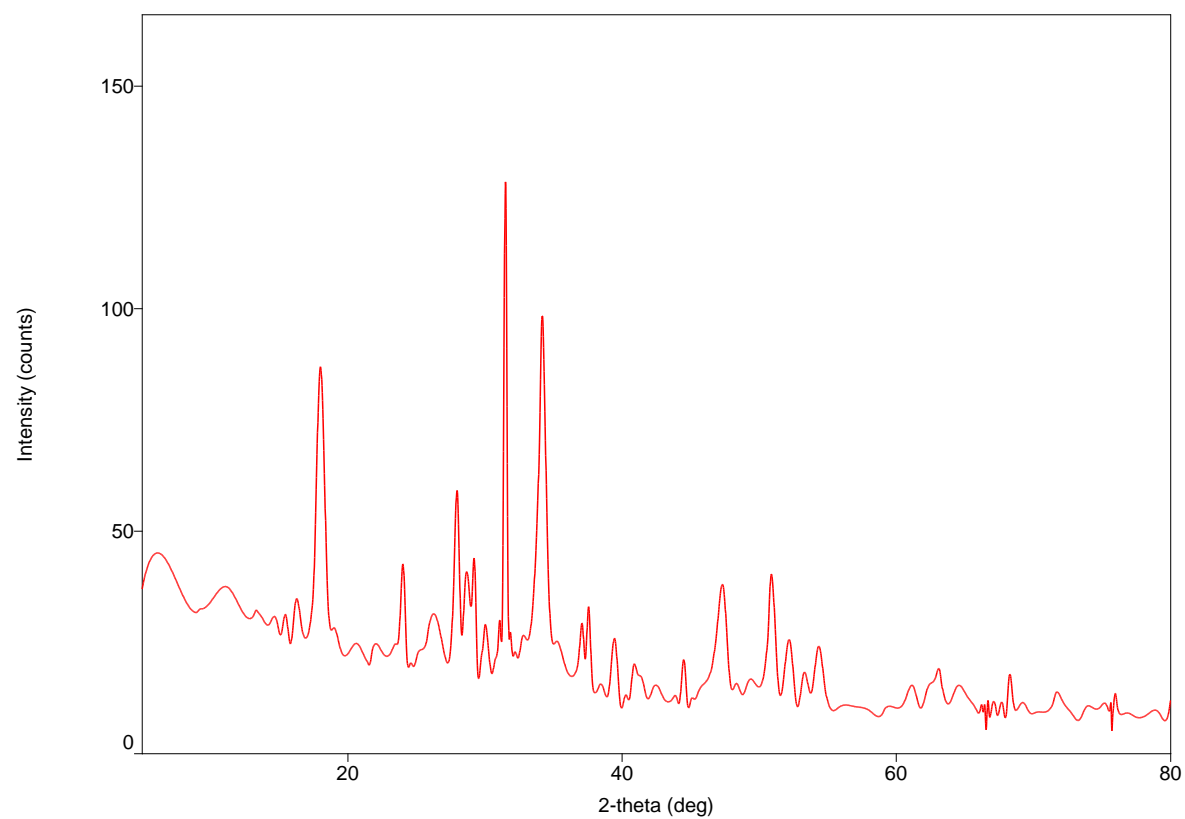


Analysis Results

General Information

Analysis date	2023/11/17 10:37:24		
Sample name	CKE3	Measurement date	2023/08/07 14:23:34
File name	CKE3.raw	Operator	USER
Comment	harpic strained		

Measurement profile



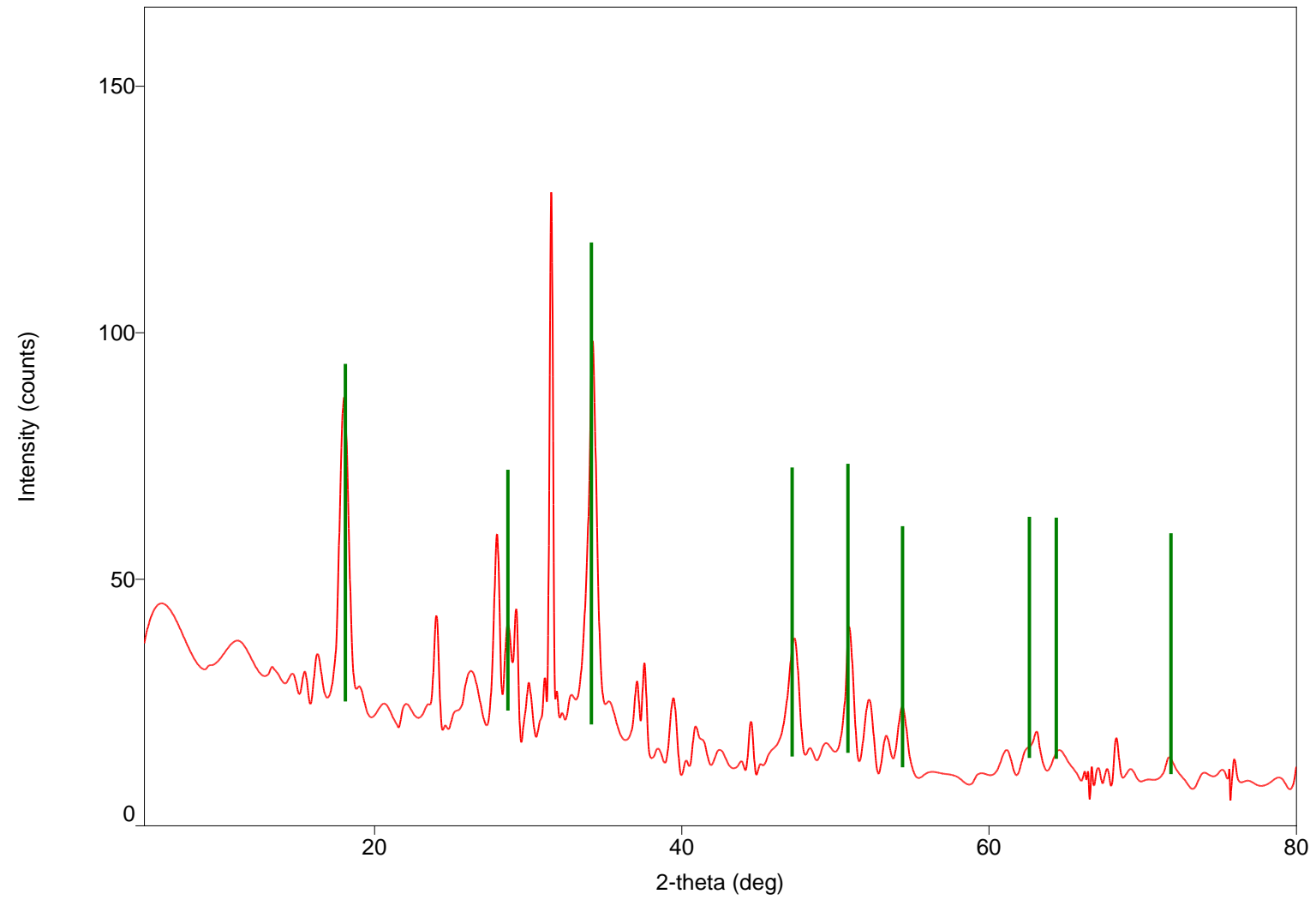
Measurement conditions

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
Portlandite	CaO · H ₂ O	1.504	ICDD (PDF-2 Release 2015 RDB)	00-002-0968

Phase name	Formula	Space group	Phase reg. detail	DB card number
Portlandite	CaO · H ₂ O	164 : P-3m1	ICDD (PDF-2 Release 2015 RDB)	00-002-0968



Peak list

No.	2-theta(deg)	d(ang.)	Height(counts)	FWHM(deg)	Size(ang.)	Phase name	Chemical formula
1	18.10(3)	4.898(9)	45(7)	0.58(3)	144(8)	Portlandite(0,0,1)	CaO · H ₂ O
2	24.08(5)	3.692(8)	16(4)	0.26(5)	324(62)	Unknown	Unknown
3	28.030(11)	3.1806(13)	25(5)	0.30(3)	284(33)	Unknown	Unknown
4	29.15(3)	3.061(3)	11(3)	0.89(16)	97(17)	Portlandite(1,0,0)	CaO · H ₂ O
5	31.52(2)	2.8364(18)	81(9)	0.204(15)	422(30)	Unknown	Unknown
6	34.15(3)	2.624(2)	54(7)	0.60(3)	144(7)	Portlandite(1,0,1)	CaO · H ₂ O
7	37.02(10)	2.427(6)	10(3)	0.34(14)	261(110)	Unknown	Unknown
8	47.20(2)	1.9241(9)	17(4)	0.61(7)	148(16)	Portlandite(1,0,2)	CaO · H ₂ O
9	50.84(2)	1.7945(8)	19(4)	0.39(6)	233(35)	Portlandite(1,1,0)	CaO · H ₂ O
10	52.15(6)	1.7524(18)	19(4)	0.25(4)	376(66)	Unknown	Unknown
11	54.28(4)	1.6885(11)	9(3)	0.56(11)	168(32)	Portlandite(1,1,1)	CaO · H ₂ O

Parameters used for WPPF

Profile parameters

Common parameter	Background	Data	CKE3
		Function name	B-spline
		param0	141.29551770331628
		param1	111.89912083624031
		param2	61.993920464658018
		param3	84.305694332293001
		param4	54.97472301069044
		param5	35.789567074808609
		param6	58.359225724875166
		param7	30.606924054949992
		param8	32.674949926337739
		param9	55.311949639527512
		param10	26.281275743440371
		param11	38.312273823870242
		param12	29.350552716540712
		param13	29.528823511061226
		param14	28.501219443541572
		node0	5
		node1	23.739999999999998
		node2	30.559999999999999
		node3	37.380000000000003
		node4	44.200000000000003
		node5	51.060000000000002
		node6	56.460000000000001
		node7	60.060000000000002
		node8	63.659999999999997
		node9	67.260000000000005
		node10	70.900000000000006
		node11	75.420000000000002
		node12	80
Common parameter	Peak shift	Function name	Shift axial displacement

		param0	0
		param1	0
		param2	0
Portlandite	Scale factor	s	1.1(2)
	FWHM	U	0.0000
		V	-0.2044
		W	0.4076
	Asym. factor	A0	1.1033
		A1	3.6345
	Decay rate factor	etaL0/mL0	0.7464
		etaL1/mL1	0.0000
		etaL2/mL2	0.0000
		etaH0/mH0	0.3146
		etaH1/mH1	0.0000
		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.
CKE3	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)
CKE3	3.590924	3.590924	4.900152	90.000000	90.000000	120.000000

Phase name	a(A)	b(A)	c(A)	alpha(deg)	beta(deg)	gamma(deg)	V(A^3)
Portlandite	3.590924	3.590924	4.900152	90.000000	90.000000	120.000000	54.720821



Crystallinity

Data set name	Crystallinity(%)
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CrystallinityGraph.emf

Crystallite size and lattice strain

Williamson-Hall method

		<u>Data set name Crystallite size(A) Strain(%)</u>		
Phase name	Crystallite size(A)	Distribution RSD	Strain(%)	Distribution type
Portlandite	-	-	-	-

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

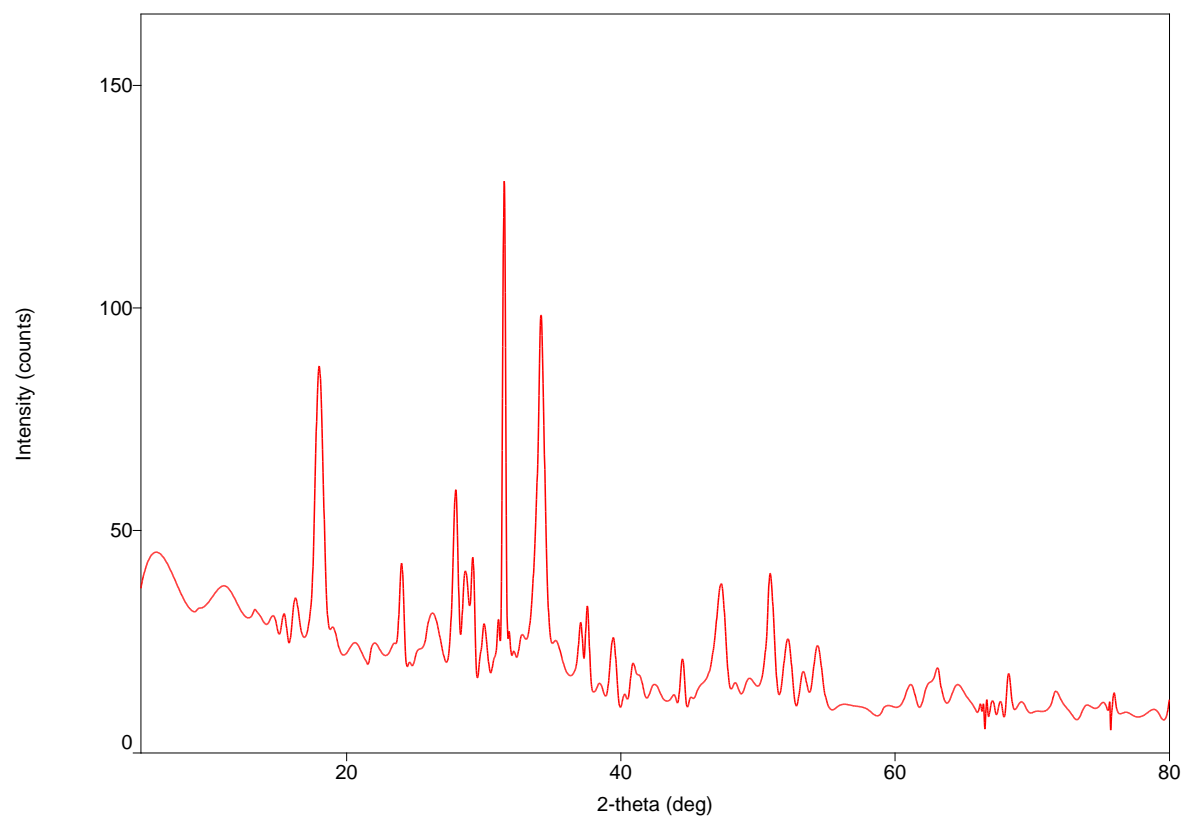
StressGraph.emf

Cluster analysis results

Dendrogram

ClusterDendrogram.emf

Measurement profiles



Cluster

Sample well

ClusterSamplePlate.emf

PCA view

ClusterPCA3DGraph.emf

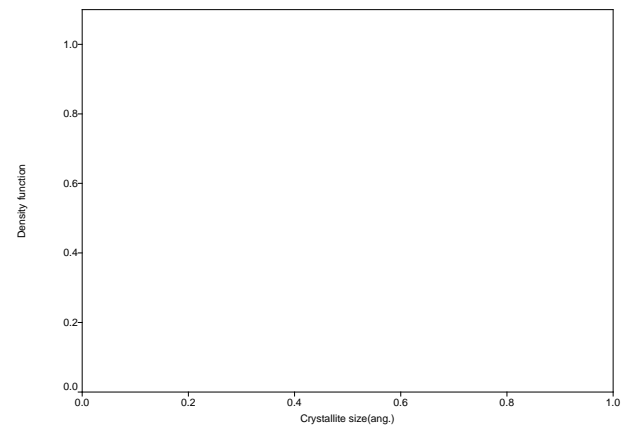
Eigenvalue graph

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
Portlandite	CaO · H ₂ O	1.504	ICDD (PDF-2 Release 2015 RDB)	00-002-0968

Quantitative analysis results

Lattice information

Phase name	a(Å)	b(Å)	c(Å)	alpha(deg)	beta(deg)	gamma(deg)	V(Å ³)
Portlandite	3.590924	3.590924	4.900152	90.000000	90.000000	120.000000	54.720821

Phase name	Space group	Z	Z'	Calc. density(g/cm ³)
Portlandite	164 : P-3m1	1	0.083	2.248

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
Portlandite	-	20

Rwp = - S = -

Crystal structure

CrystalGraph.emf