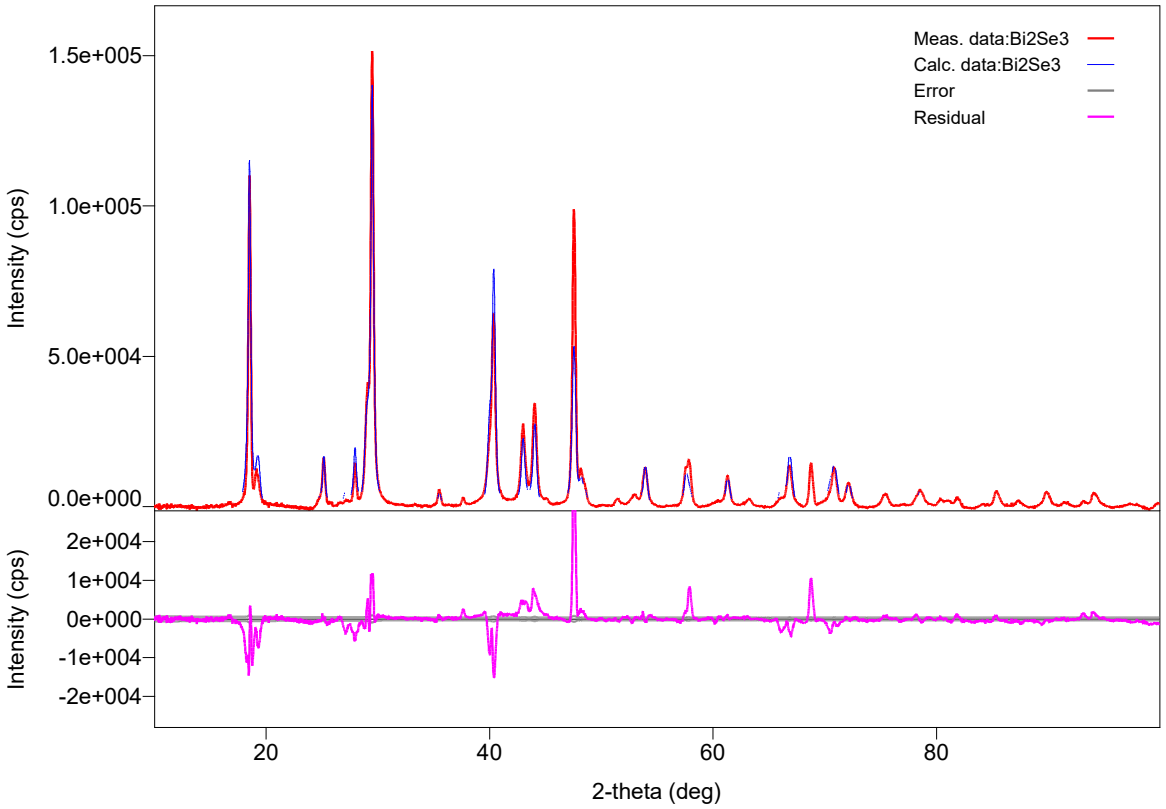
Analysis Results

General Information

Analysis date	2025/02/13 11:24:56		
Sample name		Measurement date	2025/02/13 10:36:45
File name	Bi2Se3.ras	Operator	Administrator
Comment			

Measurement profile



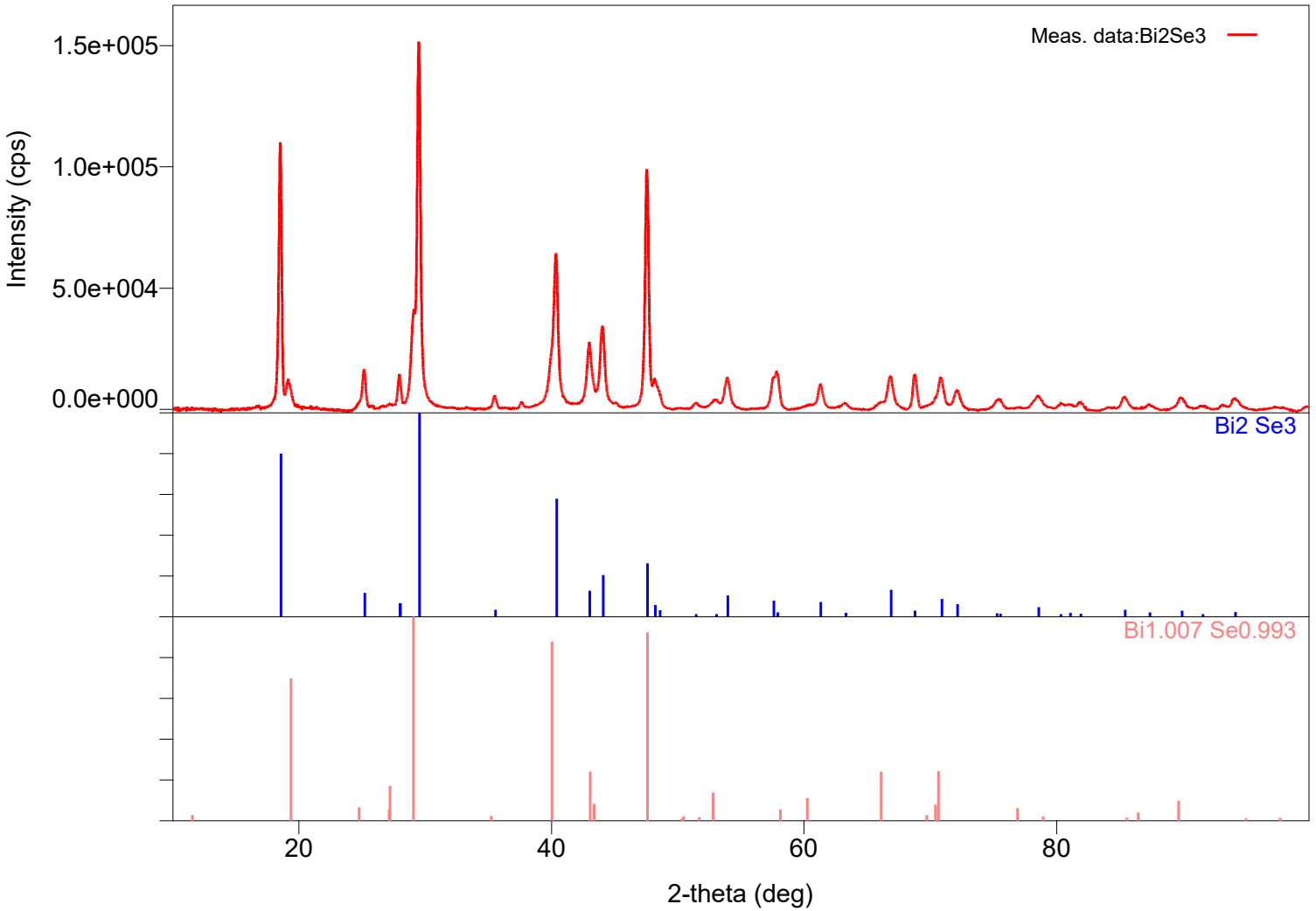
Measurement conditions

X-Ray	40 kV , 44 mA	Scan speed / Duration time	3.0293 deg/min (effective speed)
Goniometer	SmartLab(In-plane)	Step width	0.0100 deg
Attachment	Standard	Scan axis	Theta/2-Theta
Filter	Cu_K-beta	Scan range	10.0000 - 99.9700 deg
CBO selection slit	BB	Incident slit	2/3deg
Diffrected beam mono.	No_unit	Length limiting slit	10.0mm
Detector	HyPix 3000(H)	Receiving slit #1	20.000mm
Scan mode	CONTINUOUS	Receiving slit #2	30.100mm

Qualitative analysis results

Phase name	Formula	Figure of merit	Phase reg. detail	DB card number
Bismuth Selenide	Bi2 Se3	0.670	ICSD	165226
Nevskite	Bi1.007 Se0.993	0.811	ICSD	79019

Phase name	Formula	Space group	Phase reg. detail	DB card number
Bismuth Selenide	Bi2 Se3	166 : R-3m,hexagonal	ICSD	165226
Nevskite	Bi1.007 Se0.993	164 : P-3m1	ICSD	79019


Meas. data:Bi2Se3
1.5e+005
1.0e+005
5.0e+004
0.0e+000
Intensity (cps)
Bi2 Se3
Bi1.007 Se0.993
20
40
60
80
2-theta (deg)

Peak list

No.	2-theta(deg)	d(ang.)	Height(cps)	FWHM(deg)	Int. I(cps deg)	Int. W(deg)	Asym. factor
1	18.5090(13)	4.7898(3)	74308(613)	0.2432(12)	23112(145)	0.311(5)	1.07(3)
2	19.185(6)	4.6225(15)	7304(192)	0.539(16)	5030(128)	0.69(4)	1.07(3)
3	25.132(7)	3.5406(10)	11396(240)	0.278(7)	4575(69)	0.401(15)	0.96(12)
4	27.19(4)	3.277(4)	719(60)	0.68(8)	603(67)	0.84(16)	1.26(11)
5	27.945(5)	3.1902(6)	8982(213)	0.257(4)	2841(74)	0.316(16)	1.26(11)
6	29.0499(16)	3.07134(16)	23585(345)	0.449(5)	13979(174)	0.593(16)	0.951(14)
7	29.4713(7)	3.02837(8)	103033(721)	0.2629(7)	35760(183)	0.347(4)	0.951(14)
8	35.457(11)	2.5296(8)	4001(142)	0.281(10)	1667(27)	0.42(2)	0.78(15)
9	37.600(5)	2.3902(3)	1683(92)	0.242(8)	453(13)	0.27(2)	0.96(7)
10	40.303(2)	2.23595(11)	47222(488)	0.345(3)	28677(85)	0.607(8)	0.91(2)
11	42.952(3)	2.10401(13)	17773(300)	0.421(3)	11097(52)	0.624(13)	0.85(3)
12	43.986(2)	2.05689(11)	24088(349)	0.366(3)	13058(46)	0.542(10)	0.85(3)
13	45.040(10)	2.0112(4)	1040(72)	0.21(3)	319(29)	0.31(5)	0.85(3)
14	47.5245(15)	1.91168(6)	74755(614)	0.2770(11)	26415(154)	0.353(5)	1.06(2)
15	48.130(9)	1.8890(3)	6983(188)	0.40(2)	3531(266)	0.51(5)	1.06(2)
16	48.497(17)	1.8756(6)	3644(136)	0.38(3)	1748(201)	0.48(7)	1.06(2)
17	51.426(8)	1.7754(3)	1663(92)	0.471(19)	1033(26)	0.62(5)	1.07(6)
18	52.896(12)	1.7295(4)	2307(108)	0.72(3)	2198(61)	0.95(7)	1.07(6)
19	53.888(5)	1.69997(16)	8948(213)	0.454(5)	5359(79)	0.60(2)	1.07(6)
20	57.655(8)	1.5975(2)	9374(218)	0.647(7)	6635(76)	0.71(2)	0.807(12)
21	60.79(4)	1.5224(8)	1059(73)	2.08(10)	2418(96)	2.3(2)	0.807(12)
22	61.242(3)	1.51230(8)	5562(168)	0.360(10)	2189(60)	0.39(2)	0.807(12)
23	63.130(14)	1.4715(3)	1366(83)	0.62(3)	927(45)	0.68(7)	0.807(12)
24	66.10(2)	1.4125(4)	2034(101)	0.79(7)	1721(159)	0.85(12)	0.99(12)
25	66.787(6)	1.39955(11)	9666(221)	0.427(11)	4395(167)	0.45(3)	0.99(12)
26	67.34(4)	1.3894(8)	1166(77)	0.44(9)	552(152)	0.47(16)	0.99(12)
27	68.7510(12)	1.36429(2)	11604(242)	0.291(2)	3591(19)	0.309(8)	1.40(2)
28	70.764(8)	1.33034(14)	8449(207)	0.452(11)	5431(73)	0.64(2)	0.89(8)
29	72.054(10)	1.30965(16)	5074(160)	0.509(17)	3675(57)	0.72(3)	0.89(8)
30	75.371(13)	1.26004(19)	2895(121)	0.659(15)	2058(45)	0.71(5)	1.26(10)
31	76.92(5)	1.2385(6)	480(49)	1.12(12)	582(50)	1.2(2)	1.26(10)
32	78.490(15)	1.2176(2)	3335(130)	0.809(15)	2910(64)	0.87(5)	1.26(10)
33	80.299(18)	1.1947(2)	1352(83)	0.30(5)	514(77)	0.38(8)	1.1(3)

34	80.90(3)	1.1873(4)	1110(75)	0.63(11)	883(103)	0.80(15)	1.1(3)
35	81.817(10)	1.17629(11)	2153(104)	0.34(3)	925(62)	0.43(5)	1.1(3)
36	84.23(4)	1.1486(4)	470(49)	0.40(11)	235(36)	0.50(13)	1.2(2)
37	85.340(19)	1.1365(2)	3978(142)	0.45(2)	2201(44)	0.55(3)	1.2(2)
38	87.25(3)	1.1165(3)	1412(84)	0.48(3)	843(33)	0.60(6)	0.7(2)
39	89.859(12)	1.09071(12)	3655(136)	0.556(13)	2451(37)	0.67(3)	1.8(2)
40	91.437(13)	1.07596(12)	950(69)	0.52(4)	621(33)	0.65(8)	0.9(3)
41	93.071(10)	1.06131(9)	1507(87)	0.34(2)	563(26)	0.37(4)	0.56(6)
42	93.995(14)	1.05329(12)	3240(128)	0.597(14)	2118(48)	0.65(4)	0.56(6)
43	97.31(19)	1.0261(15)	504(50)	0.8(2)	403(92)	0.8(3)	1.0(12)
44	97.96(5)	1.0209(4)	434(47)	0.18(9)	82(65)	0.19(17)	1.0(12)

Parameters used for WPPF

Profile parameters

Common parameter	Background	Data	Bi2Se3
		Function name	B-spline
		param0	79307.693728878847
		param1	63842.930636349716
		param2	54417.206798879917
		param3	27977.346686271343
		param4	24152.688083933997
		param5	18570.395479057795
		param6	20119.771637460741
		param7	17457.007001890113
		param8	18515.583031792154
		param9	16615.722650039577
		param10	19174.168094614397
		param11	19020.353345113966
		param12	17584.686320520486
		param13	18781.482710008277
		param14	18604.033221194186
		param15	18489.56253601981
		param16	20661.661168814284
		node0	10
		node1	19.48
		node2	28.960000000000001
		node3	34.990000000000002
		node4	41.020000000000003
		node5	47.049999999999997
		node6	53.079999999999998
		node7	58.240000000000002
		node8	63.399999999999999
		node9	67.430000000000007
		node10	71.459999999999994
		node11	75.489999999999995
		node12	79.519999999999996

		node13	86.840000000000003
		node14	99.969999999999999
Common parameter	Peak shift		
		Function name	Shift axial displacement
		param0	-0.097373839889294531
		param1	0
		param2	0
Bismuth Selenide	Scale factor	s	855(3)
	FWHM	U	0.2127
		V	0.0431
		W	0.0500
	Asym. factor	A0	-0.2191
		A1	0.0000
	Decay rate factor	etaL0/mL0	1.1606
		etaL1/mL1	0.1532
		etaL2/mL2	0.0000
		etaH0/mH0	1.0468
		etaH1/mH1	-0.6106
		etaH2/mH2	0.0000
	Preferred orientationMarch-Dollase	h	0
		k	0
		l	3
		March coefficient	0.664350
Nevskite	Scale factor	s	145(3)
	FWHM	U	1.0588
		V	-0.8924
		W	0.3028
	Asym. factor	A0	0.1672
		A1	0.0000
	Decay rate factor	etaL0/mL0	0.0000
		etaL1/mL1	0.0000
		etaL2/mL2	0.0000
		etaH0/mH0	0.2673
		etaH1/mH1	0.0000
		etaH2/mH2	0.0000
	Preferred orientationMarch-Dollase	h	0
		k	0

	I	1
	March coefficient	0.538411

Structure parameters

Data set name	Phase Name	Element	x	y	z	Occupancy	Temperature factor
Bi2Se3	Bismuth Selenide	Bi	0.000000	0.000000	0.399813	1.000	1.353
Bi2Se3	Bismuth Selenide	Se	0.000000	0.000000	0.000000	1.000	2.193
Bi2Se3	Bismuth Selenide	Se	0.000000	0.000000	0.209695	1.000	0.014
Bi2Se3	Nevskite	Bi	0.333333	0.666667	0.04(2)	0.740	1(3)
Bi2Se3	Nevskite	Se	0.333333	0.666667	0.04(16)	0.260	1(207)
Bi2Se3	Nevskite	Se	0.000000	0.000000	0.125(9)	1.000	1(7)
Bi2Se3	Nevskite	Bi	0.666667	0.333333	0.206(6)	1.000	1.4(18)
Bi2Se3	Nevskite	Se	0.333333	0.666667	0.29(2)	1.000	0(2)
Bi2Se3	Nevskite	Bi	0.000000	0.000000	0.378(4)	1.000	1(8)
Bi2Se3	Nevskite	Se	0.666667	0.333333	0.46(14)	0.720	2(27)
Bi2Se3	Nevskite	Bi	0.666667	0.333333	0.46(15)	0.280	2(187)

Data set name	Rwp	Rp	Re	S	Chi^2	Maximum shift/e.s.d.
Bi2Se3	6.53	3.65	1.29	5.0556	25.5586	0.556

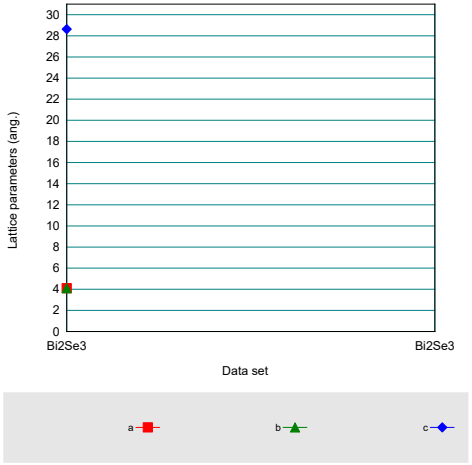
Lattice parameters

Angular correction

Analysis results

Data set name	a(A)	b(A)	c(A)	alpha(deg)	beta(deg)	gamma(deg)
Bi2Se3	4.104472	4.104472	28.629552	90.000000	90.000000	120.000000
Bi2Se3	4.197004	4.197004	22.906802	90.000000	90.000000	120.000000

Phase name	a(A)	b(A)	c(A)	alpha(deg)	beta(deg)	gamma(deg)	V(A^3)
Bismuth Selenide	4.104472	4.104472	28.629552	90.000000	90.000000	120.000000	417.695562
Nevskite	4.197004	4.197004	22.906802	90.000000	90.000000	120.000000	349.441081



Crystallinity

Data set name	Crystallinity(%)

CrystallinityGraph.emf

Crystallite size and lattice strain

Williamson-Hall method

Data set name	Crystallite size(A)	Strain(%)
Bi2Se3	247.8(3)	0.218(3)
Bi2Se3	173(2)	0.25(6)

Phase name	Crystallite size(A)	Distribution RSD	Strain(%)	Distribution type
Bismuth Selenide	247.8(3)	-	0.218(3)	-
Nevskite	173(2)	-	0.25(6)	-

CSSGraph.emf

Quantitative analysis results (RIR)

RIRGraph.emf

Quantitative analysis results (WPPF)

	Phase name	Content(%)
-	Bismuth Selenide	86.9(2)
-	Nevskite	13.1(2)

Quantitative analysis results (standard addition method)

Calibration data

QuantityCalibration.emf

Quantitative analysis results (External Standard method)

Calibration data

QuantityCalibration.emf

Quantitative analysis results (internal standard method)

Calibration Data

QuantityCalibration.emf

Stress

Stress constants

Analytical conditions

Analysis results

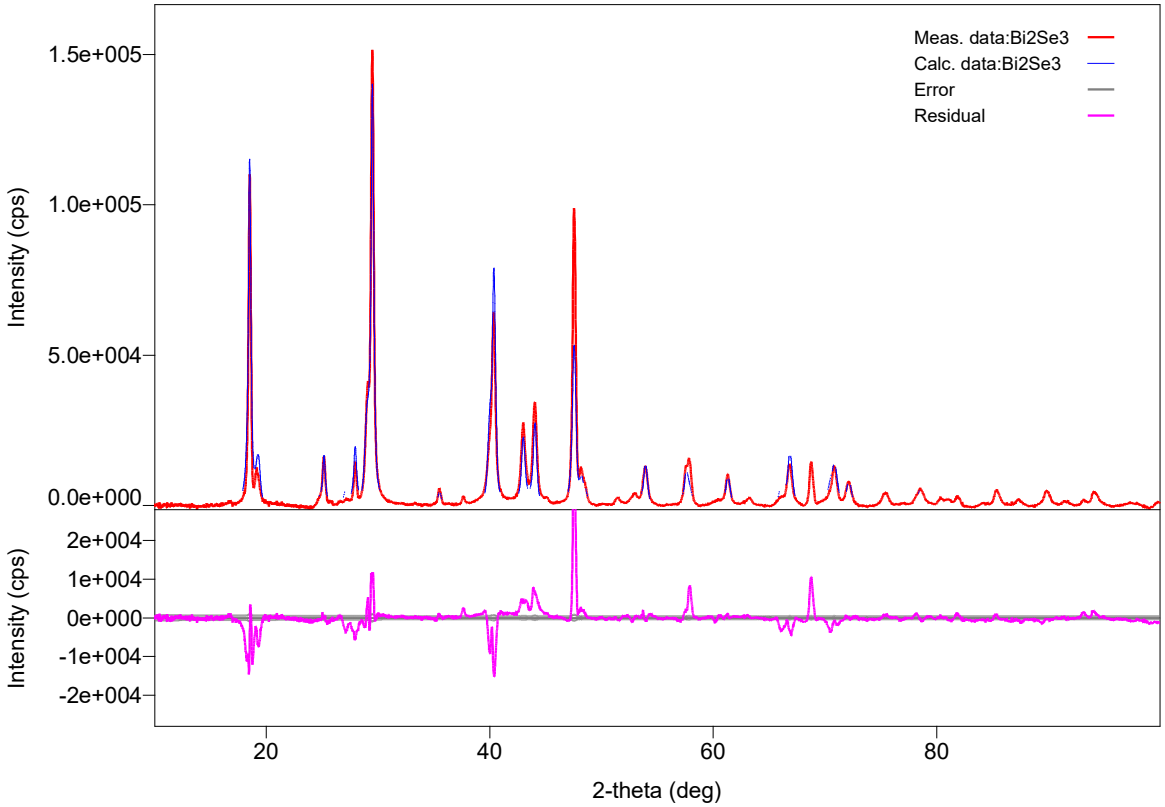
StressGraph.emf

Cluster analysis results

Dendrogram

ClusterDendrogram.emf

Measurement profiles



Cluster

Sample well

ClusterSamplePlate.emf

PCA view

ClusterPCA3DGraph.emf

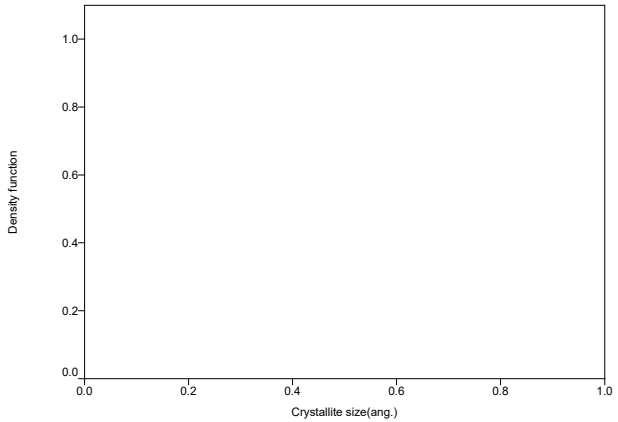
Eigenvalue graph

ClusterPCAGraph.emf

Crystallite size distribution analysis results

Crystallite size distribution

Crystallite size distribution graph



Crystal structure analysis results

Indexing

Phase name	Formula	Figure of merit	Phase reg. detail	DB card number
Bismuth Selenide	Bi2 Se3	0.670	ICSD	165226
Nevskite	Bi1.007 Se0.993	0.811	ICSD	79019

Quantitative analysis results

	Phase name	Content(%)
-	Bismuth Selenide	86.9(2)
-	Nevskite	13.1(2)

Lattice information

Phase name	a(A)	b(A)	c(A)	alpha(deg)	beta(deg)	gamma(deg)	V(A^3)
Bismuth Selenide	4.104472	4.104472	28.629552	90.000000	90.000000	120.000000	417.695562
Nevskite	4.197004	4.197004	22.906802	90.000000	90.000000	120.000000	349.441081

Phase name	Space group	Z	Z'	Calc. density(g/cm^3)
Bismuth Selenide	166 : R-3m,hexagonal	3	0.083	7.810
Nevskite	164 : P-3m1	6	0.500	8.234

Structure determination

Refinement

Measurement range: 10.0000-99.9700deg Refinement range: 10.0000-99.9700deg (1.01 A)
Number of refined parameters: 19

Phase name	Atomic coords	# of indep. reflns
Bismuth Selenide	Fractional coords	76
Nevskite	Fractional coords	186

Rwp = 6.53% S = 5.0556

Crystal structure

CrystalGraph.emf