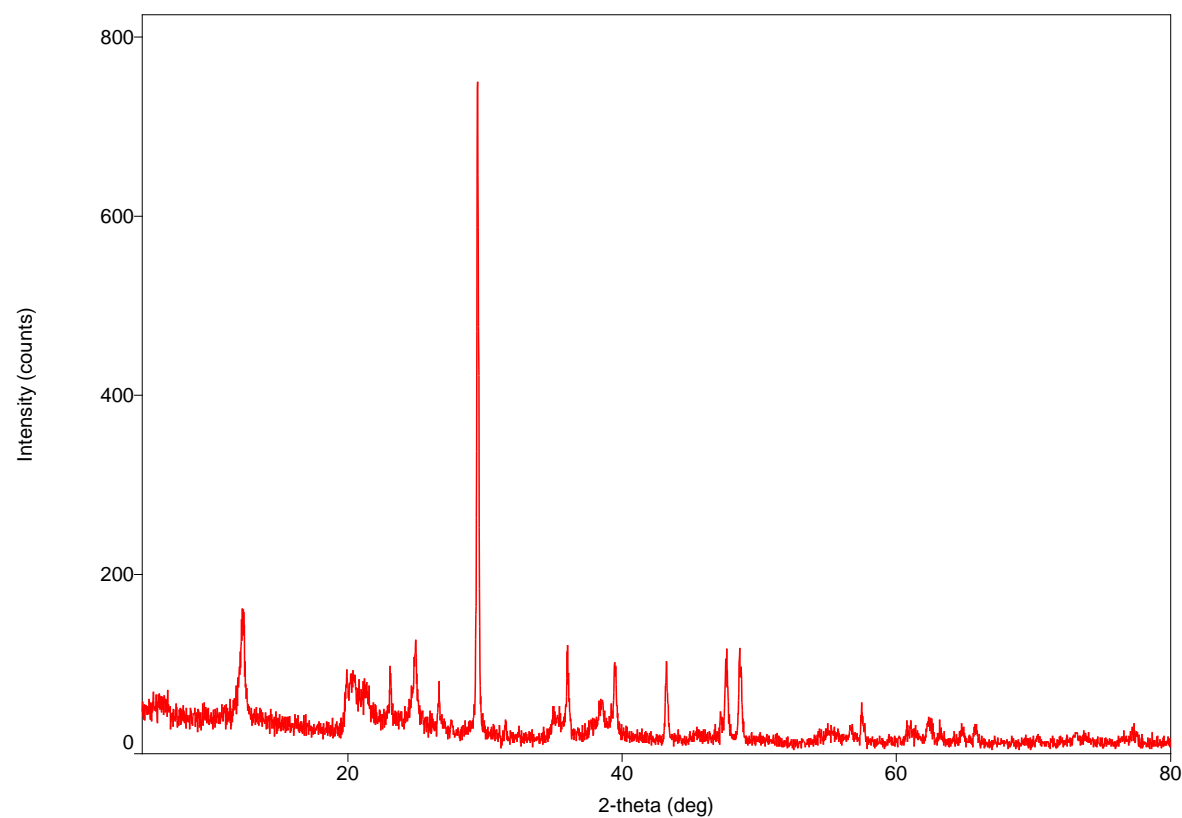


Analysis Results

General Information

Analysis date	2023/11/17 10:41:11		
Sample name	RKE3	Measurement date	2023/08/07 14:00:38
File name	RKE3.raw	Operator	USER
Comment	harpic strained		

Measurement profile



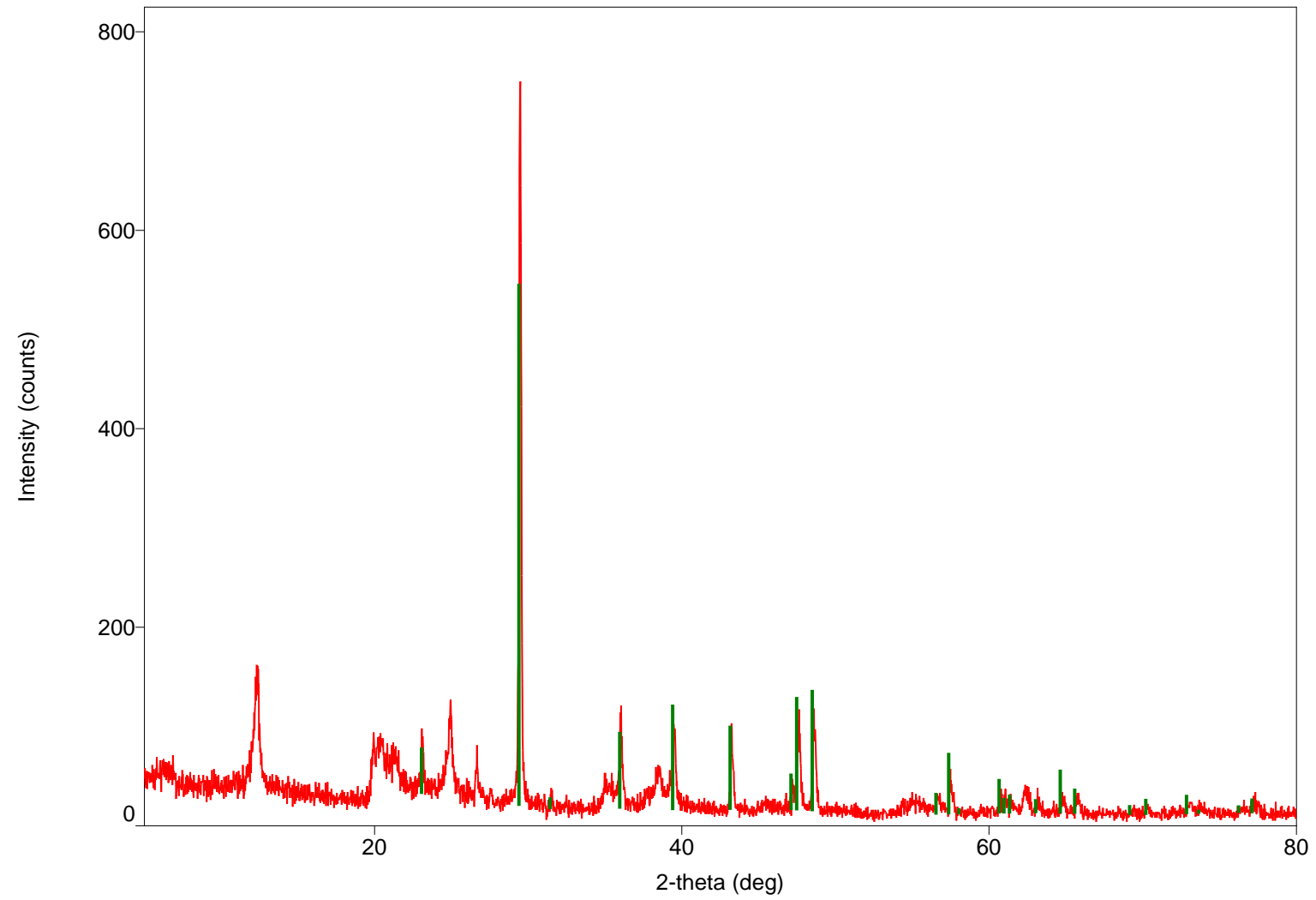
Measurement conditions

X-Ray	40 kV , 30 mA	Scan speed / Duration time	4.0000 deg./min.
Goniometer		Step width	0.0200 deg.
Attachment	-	Scan axis	2theta/theta
Filter	K-beta filter	Scan range	5.0000 - 80.0000 deg.
CBO selection slit	-	Incident slit	2/3 deg.
Diffrected beam mono.		Length limiting slit	-
Detector	Scintillation counter	Receiving slit #1	2/3 deg.
Scan mode	CONTINUOUS	Receiving slit #2	0.3mm

Qualitative analysis results

Phase name	Formula	Figure of merit	Phase reg. detail	DB card number
Calcite	CaCO ₃	0.654	ICDD (PDF-2 Release 2015 RDB)	00-047-1743

Phase name	Formula	Space group	Phase reg. detail	DB card number
Calcite	CaCO ₃	167 : R-3c,hexagonal	ICDD (PDF-2 Release 2015 RDB)	00-047-1743



Peak list

No.	2-theta(deg)	d(ang.)	Height(counts)	FWHM(deg)	Size(ang.)	Phase name	Chemical formula
1	12.409(14)	7.127(8)	76(9)	0.39(2)	214(13)	Unknown	Unknown
2	20.42(2)	4.346(5)	33(6)	1.67(5)	50.4(16)	Unknown	Unknown
3	23.076(8)	3.8511(12)	35(6)	0.15(2)	567(79)	Calcite(0,1,2)	CaCO ₃
4	24.888(10)	3.5747(13)	59(8)	0.24(3)	352(40)	Unknown	Unknown
5	26.64(3)	3.344(4)	24(5)	0.13(4)	651(178)	Unknown	Unknown
6	29.467(4)	3.0287(4)	609(25)	0.115(5)	746(31)	Calcite(1,0,4)	CaCO ₃
7	35.25(8)	2.544(6)	14(4)	0.89(15)	97(16)	Unknown	Unknown
8	36.00(2)	2.4927(16)	45(7)	0.24(2)	367(35)	Calcite(1,1,0)	CaCO ₃
9	38.46(4)	2.339(2)	24(5)	0.58(7)	152(19)	Unknown	Unknown
10	39.462(11)	2.2816(6)	68(8)	0.16(3)	545(86)	Calcite(1,1,3)	CaCO ₃
11	43.243(11)	2.0905(5)	70(8)	0.135(12)	663(57)	Calcite(2,0,2)	CaCO ₃
12	47.202(11)	1.9240(4)	28(5)	0.09(2)	1017(224)	Calcite(0,2,4)	CaCO ₃
13	47.572(15)	1.9099(6)	77(9)	0.168(19)	540(60)	Calcite(0,1,8)	CaCO ₃
14	48.561(4)	1.87325(14)	88(9)	0.150(12)	605(49)	Calcite(1,1,6)	CaCO ₃
15	55.26(9)	1.661(2)	8(3)	1.48(14)	63(6)	Unknown	Unknown
16	56.65(2)	1.6233(5)	13(4)	0.17(4)	549(135)	Calcite(2,1,1)	CaCO ₃
17	57.466(10)	1.6023(3)	30(6)	0.156(17)	607(66)	Calcite(1,2,2)	CaCO ₃
18	60.99(6)	1.5178(14)	9(3)	0.62(13)	155(32)	Calcite(2,1,4)	CaCO ₃
19	62.34(3)	1.4883(5)	21(5)	0.22(4)	432(77)	Unknown	Unknown
20	64.76(4)	1.4383(8)	13(4)	0.17(4)	579(138)	Calcite(3,0,0)	CaCO ₃
21	65.701(16)	1.4200(3)	14(4)	0.19(4)	527(117)	Calcite(0,0,12)	CaCO ₃
22	72.99(3)	1.2952(5)	9(3)	0.30(13)	348(158)	Calcite(1,2,8)	CaCO ₃

Parameters used for WPPF

Profile parameters

Common parameter	Background	Data	RKE3
		Function name	B-spline
		param0	174.82721795483283
		param1	150.60607537089101
		param2	115.34344976730381
		param3	124.86313270239458
		param4	60.317346985289348
		param5	140.28993342628635
		param6	43.717944078157863
		param7	62.828047824224228
		param8	46.258950278935551
		param9	61.233425278763583
		param10	31.740462805809543
		param11	38.317677642221454
		param12	44.286348930778054
		param13	32.071077361300176
		param14	43.70790931868234
		param15	42.007487590162405
		param16	33.856906818598105
		node0	5
		node1	9.839999999999999
		node2	14.68
		node3	19.52
		node4	24.399999999999999
		node5	29.739999999999998
		node6	35.079999999999998
		node7	40.420000000000002
		node8	45.759999999999998
		node9	52.039999999999999
		node10	58.32
		node11	64.599999999999994
		node12	69.719999999999999

		node13	74.840000000000003
		node14	80
Common parameter	Peak shift	Function name	Shift axial displacement
		param0	0.083453591301635349
		param1	0
		param2	0
Calcite	Scale factor	s	4.1(2)
		U	0.0932
		V	-0.0589
		W	0.0306
		A0	0.1608
		A1	0.9195
		etaL0/mL0	0.6611
		etaL1/mL1	-0.1458
		etaL2/mL2	0.0000
		etaH0/mH0	0.8013
		etaH1/mH1	-0.1302
		etaH2/mH2	0.0000
		Preferred orientationMarch-Dollase	
		h	0
		k	0
		l	0
		March coefficient	1.000000

Structure parameters

Data set name	Phase Name	Element	x	y	z	Occupancy	Temperature factor
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Data set name	Rwp	Rp	Re	S	Chi^2	Maximum shift/e.s.d.
RKE3	0	0	0	0	0	0

Lattice constants

Angular correction

Analysis results

Data set name	a(A)	b(A)	c(A)	alpha(deg)	beta(deg)	gamma(deg)
RKE3	4.990553	4.990553	17.070047	90.000000	90.000000	120.000000

Phase name	a(A)	b(A)	c(A)	alpha(deg)	beta(deg)	gamma(deg)	V(A^3)
Calcite	4.990553	4.990553	17.070047	90.000000	90.000000	120.000000	368.182111



Crystallinity

Data set name	Crystallinity(%)
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CrystallinityGraph.emf

Crystallite size and lattice strain

Williamson-Hall method

<table><tr><th>Data set name</th><th>Crystallite size(A)</th><th>Strain(%)</th></tr></table>					Data set name	Crystallite size(A)	Strain(%)
Data set name	Crystallite size(A)	Strain(%)					
Phase name	Crystallite size(A)	Distribution RSD	Strain(%)	Distribution type			
Calcite	-	-	-	-			

CSSGraph.emf

Quantitative analysis results (RIR)

RIRGraph.emf

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

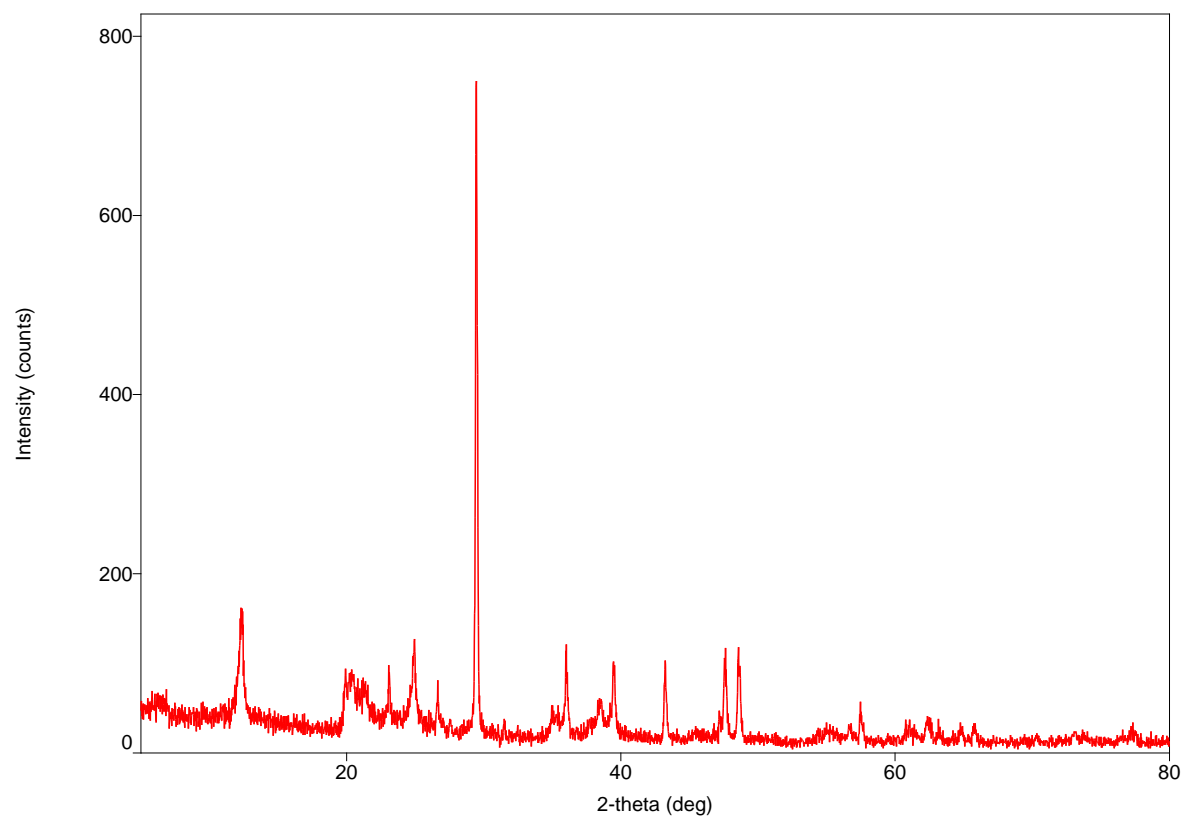
StressGraph.emf

Cluster analysis results

Dendrogram

ClusterDendrogram.emf

Measurement profiles



Cluster

Sample well

ClusterSamplePlate.emf

PCA view

ClusterPCA3DGraph.emf

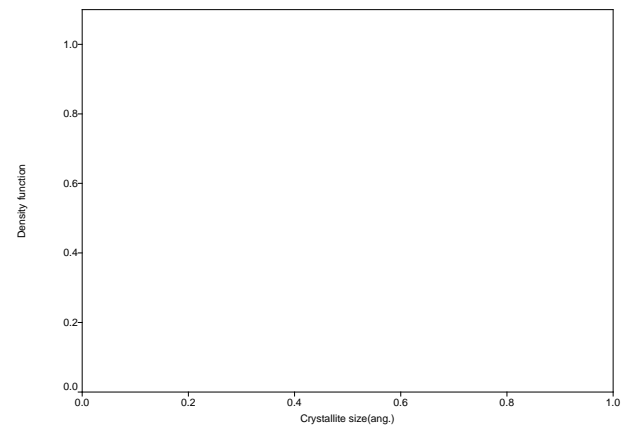
Eigenvalue graph

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
Calcite	CaCO ₃	0.654	ICDD (PDF-2 Release 2015 RDB)	00-047-1743

Quantitative analysis results

Lattice information

Phase name	a(A)	b(A)	c(A)	alpha(deg)	beta(deg)	gamma(deg)	V(A^3)
Calcite	4.990553	4.990553	17.070047	90.000000	90.000000	120.000000	368.182111

Phase name	Space group	Z	Z'	Calc. density(g/cm^3)
Calcite	167 : R-3c,hexagonal	6	0.167	2.708

Structure determination

Refinement

Measurement range: 5.0000-80.0000deg Refinement range: 5.0000-80.0000deg (1.20 Å)

Number of refined parameters: 0

Phase name	Atomic coords	# of indep. reflns
Calcite	-	26

Rwp = - S = -

Crystal structure

CrystalGraph.emf