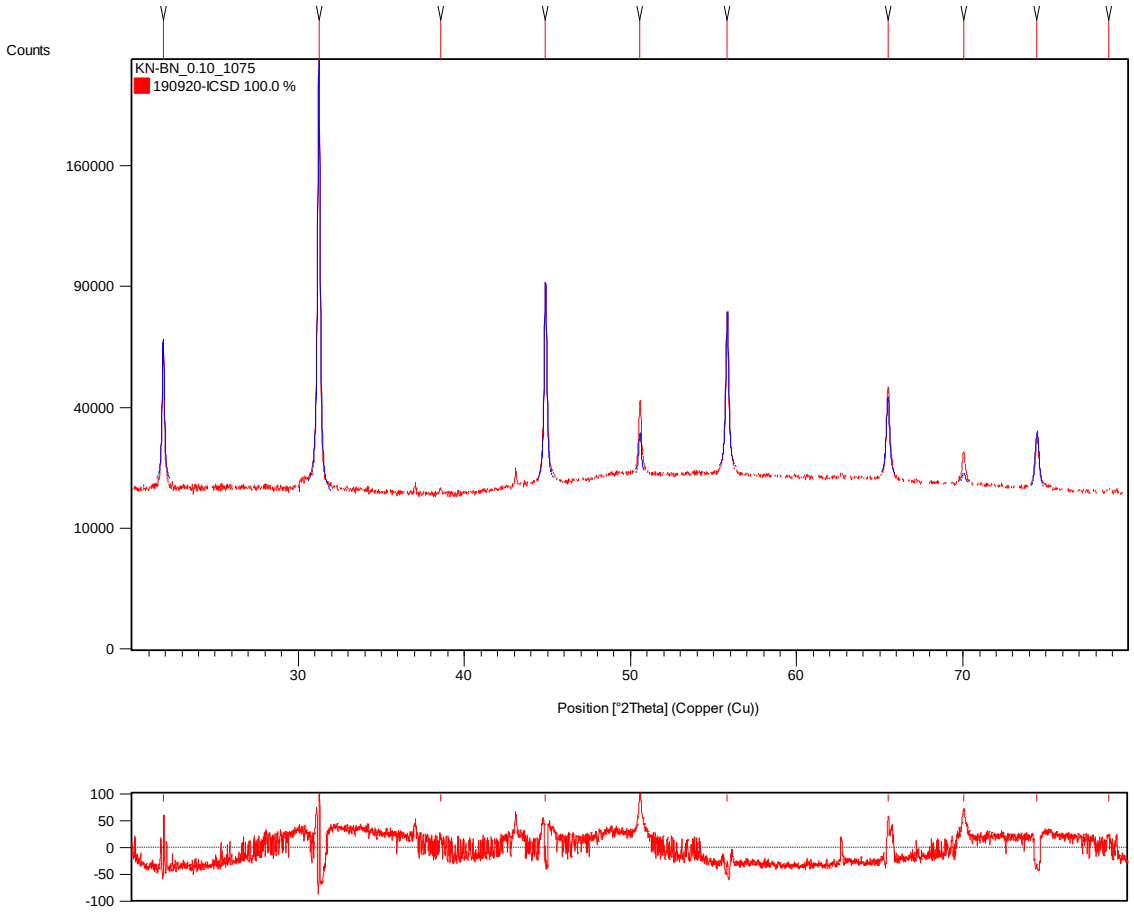

Figure F. 4: Experimental X-ray diffraction data (red), calculated fitting profile (blue) and difference plot for KNBN x=0.10.

Atom	Wyck.	s.o.f.	x	y	z	Biso/ 10^4 pm^2
K1	1b	0.900000	0.500000	0.500000	0.500000	0.020500
Nb1	1a	0.900000	0.000000	0.000000	0.000000	0.015490
O1	3d	1.000000	0.500000	0.000000	0.000000	0.000000
Bi	1b	0.100000	0.500000	0.500000	0.500000	0.020500
Ni	1a	0.100000	0.000000	0.000000	0.000000	0.000000

Table F. 3: Occupancy, atomic fract. coordinates and Biso for orthorhombic KNBN x=0.10

F.1.1.2.1 Alternative Rietveld refinement for x=0.10 into orthorhombic symmetry.

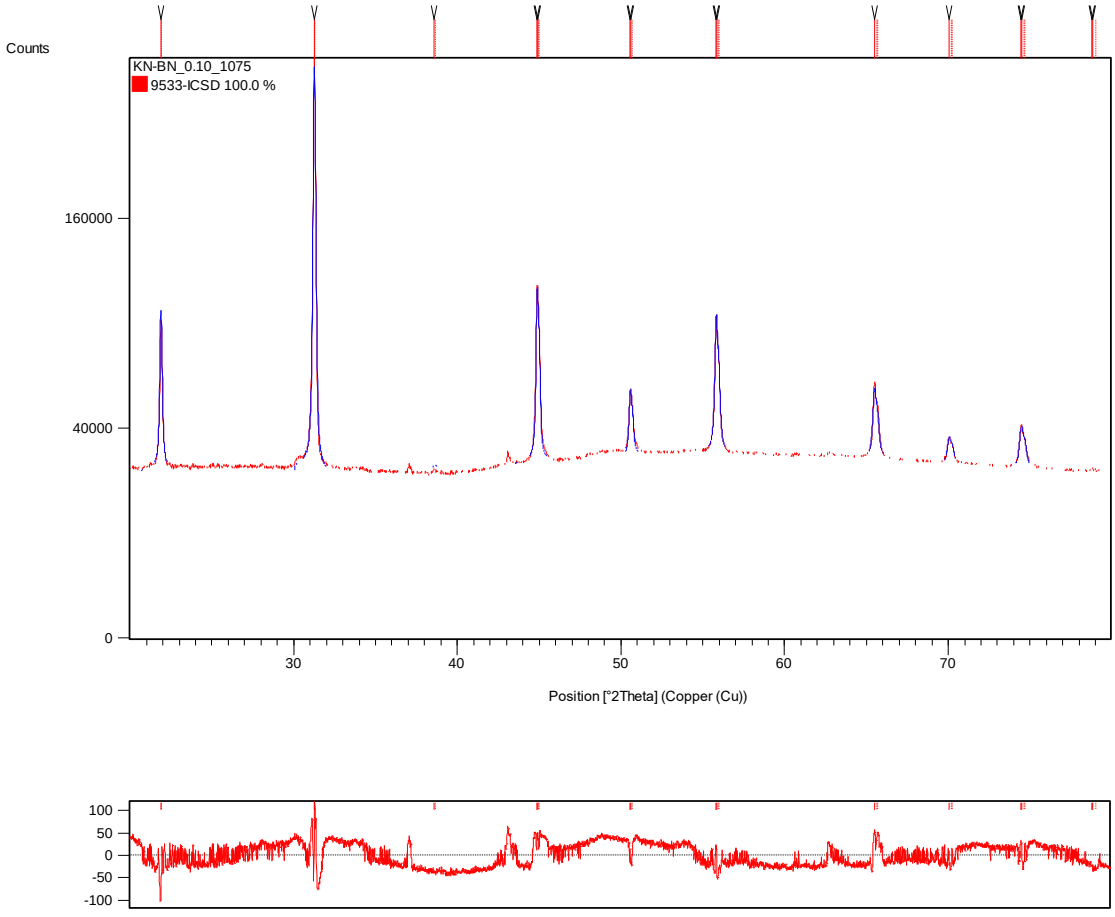

Figure F. 5: Alternative refinement. Experimental X-ray diffraction data (red), calculated fitting profile (blue) and difference plot for KNBN x=0.10 into orthorhombic phase.

Space Group	Amm2
Density (Experimental) (g/cm^3)	4.2(2)
Density (calculated) (g/cm^3)	4.971(3)
Relative Density (%)	84(1)
a (Å)	4.0148(1)
b (Å)	5.6770(2)
c (Å)	5.6731(7)
$V/10^6$ (pm^3)	64.651(2)
R_{exp}	0.8102
R_p	2.1539
R_{wp}	2.6282
GOF	10.5211

Table F. 4: Experimental and theoretical density, lattice parameters and agreement indices calculated by Rietveld Refinement for KNBN (x=0.10)

F.1.1.3. X=0.15

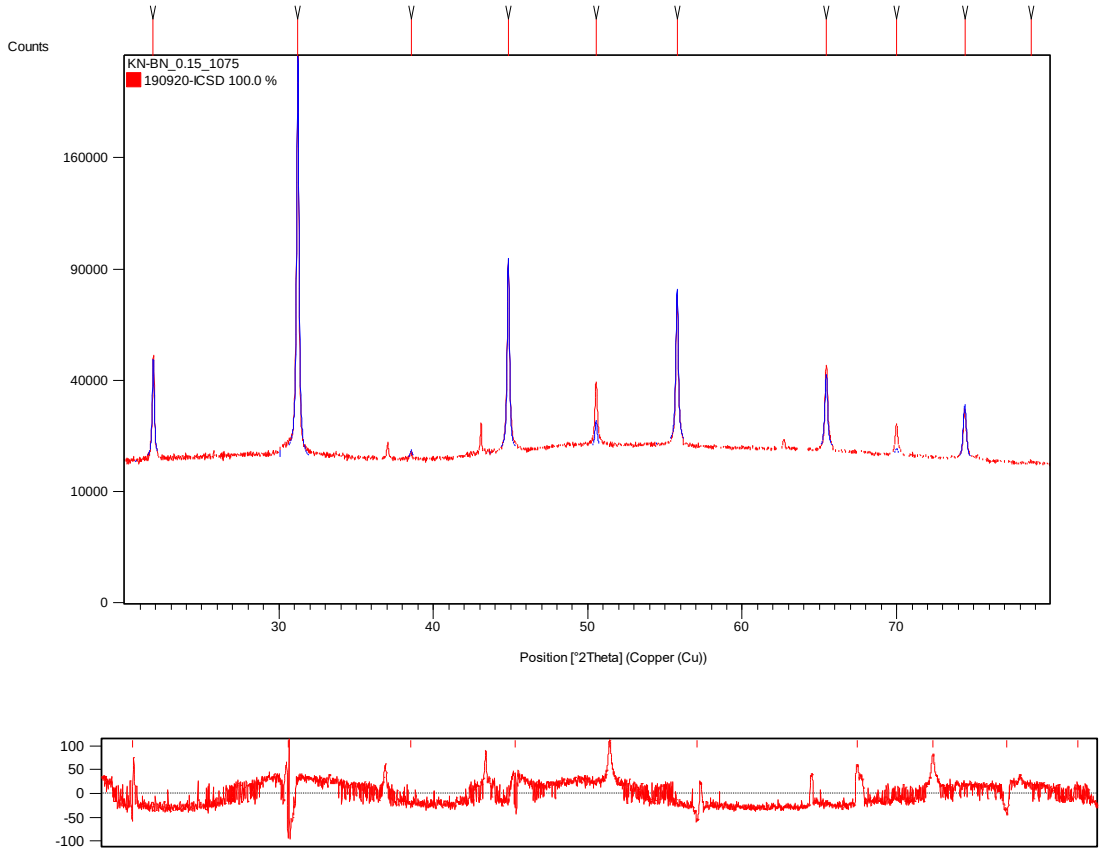

Figure F. 6: Experimental X-ray diffraction data (red), calculated fitting profile (blue) and difference plot for KNBN x=0.15.

Atom	Wyck.	s.o.f.	x	y	z	Biso/ 10^4 pm^2
K1	1b	0.850000	0.500000	0.500000	0.500000	0.020500
Nb1	1a	0.850000	0.000000	0.000000	0.000000	0.015490
O1	3d	1.000000	0.500000	0.000000	0.000000	0.000000
Bi	1b	0.150000	0.500000	0.500000	0.500000	0.000000
Ni	1a	0.150000	0.000000	0.000000	0.000000	0.000000

Table F. 5: Occupancy, atomic fract. coordinates and Biso for orthorhombic KNBN x=0.15.

F.1.1.4. X=0.20

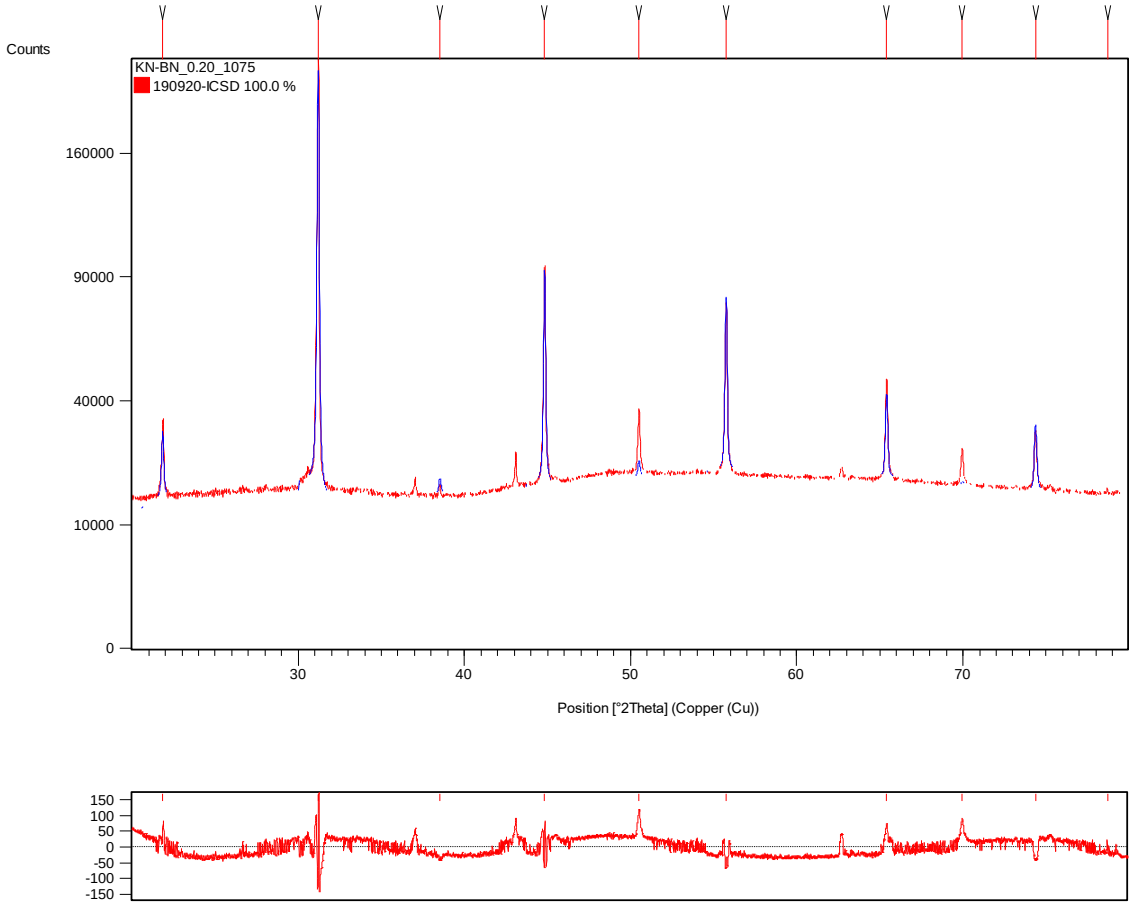

Figure F. 7: Experimental X-ray diffraction data (red), calculated fitting profile (blue) and difference plot for KNBN x=0.20.

Atom	Wyck.	s.o.f.	x	y	z	Biso/ 10^4 pm^2
K1	1b	0.800000	0.500000	0.500000	0.500000	0.020500
Nb1	1a	0.800000	0.000000	0.000000	0.000000	0.015490
O1	3d	1.000000	0.500000	0.000000	0.000000	0.000000
Bi	1b	0.200000	0.500000	0.500000	0.500000	0.000000
Ni	1a	0.200000	0.000000	0.000000	0.000000	0.000000

Table F. 6: Occupancy, atomic fract. coordinates and Biso for orthorhombic KNBN x=0.20

F.1.1.5. X=0.25

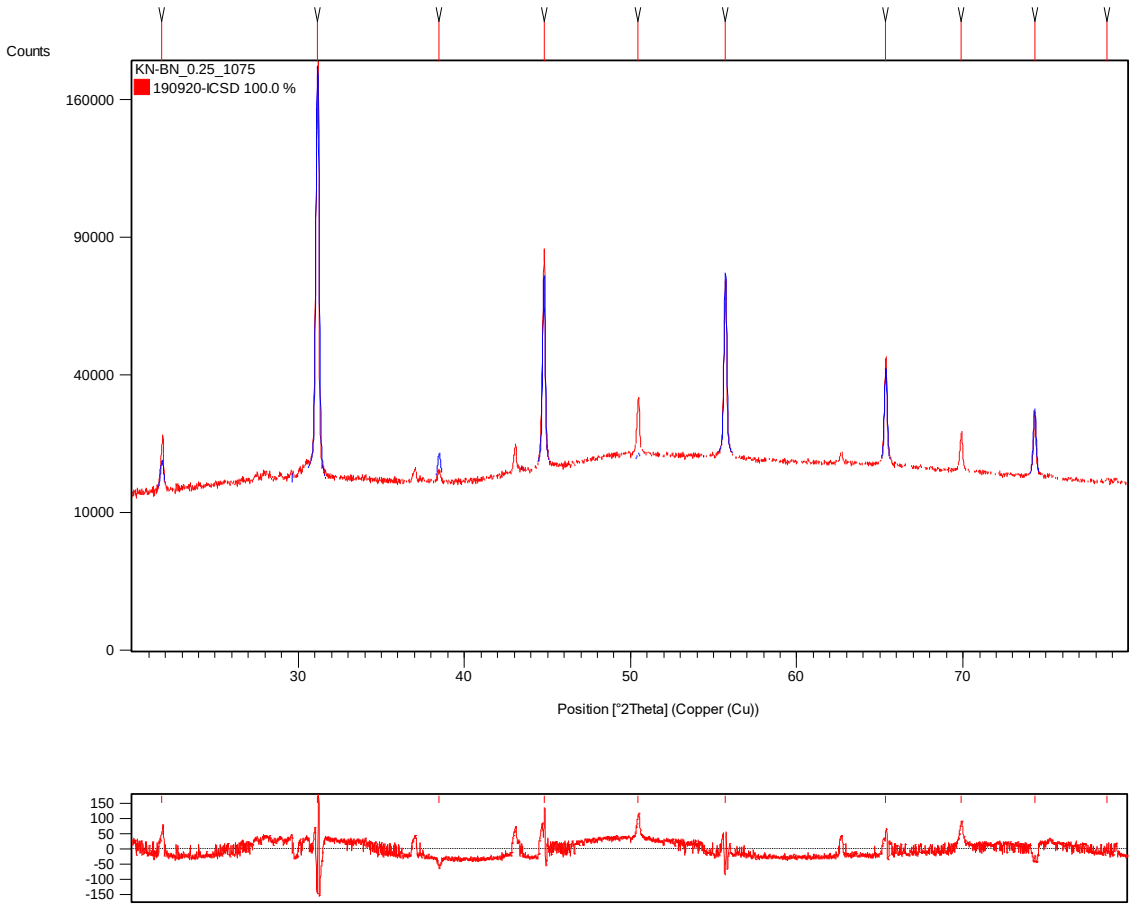

Figure F. 8: Experimental X-ray diffraction data (red), calculated fitting profile (blue) and difference plot for KNBN x=0.25.

Atom	Wyck.	s.o.f.	x	y	z	Biso/ 10^4 pm^2
K1	1b	0.750000	0.500000	0.500000	0.500000	0.020500
Nb1	1a	0.750000	0.000000	0.000000	0.000000	0.015490
O1	3d	1.000000	0.500000	0.000000	0.000000	0.000000
Bi	1b	0.250000	0.500000	0.500000	0.500000	0.020500
Ni	1a	0.250000	0.000000	0.000000	0.000000	0.015490

Table F. 7.: Occupancy, atomic fract. coordinates and Biso for orthorhombic KNBF x=0.25.

F.2. EDX measurements

F.2.1. (1-x) $KNbO_3$- x $BiNiO_3$

F.2.1.1. x=0.05

K (%)	Nb (%)	Bi (%)	Ni (%)	K/Nb	K/Bi	K/Ni
47.5	47.5	2.5	2.5	1	19	19

Table F. 8: Atomic percent of K, Nb, Bi, Ni and molar relations for the nominal KNBN x=0.05composition.

	K (%)	Nb (%)	Bi (%)	Ni (%)	K/Nb	K/Bi	K/Ni
1	46.7	47.3	3.6	2.4	0.988	13	19
2	47.6	46.5	3.7	2.3	1.025	13	21
3	48.4	46.6	3.0	2.0	1.039	16	24
4	46.0	50.1	2.1	1.8	0.917	22	26
5	46.8	47.9	3.6	1.7	0.979	13	28
6	44.6	52.3	1.7	1.4	0.854	27	31
7	48.5	48.1	2.0	1.4	1.007	24	35
8	47.6	49.6	1.5	1.3	0.960	31	37
9	47.6	49.6	1.5	1.3	0.960	31	37
10	47.6	49.6	1.5	1.3	0.960	31	37
11	48.7	47.3	3.0	1.0	1.029	16	51

Table F. 9: Experimental atomic percent of K, Nb, Bi, Ni and molar relations for KNBN x=0.05 composition by EDX spectra.

F.2.1.2. x=0.10

K (%)	Nb (%)	Bi (%)	Ni (%)	K/Nb	K/Bi	K/Ni
45	45	5	5	1	9	9

Table F. 10: Atomic percent of K, Nb, Bi, Ni and molar relations for the nominal KNBN x=0.10 composition

	K (%)	Nb (%)	Bi (%)	Ni (%)	K/Nb	K/Bi	K/Ni
1	35.6	37.5	7.3	19.6	0.950	5	2
2	46.5	41.4	6.7	5.4	1.122	7	9
3	46.2	44.0	5.1	4.7	1.051	9	10
4	44.9	43.3	7.3	4.5	1.036	6	10
5	60.9	31.2	3.9	3.9	1.951	15	16
6	49.6	41.6	5.2	3.6	1.190	10	14
7	45.9	43.6	6.9	3.6	1.052	7	13
8	57.7	31.8	7.0	3.5	1.813	8	16
9	47.3	43.2	6.2	3.3	1.095	8	15
10	47.0	43.8	6.0	3.3	1.072	8	14
11	65.4	29.5	2.1	3.0	2.217	32	22
12	47.2	45.2	4.8	2.8	1.043	10	17
13	49.6	43.3	4.3	2.8	1.145	12	18
14	47.2	45.5	4.7	2.7	1.036	10	17
15	49.3	45.8	2.3	2.6	1.078	21	19
16	48.6	45.8	3.2	2.4	1.062	15	20
17	47.7	45.6	4.4	2.3	1.048	11	21
18	48.0	45.9	3.9	2.2	1.046	12	22
19	48.4	45.5	4.4	1.7	1.064	11	28
20	48.3	47.2	2.9	1.5	1.025	16	31

Table F. 11: Experimental atomic percent of K, Nb, Bi, Ni and molar relations for KNBN x=0.10 composition by EDX spectra.

F.2.1.3. x=0.15

K (%)	Nb (%)	Bi (%)	Ni (%)	K/Nb	K/Bi	K/Ni
42.5	42.5	7.5	7.5	1	5.67	5.67

Table F. 12: Atomic percent of K, Nb, Bi, Ni and molar relations for the nominal KNBN x=0.15 composition.

	K (%)	Nb (%)	Bi (%)	Ni (%)	K/Nb	K/Bi	K/Ni
1	41.3	41.3	9.9	7.5	1.001	4	6
2	40.4	45.5	8.2	5.9	0.889	5	7
3	40.9	42.6	10.7	5.8	0.961	4	7
4	42.4	41.8	10.3	5.5	1.014	4	8
5	42.9	43.0	8.7	5.3	0.998	5	8
6	43.3	44.4	7.4	4.8	0.974	6	9
7	46.2	44.0	5.1	4.7	1.051	9	10
8	43.1	43.6	8.8	4.5	0.988	5	9
9	44.0	44.8	6.9	4.3	0.983	6	10
10	42.8	45.0	8.0	4.2	0.951	5	10
11	44.7	44.1	7.3	4.0	1.014	6	11
12	44.1	45.0	6.9	4.0	0.979	6	11
13	45.1	43.6	7.5	3.8	1.036	6	12
14	46.4	44.0	5.8	3.8	1.054	8	12
15	45.3	44.2	6.9	3.6	1.025	7	13
16	44.9	44.9	6.6	3.6	0.999	7	12

Table F. 13: Experimental atomic percent of K, Nb, Bi, Ni and molar relations for KNBN x=0.15 composition by EDX spectra.

F.2.1.4. x=0.20

K (%)	Nb (%)	Bi (%)	Ni (%)	K/Nb	K/Bi	K/Ni
40	40	10	10	1	4	4

Table F. 14: Atomic percent of K, Nb, Bi, Ni and molar relations for the nominal KNBN x=0.20 composition.

	K (%)	Nb (%)	Bi (%)	Ni (%)	K/Nb	K/Bi	K/Ni
1	38.6	44.8	9.2	7.4	0.862	4	5
2	39.3	43.4	10.1	7.2	0.907	4	5
3	40.3	41.5	11.7	6.5	0.972	3	6
4	39.5	42.6	11.6	6.4	0.927	3	6
5	41.1	42.0	10.8	6.1	0.978	4	7
6	41.7	43.0	9.5	5.8	0.970	4	7
7	41.0	42.2	11.1	5.7	0.972	4	7
8	40.2	42.6	11.6	5.6	0.945	3	7
9	40.2	42.6	11.6	5.6	0.945	3	7
10	42.2	44.4	7.9	5.5	0.951	5	8
11	42.1	43.0	9.5	5.4	0.980	4	8
12	42.8	43.8	8.0	5.4	0.976	5	8

Table F. 15: Experimental atomic percent of K, Nb, Bi, Ni and molar relations for KNBN x=0.20 composition by EDX spectra.

F.2.1.5. x=0.25

K (%)	Nb (%)	Bi (%)	Ni (%)	K/Nb	K/Bi	K/Ni
37.5	37.5	12.5	12.5	1	3	3

Table F. 76: Atomic percent of K, Nb, Bi, Ni and molar relations for the nominal KNBN x=0.25 composition

	K (%)	Nb (%)	Bi (%)	Ni (%)	K/Nb	K/Bi	K/Ni
1	32.1	43.2	10.9	13.8	0.743	3	2
2	37.6	39.3	12.8	10.3	0.958	3	4
3	37.5	39.5	13.6	9.4	0.950	3	4
4	37.4	42.0	12.0	8.6	0.889	3	4
5	37.3	42.1	12.0	8.6	0.887	3	4
6	38.2	40.3	13.3	8.3	0.947	3	5

7	40.2	39.7	11.9	8.1	1.013	3	5
8	38.9	40.8	12.4	7.8	0.955	3	5
9	38.9	40.8	12.4	7.8	0.955	3	5
10	38.5	40.4	13.3	7.8	0.954	3	5
11	40.3	40.9	11.4	7.4	0.983	4	5
12	39.4	42.2	11.0	7.4	0.933	4	5
13	39.6	43.2	9.8	7.4	0.917	4	5
14	39.6	43.2	9.8	7.4	0.917	4	5
15	41.4	40.3	11.3	6.9	1.028	4	6
16	41.4	40.3	11.3	6.9	1.028	4	6
17	41.9	42.9	9.5	5.7	0.977	4	7
18	73.0	18.5	5.2	3.2	3.936	14	23

Table F. 17: Experimental atomic percent of K, Nb, Bi, Ni and molar relations for KNBN x=0.25 composition by EDX spectra.

APPENDIX G

Chapter 9:

Ferroelectric and optical properties for:

$KNbO_3$ vs $K_{0.90}Ba_{0.1}Nb_{0.95}Ni_{0.05}O_3$

$K_{0.5}Na_{0.5}NbO_3$ vs $K_{0.49}Na_{0.49}Ba_{0.02}Nb_{0.99}Ni_{0.01}O_3$

G.1. Rietveld Refinements plots

G.1.1. $KNbO_3$.

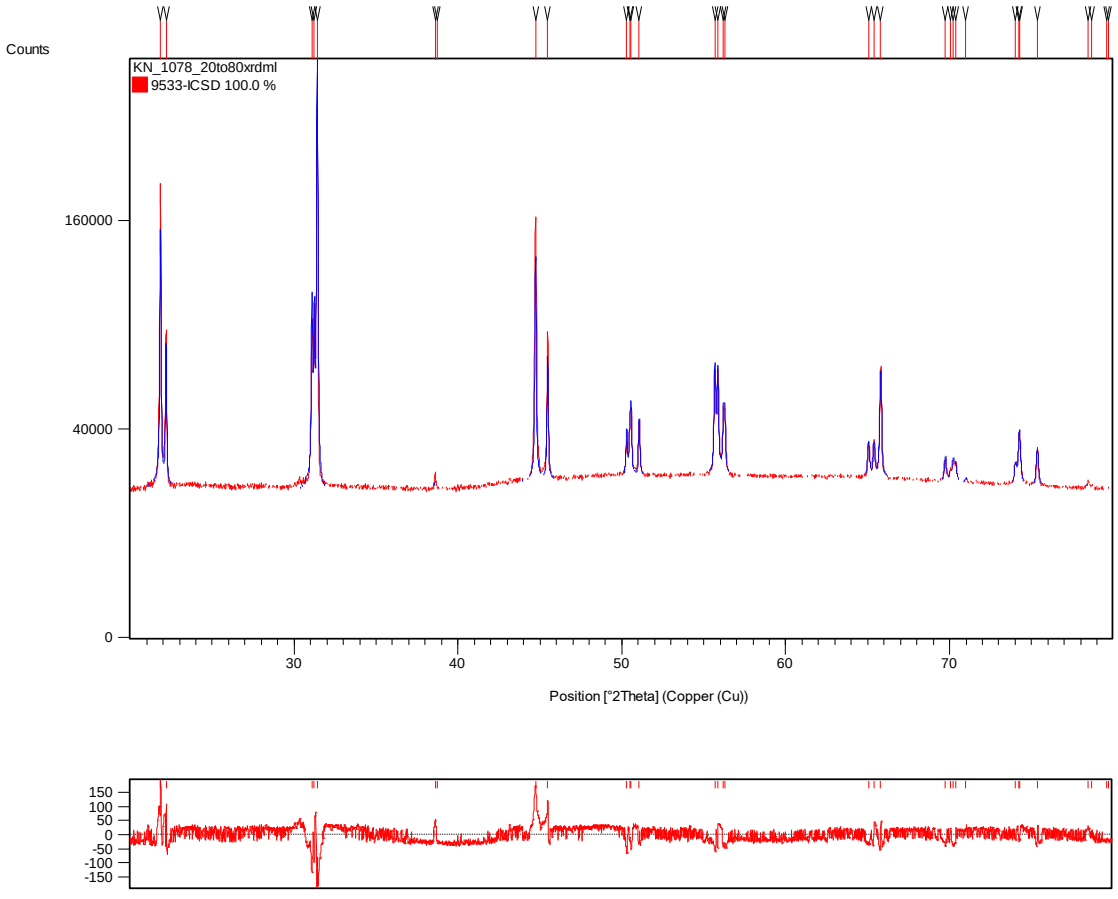

Figure G. 1.: Experimental X-ray diffraction data (red), calculated fitting profile (blue) and difference plot for $KNbO_3$ ceramic.

Atom	Wyck.	s.o.f.	x	y	z	Biso/ 10^4 pm^2
K1	2b	1.000000	0.500000	0.000000	0.528924	0.000000
Nb1	2a	1.000000	0.000000	0.000000	0.000000	0.000000
O1	2b	1.000000	0.500000	0.000000	-0.007275	0.000000
O2	4d	1.000000	0.000000	0.252400	0.335(5)	0.000000

Table G. 1.: Occupancy, atomic fract. coordinates and Biso for orthorhombic KN.

G.1.2. 0.9 $KNbO_3$- 0.1 $BaNb_{0.5}Ni_{0.5}O_3$ (KN-BNN)

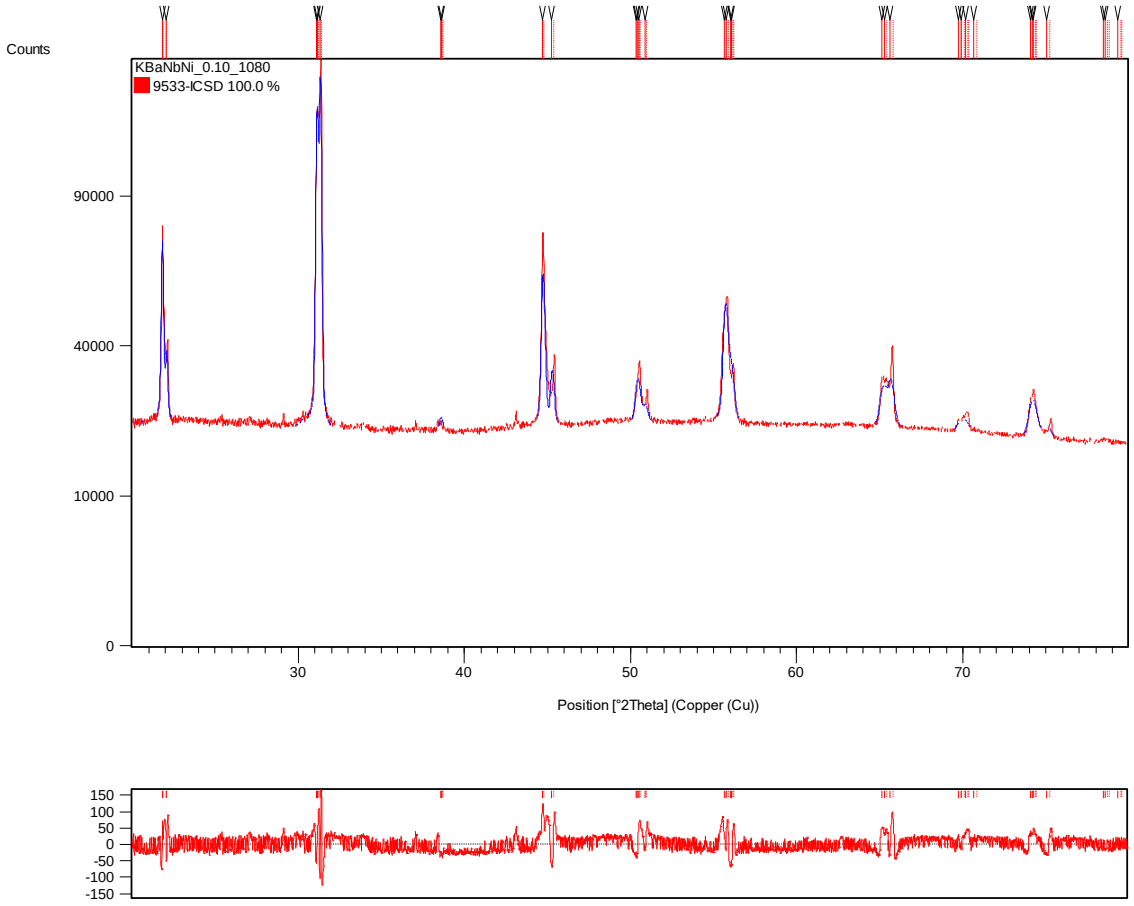

Figure G. 2: Experimental X-ray diffraction data (red), calculated fitting profile (blue) and difference plot for KN-BNN ceramic.

Atom	Wyck.	s.o.f.	x	y	z	Biso/ 10^4 pm^2
K1	2b	0.900000	0.500000	0.000000	0.513800	0.000000
Nb1	2a	1.000000	0.000000	0.000000	0.000000	0.000000
O1	2b	1.000000	0.500000	0.000000	0.036400	0.000000
O2	4d	1.000000	0.000000	0.252400	0.284200	0.000000
Ba	2b	0.100000	0.500000	0.000000	0.513800	0.000000
Ni	2a	0.100000	0.000000	0.000000	0.000000	0.000000

Table G. 2: Occupancy, atomic fract. coordinates and Biso for orthorhombic KN-BNN.

G.1.3. $K_{0.5}Na_{0.5}NbO_3$

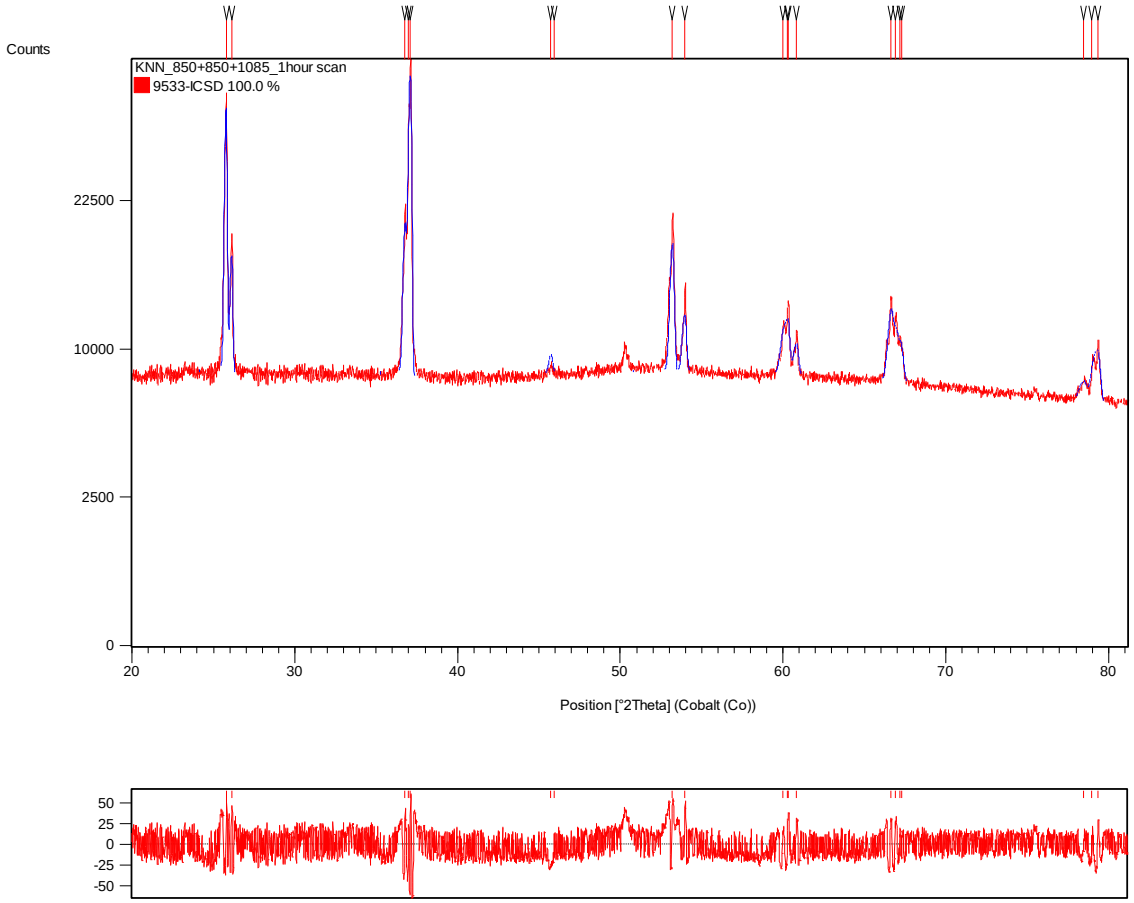

Figure G. 3.: Experimental X-ray diffraction data (red), calculated fitting profile (blue) and difference plot for KNN ceramic.

Atom	Wyck.	s.o.f.	x	y	z	Biso/ 10^4 pm^2
K1	2b	0.500000	0.500000	0.000000	0.513800	0.000000
Nb1	2a	1.000000	0.000000	0.000000	0.000000	0.000000
O1	2b	1.000000	0.500000	0.000000	0.036400	0.000000
O2	4d	1.000000	0.000000	0.252400	0.284200	0.000000
Na	2b	0.500000	0.500000	0.000000	0.574535	0.000000

Table G. 3.: Occupancy, atomic fract. coordinates and Biso for orthorhombic KNN.

G.1.4. 0.98 $K_{0.5}Na_{0.5}NbO_3$- 0.02 $BaNb_{0.5}Ni_{0.5}O_3$ (KNN-BNN)

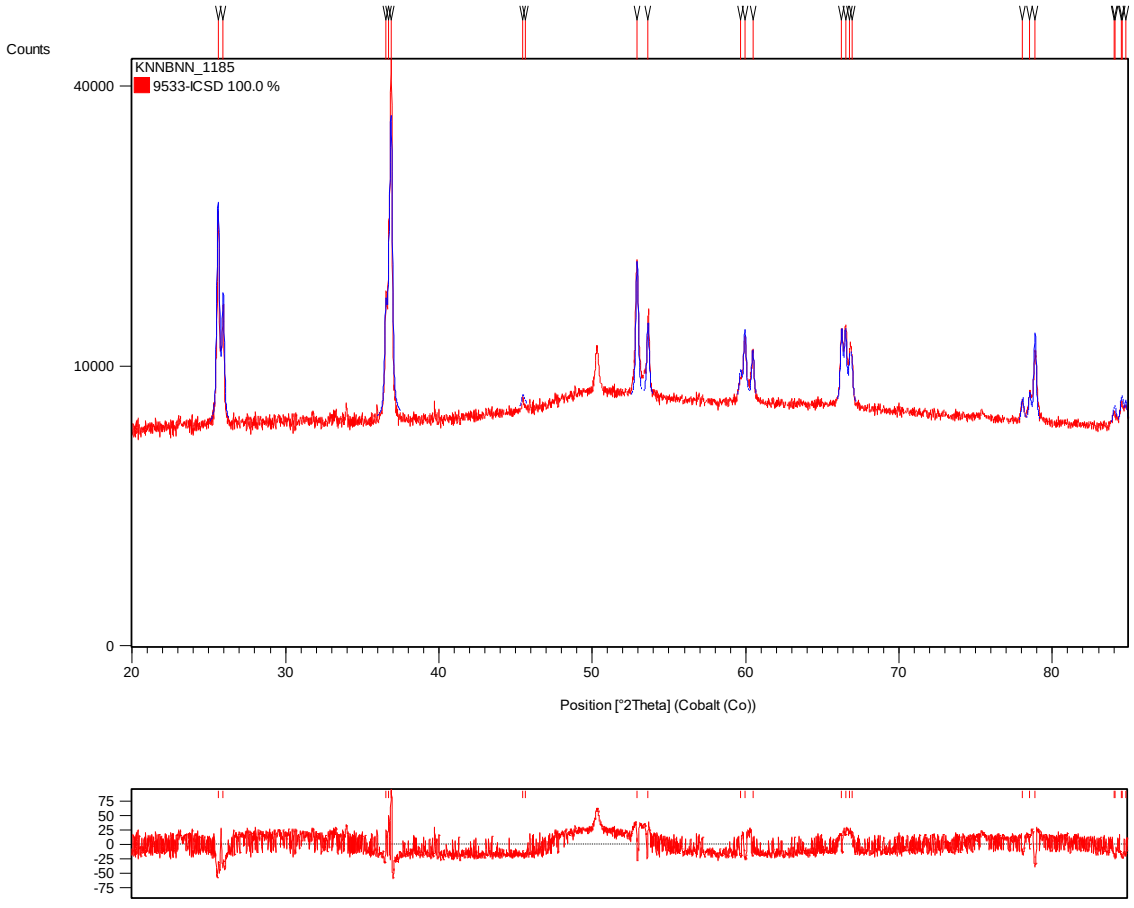

Figure G. 4.: Experimental X-ray diffraction data (red), calculated fitting profile (blue) and difference plot for 0.98 $K_{0.5}Na_{0.5}NbO_3$- 0.02 $BaNb_{0.5}Ni_{0.5}O_3$ ceramic.

Atom	Wyck.	s.o.f.	x	y	z	Biso/ 10^4 pm^2
K1	2b	0.490000	0.500000	0.000000	0.513800	0.000000
Nb1	2a	1.000000	0.000000	0.000000	0.000000	0.000000
O1	2b	1.000000	0.500000	0.000000	0.036400	0.000000
O2	4d	1.000000	0.000000	0.252400	0.284200	0.000000
Na	2b	0.490000	0.500000	0.000000	0.513800	0.000000
Ba	2a	0.020000	0.000000	0.000000	0.000000	0.000000
Ni	2a	0.020000	0.000000	0.000000	0.000000	0.000000

Table G. 4.: Occupancy, atomic fract. coordinates and Biso for orthorhombic KNN-BNN.

G.2. EDX measurements and spectra

G.2.1. $KNbO_3$

K (%)	Nb (%)	K/Nb
50	50	1

Table G. 5: Atomic percent of K, Nb molar relation for the nominal KN.

Measurements	K (%)	Nb (%)	K/Nb
1	52	48	1.073
2	52	48	1.063
3	51	49	1.058
4	51	49	1.053
5	51	49	1.048
6	51	49	1.043
7	51	49	1.033
8	51	49	1.023
9	50	50	1.018
10	50	50	1.009
11	49	51	0.963

Table G. 6: Experimental atomic percent of K, Nb, and molar relations for KN composition by EDX analyses.

G.2.2. 0.9 $KNbO_3$- 0.1 $BaNb_{0.5}Ni_{0.5}O_3$ (KN-BNN)

K (%)	Nb (%)	Ba (%)	Ni (%)	K/Nb	K/Ba	K/Ni
45	47.5	5	2.5	~0.95	9	18

Table G. 7: Atomic percent of K, Nb, Ba, Ni and molar relations for the nominal KN-BNN composition.

	K (%)	Nb (%)	Ba (%)	Ni (%)	K/Nb	K/Ba	K/Ni
1	49.1	49.5	1.4	0.0	0.992	35	-
2	47.2	48.8	4.0	0.0	0.967	12	-
3	48.5	50.9	0.5	0.0	0.953	97	-
4	48.2	51.0	0.9	0.0	0.945	54	-
5	48.8	50.0	0.8	0.4	0.976	61	122
6	43.5	47.7	8.1	0.7	0.912	5	62
7	48.4	49.5	1.3	0.8	0.978	37	61
8	43.4	45.4	7.8	0.8	0.956	6	54
9	46.6	49.9	2.4	1.0	0.934	19	47
10	46.8	48.6	3.5	1.1	0.963	13	43
11	42.5	49.9	6.2	1.4	0.852	7	30
12	45.2	48.9	3.7	2.2	0.924	12	21
13	46.3	46.3	5.1	2.4	1.000	9	19
14	45.8	47.6	3.8	2.8	0.962	12	16
15	46.2	47.2	3.4	3.2	0.979	14	14
16	40.9	46.6	9.4	3.0	0.878	4	14
17	40.4	49.1	7.5	3.0	0.823	5	13
18	40.9	44.7	10.0	4.3	0.915	4	10
19	40.9	44.7	10.0	4.3	0.915	4	10

Table G. 8.: Experimental atomic percent of K, Ba, Nb, Ni and molar relations for KN-BNN composition by EDX analyses.

G.2.3.: $K_{0.5}Na_{0.5}NbO_3$

K (%)	Na (%)	Nb (%)	K/Na	K/Nb
25	25	50	1	0.5

Table G. 9: Atomic percent of K, Na, Nb, Ni and molar relations for the nominal KNN composition.

	K (%)	Na (%)	Nb (%)	K/Na	K/Nb
1	32.3	17.0	50.7	1.9	0.6
2	28.0	15.0	57.0	1.9	0.5
3	27.3	22.2	50.6	1.2	0.5
4	27.4	22.5	50.1	1.2	0.5
5	26.0	25.0	49.0	1.0	0.5
6	25.3	24.9	49.7	1.0	0.5
7	28.3	28.0	43.7	1.0	0.6
8	22.9	24.5	52.7	0.9	0.4
9	22.9	24.7	52.4	0.9	0.4
10	22.0	24.6	53.4	0.9	0.4
11	21.9	27.4	50.7	0.8	0.4
12	21.2	29.5	49.3	0.7	0.4
13	22.4	31.3	46.3	0.7	0.5
14	19.1	28.3	52.6	0.7	0.4
15	19.5	29.1	51.5	0.7	0.4
16	19.1	28.7	52.2	0.7	0.4
17	19.6	31.3	49.0	0.6	0.4
18	20.0	32.2	47.8	0.6	0.4
19	18.6	30.3	51.1	0.6	0.4
20	19.6	32.5	48.0	0.6	0.4
21	16.9	30.0	53.1	0.6	0.3
22	18.7	33.5	47.8	0.6	0.4
23	18.5	33.4	48.1	0.6	0.4
24	17.3	31.4	51.4	0.6	0.3

Table G. 10.: Experimental atomic percent of K, Na, Nb, and molar relations for KNN composition by EDX analyses.

G.2.4.: 0.98 $K_{0.5}Na_{0.5}NbO_3$- 0.02 $BaNb_{0.5}Ni_{0.5}O_3$ (KNN-BNN)

K (%)	Na (%)	Ba (%)	Nb (%)	Ni (%)	K/Na	K/Ba	K/Nb	K/Ni
24.5	24.5	1	49.5	0.5	1	24.5	0.5	49

Table G. 11: Atomic percent of K, Na, Ba, Nb, Ni and molar relations for the nominal KNN-BNN composition

	K (%)	Na (%)	Ba (%)	Nb (%)	Ni (%)	K/Na	K/Ba	K/Nb	K/Ni
1	21.8	30.2	0.9	47.1	0.0	0.7	24	0.5	-
2	25.3	21.9	1.0	51.8	0.0	1.2	25	0.5	-
3	33.6	15.8	0.3	50.3	0.0	2.1	112	0.7	-
4	28.9	19.8	1.1	50.2	0.0	1.5	26	0.6	-
5	32.6	19.1	1.4	46.9	0.0	1.7	23	0.7	-
6	31.5	19.0	1.5	48.0	0.0	1.7	21	0.7	-
7	25.4	23.6	0.9	50.1	0.0	1.1	28	0.5	-
8	21.2	25.2	1.2	52.4	0.0	0.8	18	0.4	-
9	14.0	13.6	10.2	62.2	0.0	1.0	1	0.2	-
10	33.2	19.0	0.6	47.2	0.0	1.7	55	0.7	-
11	27.7	21.4	1.0	49.9	0.0	1.3	28	0.6	-
12	25.0	24.7	0.5	49.9	0.0	1.0	50	0.5	-
13	28.3	21.8	0.9	48.9	0.1	1.3	31	0.6	283
14	20.1	29.7	1.5	48.5	0.2	0.7	13	0.4	101
15	30.1	20.1	0.9	48.6	0.3	1.5	33	0.6	100
16	37.9	13.6	1.4	46.5	0.5	2.8	27	0.8	76
17	26.7	23.7	0.5	48.6	0.4	1.1	53	0.5	67
18	23.1	25.2	1.3	50.1	0.4	0.9	18	0.5	58
19	27.9	23.4	0.7	47.5	0.6	1.2	40	0.6	47
20	30.4	16.9	2.0	50.0	0.7	1.8	15	0.6	43
21	29.0	16.8	1.1	52.4	0.7	1.7	26	0.6	41
22	25.8	23.6	1.3	48.4	0.8	1.1	20	0.5	32
23	26.1	22.0	2.0	49.1	0.9	1.2	13	0.5	29
24	20.2	23.7	1.4	53.6	1.1	0.9	14	0.4	18
25	18.9	30.7	0.9	48.4	1.1	0.6	21	0.4	17
26	20.0	27.1	0.6	51.0	1.2	0.7	33	0.4	17
27	24.5	25.7	1.6	46.6	1.5	1.0	15	0.5	16

28	18.7	28.7	1.5	49.8	1.3	0.7	12	0.4	14
29	19.9	23.8	1.3	53.2	1.8	0.8	15	0.4	11
30	13.8	13.4	12.7	58.4	1.7	1.0	1	0.2	8
31	13.0	18.0	10.2	57.1	1.7	0.7	1	0.2	8

Table G. 12: Experimental atomic percent of K, Na, Ba, Nb, Ni and molar relations for KNN-BNN composition by EDX analyses.

APPENDIX H

H.1. Publications and Scientific Results

H.1.1. Published papers

1. Uchechukwu Obilor, Cristina Pascual-Gonzalez, Shunsuke Murakami, Ian M. Reaney and Antonio Feteira. *Study of the temperature dependence of the giant electric field-induced strain in Nb-doped BNT-BT-BKT piezoceramics*, Materials Research Bulletin, 2017, ISSN 0025-5408.

2. Journal American Ceramic Society. Invited feature article + cover devoted to Band Gap Engineering of $KNbO_3$ to be published in 2018.

3. C. Pascual-Gonzalez, G. Schileo, S. Murakami, A. Khesro, D. Wang, I. M. Reaney and A. Feteira. *Continuously controllable optical band gap in orthorhombic ferroelectric $KNbO_3$-$BiFeO_3$ ceramics.* Applied Physics Letters, 110, 179202 (2017).

4. C. Pascual-González, G. Schileo, A. Kherso, I. Sterianou, D. Wang, I. M. Reaney and A. Feteira. *Band gap evolution and piezoelectric-to-electrostrictive crossover in (1-x)$KNbO_3$ - x($Ba_{0.5}Bi_{0.5}$)($Nb_{0.5}Zn_{0.5}$)O_3 ceramics.* Journal of Materials Chemistry C, 5 (8). pp. 1990-1996. (2017). Electronic Supplementary Information (ESI) available.

5. C. Pascual-González, G. Schileo and A. Feteira. *Band gap narrowing in KNbO3-Bi(Yb,Me)O3 (Me=Fe or Mn) ferroelectric ceramic*s. Applied Physics Letters, 109, 132902 (2016).

6. G. Schileo, C. Pascual-Gonzalez, M. Alguero, I. M. Reaney, P. Postolache, L. Mitoseriu, K. Reichmann and A. Feteira. *Yttrium Iron Garnet/Barium Titanate Multiferroic Composites*. Journal American Ceramic Society 1-6 (2016).

H.1.2. Chapter book

1. Chapter 22: Single Phase, Composite and Laminate Multiferroics in Magnetic, Ferroelectric, and Multiferroic Metal Oxides, Elsevier, awaiting final proofs.

H.2. Attendance

H.2.1. Placements

1. Short-Term Scientific Mission (STSM) (From 20/02/2017 to 10/3/2013)

Institut de Ciència de Materials de Barcelona (ICMAB-CSIC)

Activity: Thin films preparation by PLD of promising photovoltaic ceramics.

Granted: TO-BE COST Action

Supervisor: Ignasi Fina.

H.2.2. Attended congresses

1. 12th Pacific Rim Conference on Ceramic and Glass Technology (PACRIM 12), including Glass & Optical Materials Division Meeting (GOMD 2017). Waikoloa, Hawaii, USA. 21-26 May 2017.

2. TO-BE Spring Meeting 2017. Luxembourg. 3-5 April 2017.

3. TO-BE Fall Meeting 2016. City Hotel Ljubljana, Ljubljana, Slovenia. 28-30 September 2016.

4. TO-BE Spring Meeting 2016. University of Warwick-England. United Kingdom. 6-8 of April 2016.

5. 14th International Conference, European Ceramic Society. Toledo. Spain. 21-25 June 2015.

H.3.2. Summer Schools

1. International School of Oxide School of Oxide Electronics 2015 (ISOE 2015). Institut D'etudes Scientifiques De Cargèse, Cargese, Corsica, France. 12-24 October 2015.

H.3 Dissemination

H.3.1 Oral contributions as presenting author:

1. C. Pascual-Gonzalez, G. Schileo and A. Feteira. Band gap engineering in KNbO3-based solid solutions. 12th Pacific Rim Conference on Ceramic and Glass Technology (PACRIM 12), including Glass & Optical Materials Division Meeting (GOMD 2017), from 21st to 26th of May 2017 in Waikoloa, Hawaii, USA.

2. Cristina Pascual-Gonzalez, Carolina Elicker, Iasmi Sterianou and Antonio Feteira. Piezoelectric-to-electrostrictive crossover in (1-x) $KNbO_3$-x$(Ba_{0.5}Bi_{0.5})(Nb_{0.5}Zn_{0.5})O_3$ ceramics. MERI Symposium. 3rd Place Award Student Talk. Sheffield Hallam University. Sheffield. United Kingdom. 17-18 May 2016.

3. G. Schileo, C. Pascual-Gonzalez, M. Alguero, I. M. Reaney, P. Postolache, L. Mitoseriu, K. Reichmann and A. Feteira. Multiferroic Composites. 14th International Conference, European Ceramic Society. Toledo Spain. 21-25 June 2015.

H.3.2 Poster contributions as presenting author

1. C. Pascual-Gonzalez, G. Schileo and A. Feteira. Band gap engineering in $KNbO_3$-$BiMeO_3$ (Me=Mn, Fe, Co and Ni). TO-BE Spring Meeting 2017. Luxembourg. 3-5 April 2017.

2. C. Pascual-Gonzalez, G. Schileo and A. Feteira. Continuously controllable optical band gap in ferroelectric $KNbO_3$-$BiFeO_3$ solid solution. TO-BE Fall Meeting 2016. Ljubljana, Slovenia. 28-30 September 2016.

3. C. Pascual-Gonzalez, G. Schileo, A. Nabok and A. Feteira. Band gap narrowing in ferroelectric $KNbO_3$-$Bi(Yb,Me)O_3$ (Me=Fe or Mn) ceramics. TO-BE Spring Meeting 2016. University of Warwick-England. 6-8 of April 2016.

4. C. Pascual-Gonzalez, G. Schileo and A. Feteira. Ferroelectric material for solar energy harvesting. MERI Symposium. Sheffield Hallam University. Sheffield. United Kingdom. 19-20 May 2015.