Apêndice - 1

Cálculo da decomposição da amônia no interior do reator

1.1 - Dados cinéticos da decomposição da amônia

Parâmetros Cinéticos	**Valores para T = 2200-3300K e P= 2.03 - 495 kPa**
Fator de frequência (A)	$5.5x10^{15}$ l/s
Energia de ativação (E_a)	451 kJ/mol
Ordem de reação (α)	1

R = 8,314 J/mol.K

1.2 - Dados do reator e do processo

C_{a0} = 0,0401 moles/L (fluxo molar)
P = 101325 Pa (pressão)
T = 273 - 1373 K (temperatura)
D = 0,03 m (diâmetro do reator)

1.3 - Parâmetros calculados

Vazão volumétrica

V_z (600^{o}C) = 0,01465 L/s
V_z (1000^{o}C) = 0,02136 L/s
V_z (1100^{o}C) = 0,02300 L/s

$$\frac{V_Z dC_a}{dZ} = -r_a \Rightarrow \frac{V_Z dC_a}{dZ} = -kC_a \Rightarrow \frac{dC_a}{C_a} = -\left(\frac{k}{V_Z}\right)dZ$$

$$\int_{Ca0}^{Ca} \frac{dC_a}{C_a} = -\left(\frac{k}{V_Z}\right)\int_0^Z dZ \Rightarrow \ln\left(\frac{C_a}{C_{a0}}\right) = -\left(\frac{k}{V_Z}\right)Z$$

$$C_a(Z) = C_{a0}.e^{\left(\frac{-k}{V_Z}\right)Z}$$

onde:

$$k = A.e^{\left(\frac{-E_A}{RT}\right)}$$

$$r_a = kC_{a0}$$

Z = 0.15 m (comprimento do reator)

r_a = (taxa de reação)

k = (constante cinética)

k (600 ^oC) = 5,68 x 10^{-12} L/s

k (1000 ^oC) = 0,01713 L/s

k (1100 ^oC) = 0,038 L/s

Tabela de valores – eixo do reator versus concentrações de NH_3 em diferentes temperaturas

Z (metros)	C_a (moles/L) - 600 C	C_a (moles/L) - 1000 C	C_a (moles/L) - 1100 C
0	0.401	0.401	0.401
0.01	0.401	0.397789527	0.394429212
0.02	0.401	0.394604757	0.387966094
0.03	0.401	0.391445485	0.38160888
0.04	0.401	0.388311506	0.375355836
0.05	0.401	0.385202619	0.369205253
0.06	0.401	0.382118622	0.363155455
0.07	0.401	0.379059316	0.357204788
0.08	0.401	0.376024504	0.351351629
0.09	0.401	0.373013989	0.34559438
0.1	0.401	0.370027576	0.339931469
0.11	0.401	0.367065073	0.334361351
0.12	0.401	0.364126288	0.328882504
0.13	0.401	0.361211032	0.323493435
0.14	0.401	0.358319116	0.31819267
0.15	0.401	0.355450353	0.312978764
0.16	0.401	0.352604557	0.307850292
0.17	0.401	0.349781546	0.302805856
0.18	0.401	0.346981136	0.297844078
0.19	0.401	0.344203147	0.292963604
0.2	0.401	0.341447399	0.288163102
0.21	0.401	0.338713713	0.28344126
0.22	0.401	0.336001915	0.27879679
0.23	0.401	0.333311827	0.274228425
0.24	0.401	0.330643276	0.269734917
0.25	0.401	0.327996091	0.26531504
0.26	0.401	0.325370099	0.260967586
0.27	0.401	0.322765131	0.256691371
0.28	0.401	0.320181019	0.252485225
0.29	0.401	0.317617596	0.248348001
0.3	0.401	0.315074696	0.24427857
0.31	0.401	0.312552155	0.24027582
0.32	0.401	0.31004981	0.23633866
0.33	0.401	0.307567499	0.232466014
0.34	0.401	0.305105062	0.228656825
0.35	0.401	0.30266234	0.224910053
0.36	0.401	0.300239174	0.221224676
0.37	0.401	0.297835409	0.217599688
0.38	0.401	0.295450889	0.214034098
0.39	0.401	0.293085459	0.210526935
0.4	0.401	0.290738968	0.20707724
0.41	0.401	0.288411263	0.203684071
0.42	0.401	0.286102194	0.200346503
0.43	0.401	0.283811611	0.197063625
0.44	0.401	0.281539368	0.193834539
0.45	0.401	0.279285317	0.190658366
0.46	0.401	0.277049311	0.187534237
0.47	0.401	0.274831208	0.184461301
0.48	0.401	0.272630863	0.181438717
0.49	0.401	0.270448135	0.178465661
0.5	0.401	0.268282881	0.175541322

Apêndice - 2

Resultados das medições de tamanho de partícula dos reagentes

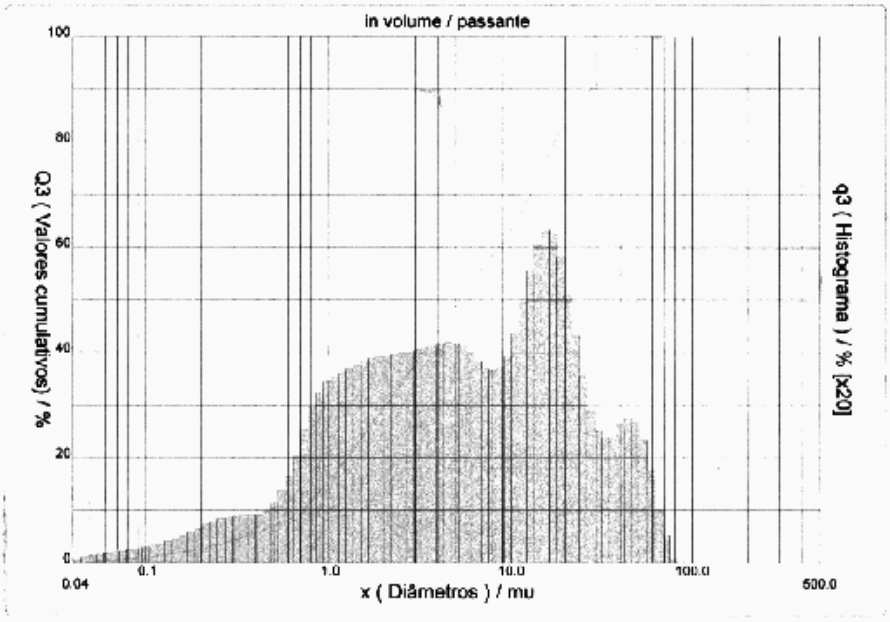
CILAS

DISTRIBUIÇÃO GRANULOMÉTRICA

CILAS 1064 Líquido

Faixa : 0.04 mu - 500.00 mu / 100 Classes

Ref da amostra	: Padrão	Ultrasom	: 60 s
Type produit	: Óxido + Carbono	Concentração	: 237
Client	: DCMM	Diâmetro a 10%	: 0.71 mu
Comentários	:	Diâmetro a 50%	: 5.21 mu
Líquido	: Water (eau)	Diâmetro a 90%	: 27.67 mu
Agente dispersante	:	Fraunhofer	
Operador	: Carlos	Densidade/Fator	----------
Empresa	:	Superfície específica	----------
Localização	:	Diluição automática	: Não / Não
Data : 01/24/2002	Hora : 02:49:52PM	Nb Medida./Limp.	: 20/20/4
Índice med.	: 250	SOP : Standard L	



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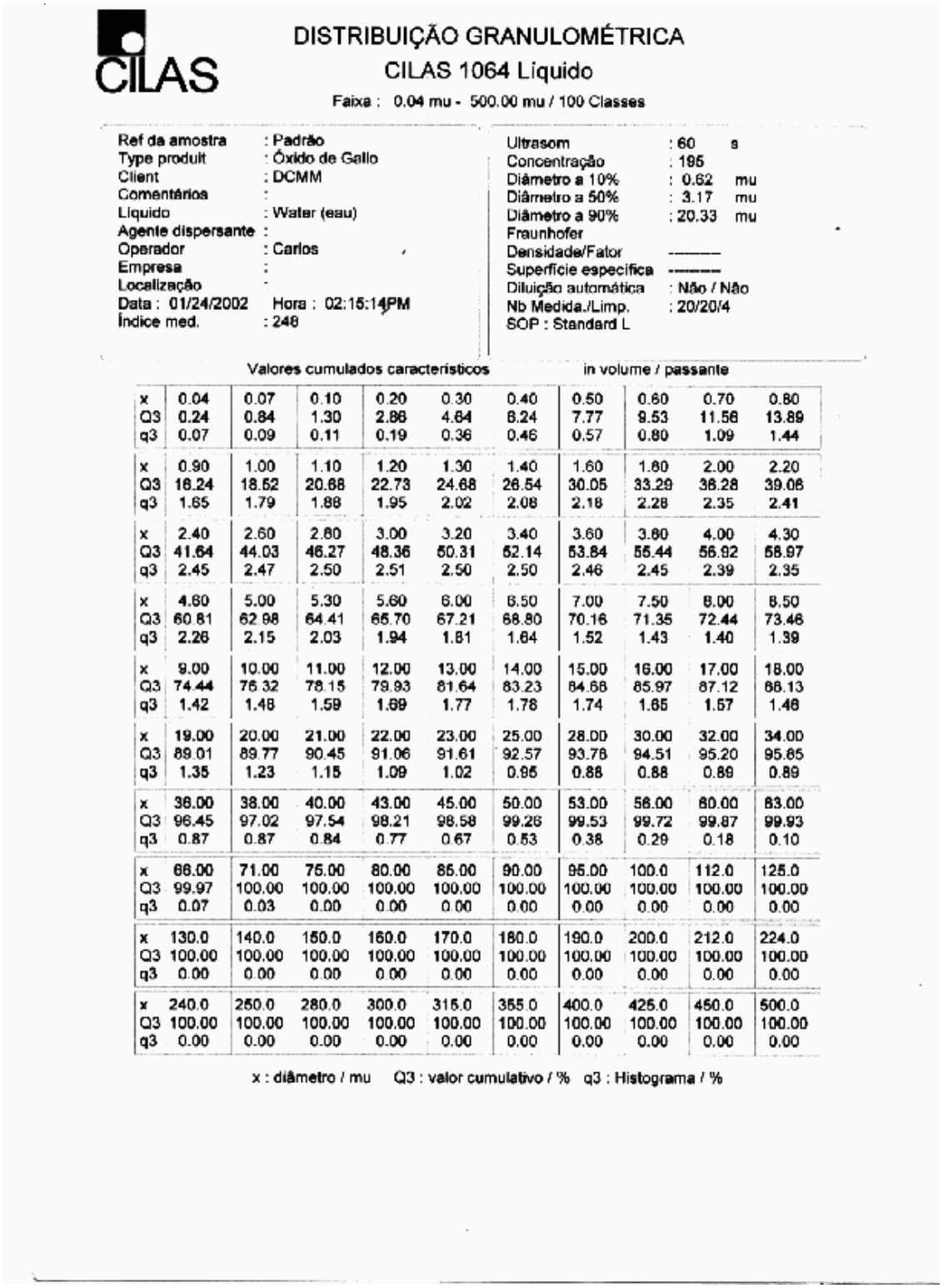


CILAS

DISTRIBUIÇÃO GRANULOMÉTRICA

CILAS 1064 Liquido

Faixa : 0.04 mu - 500.00 mu / 100 Classes

Ref da amostra	: Padrão
Type produit	: Óxido de Gallo
Client	: DCMM
Comentários	:
Liquido	: Water (eau)
Agente dispersante	:
Operador	: Carlos
Empresa	:
Localização	:
Data : 01/24/2002	Hora : 02:15:14PM
Índice med.	: 248

Ultrasom	: 60 s
Concentração	: 195
Diâmetro a 10%	: 0.62 mu
Diâmetro a 50%	: 3.17 mu
Diâmetro a 90%	: 20.33 mu
Fraunhofer	
Densidade/Fator	-------
Superfície especifica	-------
Diluição automática	: Não / Não
Nb Medida./Limp.	: 20/20/4
SOP : Standard L	

Valores cumulados caracteristicos in volume / passante

x	0.04	0.07	0.10	0.20	0.30	0.40	0.50	0.60	0.70	0.80
Q3	0.24	0.84	1.30	2.86	4.64	6.24	7.77	9.53	11.56	13.89
q3	0.07	0.09	0.11	0.19	0.36	0.46	0.57	0.80	1.09	1.44
x	0.90	1.00	1.10	1.20	1.30	1.40	1.60	1.80	2.00	2.20
Q3	16.24	18.52	20.68	22.73	24.68	26.54	30.05	33.29	36.28	39.06
q3	1.65	1.79	1.88	1.95	2.02	2.08	2.18	2.28	2.35	2.41
x	2.40	2.60	2.80	3.00	3.20	3.40	3.60	3.80	4.00	4.30
Q3	41.64	44.03	46.27	48.36	50.31	52.14	53.84	55.44	56.92	58.97
q3	2.45	2.47	2.50	2.51	2.50	2.50	2.46	2.45	2.39	2.35
x	4.60	5.00	5.30	5.60	6.00	6.50	7.00	7.50	8.00	8.50
Q3	60.81	62.98	64.41	65.70	67.21	68.80	70.16	71.35	72.44	73.46
q3	2.26	2.15	2.03	1.94	1.81	1.64	1.52	1.43	1.40	1.39
x	9.00	10.00	11.00	12.00	13.00	14.00	15.00	16.00	17.00	18.00
Q3	74.44	76.32	78.15	79.93	81.64	83.23	84.66	85.97	87.12	88.13
q3	1.42	1.48	1.59	1.69	1.77	1.78	1.74	1.65	1.57	1.46
x	19.00	20.00	21.00	22.00	23.00	25.00	28.00	30.00	32.00	34.00
Q3	89.01	89.77	90.45	91.06	91.61	92.57	93.78	94.51	95.20	95.85
q3	1.35	1.23	1.15	1.09	1.02	0.95	0.88	0.88	0.89	0.89
x	36.00	38.00	40.00	43.00	45.00	50.00	53.00	56.00	60.00	63.00
Q3	96.45	97.02	97.54	98.21	98.58	99.26	99.53	99.72	99.87	99.93
q3	0.87	0.87	0.84	0.77	0.67	0.53	0.38	0.29	0.18	0.10
x	66.00	71.00	75.00	80.00	85.00	90.00	95.00	100.0	112.0	125.0
Q3	99.97	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00
q3	0.07	0.03	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
x	130.0	140.0	150.0	160.0	170.0	180.0	190.0	200.0	212.0	224.0
Q3	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00
q3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
x	240.0	250.0	280.0	300.0	315.0	355.0	400.0	425.0	450.0	500.0
Q3	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00
q3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

x : diâmetro / mu Q3 : valor cumulativo / % q3 : Histograma / %

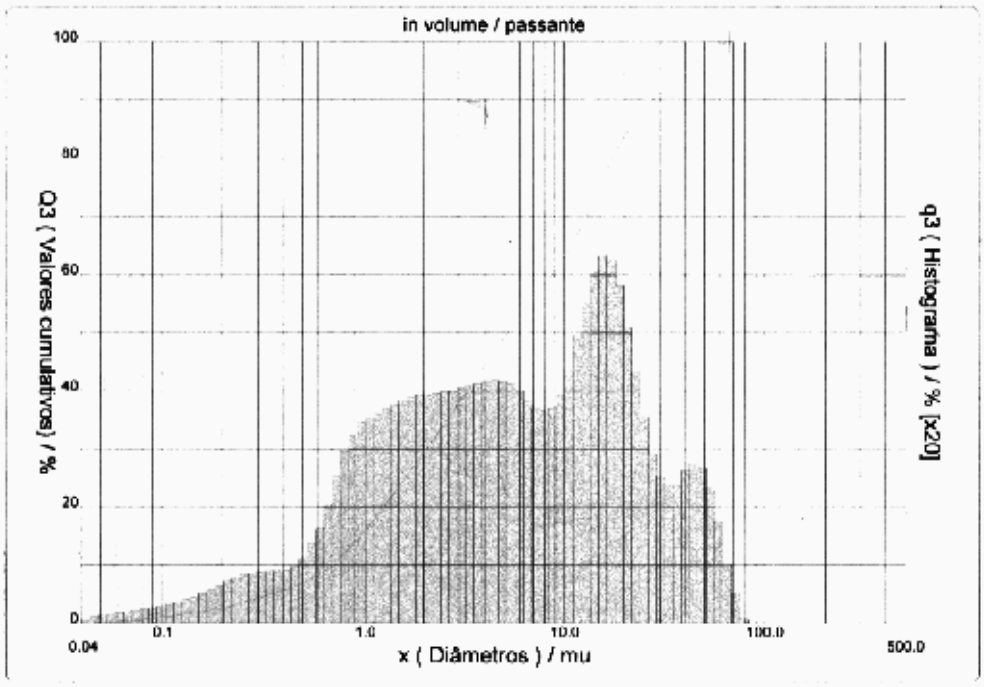
CILAS

DISTRIBUIÇÃO GRANULOMÉTRICA

CILAS 1064 Liquido

Faixa : 0.04 mu - 500.00 mu / 100 Classes

Ref da amostra	: Padrão	Ultrasom	: 60	s
Type produit	: Óxido + Carbono	Concentração	: 237	
Client	: DCMM	Diâmetro a 10%	: 0.71	mu
Comentários	:	Diâmetro a 50%	: 5.21	mu
Liquido	: Water (sau)	Diâmetro a 90%	: 27.67	mu
Agente dispersante	:	Fraunhofer		
Operador	: Carlos	Densidade/Fator	-------	
Empresa	:	Superfície específica	-------	
Localização	:	Diluição automática	: Não / Não	
Data : 01/24/2002	Hora : 02:49:52PM	Nb Medida./Limp.	: 20/20/4	
Índice med.	: 250	SOP : Standard L		



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DISTRIBUIÇÃO GRANULOMÉTRICA

CILAS 1064 Líquido

Faixa : 0.04 mu - 500.00 mu / 100 Classes

Ref da amostra	: Padrão	Ultrasom	: 60 s
Type produit	: Óxido + Carbono	Concentração	: 237
Client	: DCMM	Diâmetro a 10%	: 0.71 mu
Comentários	:	Diâmetro a 50%	: 5.21 mu
Liquido	: Water (eau)	Diâmetro a 90%	: 27.67 mu
Agente dispersante	:	Fraunhofer	
Operador	: Carlos	Densidade/Fator	--------
Empresa	:	Superfície especifica	--------
Localização	:	Diluição automática	: Não / Não
Data : 01/24/2002	Hora : 02:49:52PM	Nb Medida./Limp.	: 20/20/4
Índice med.	: 250	SOP : Standard L	

Valores cumulados característicos in volume / passante

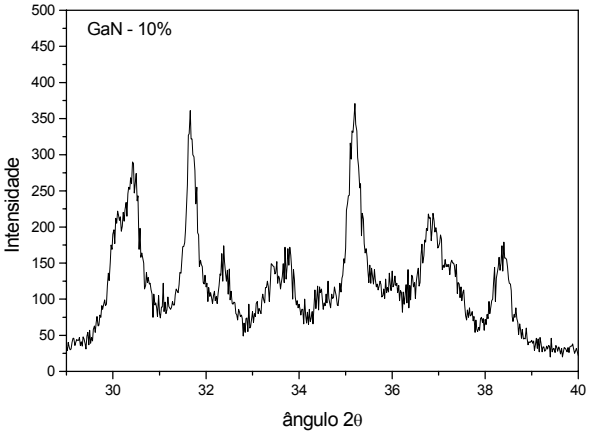
x	0.04	0.07	0.10	0.20	0.30	0.40	0.50	0.60	0.70	0.80
Q3	0.05	0.45	0.90	2.56	4.27	5.61	6.77	8.14	9.79	11.75
q3	0.01	0.06	0.10	0.19	0.33	0.37	0.41	0.59	0.85	1.16
x	0.90	1.00	1.10	1.20	1.30	1.40	1.60	1.80	2.00	2.20
Q3	13.74	15.66	17.43	19.09	20.65	22.11	24.80	27.22	29.41	31.39
q3	1.34	1.44	1.47	1.51	1.54	1.56	1.59	1.62	1.64	1.64
x	2.40	2.60	2.80	3.00	3.20	3.40	3.60	3.80	4.00	4.30
Q3	33.21	34.89	36.45	37.92	39.31	40.62	41.86	43.05	44.18	45.78
q3	1.65	1.66	1.66	1.68	1.70	1.71	1.72	1.74	1.74	1.75
x	4.60	5.00	5.30	5.60	6.00	6.50	7.00	7.50	8.00	8.50
Q3	47.27	49.10	50.37	51.55	52.99	54.60	56.05	57.38	58.62	59.80
q3	1.75	1.74	1.72	1.69	1.65	1.59	1.55	1.52	1.52	1.54
x	9.00	10.00	11.00	12.00	13.00	14.00	15.00	16.00	17.00	18.00
Q3	60.95	63.23	65.59	68.00	70.44	72.64	75.15	77.30	79.26	81.05
q3	1.59	1.71	1.96	2.19	2.41	2.56	2.65	2.63	2.58	2.45
x	19.00	20.00	21.00	22.00	23.00	25.00	28.00	30.00	32.00	34.00
Q3	82.59	83.95	85.13	86.16	87.06	88.52	90.17	91.05	91.85	92.60
q3	2.25	2.10	1.91	1.75	1.60	1.38	1.15	1.01	0.98	0.98
x	36.00	38.00	40.00	43.00	45.00	50.00	53.00	56.00	60.00	63.00
Q3	93.33	94.07	94.81	95.85	96.50	97.91	98.56	99.07	99.52	99.74
q3	1.01	1.08	1.14	1.14	1.13	1.06	0.88	0.73	0.52	0.36
x	66.00	71.00	75.00	80.00	85.00	90.00	95.00	100.0	112.0	125.0
Q3	99.89	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00
q3	0.25	0.12	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
x	130.0	140.0	150.0	160.0	170.0	180.0	190.0	200.0	212.0	224.0
Q3	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00
q3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
x	240.0	250.0	280.0	300.0	315.0	355.0	400.0	425.0	450.0	500.0
Q3	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00
q3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

x : diâmetro / mu Q3 : valor cumulativo / % q3 : Histograma / %

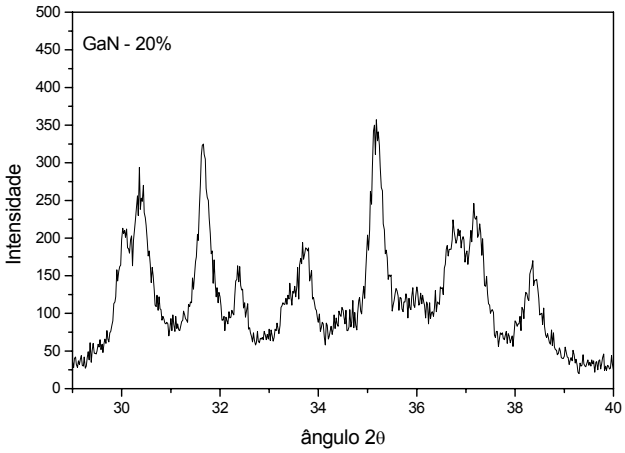
Apêndice - 3

Difração de raios-X

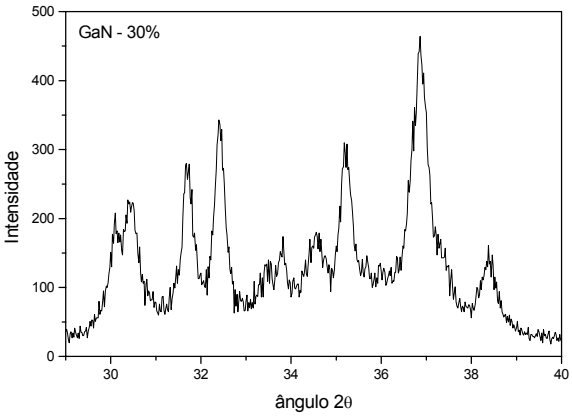
Curva de calibração:



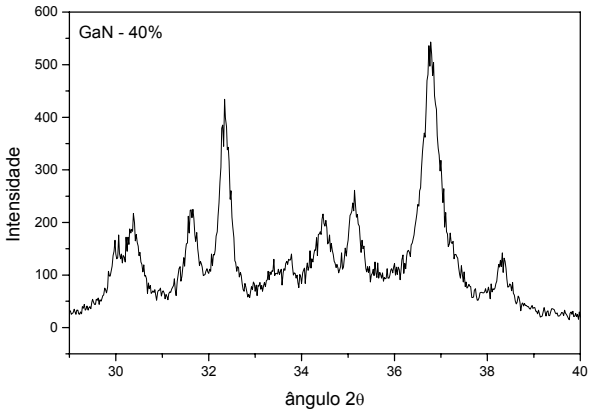
DRX de pó padrão:
10% GaN
90% Ga_2O_3



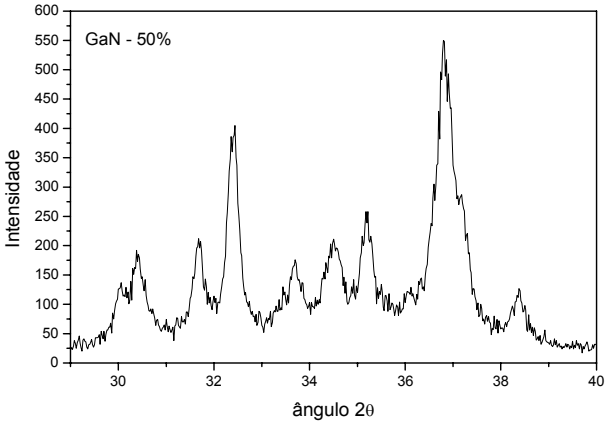
DRX de pó padrão:
20% GaN
80% Ga_2O_3



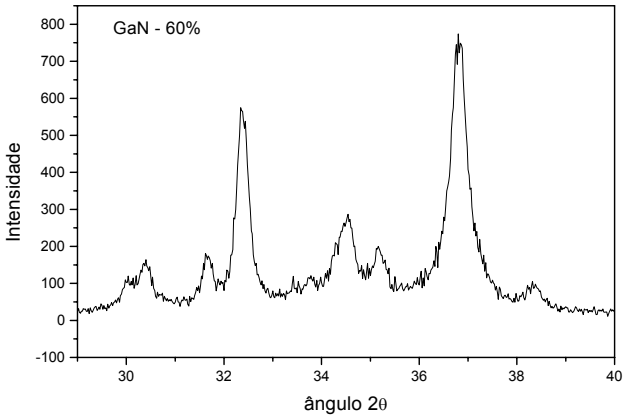
DRX de pó padrão:
30% GaN
70% Ga_2O_3



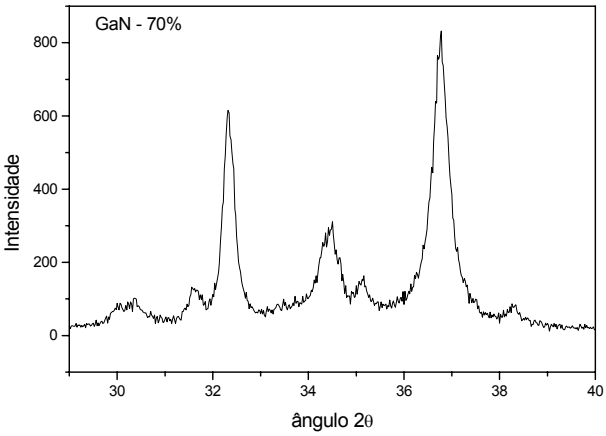
DRX de pó padrão:
40% GaN
60% Ga_2O_3



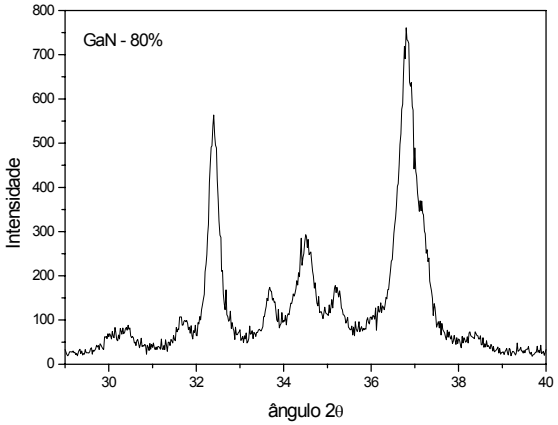
DRX de pó padrão:
50% GaN
50% Ga_2O_3



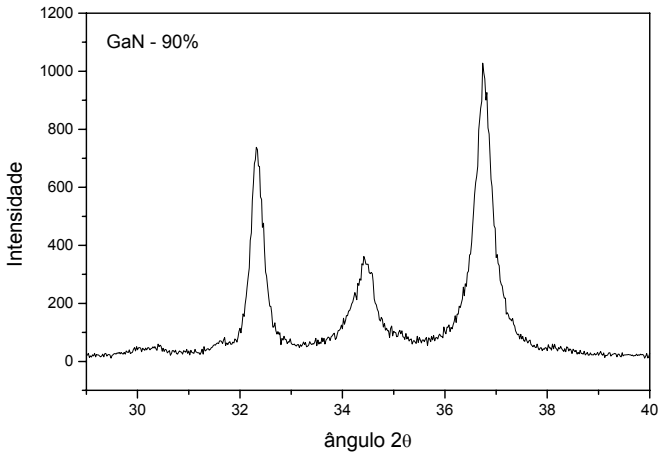
DRX de pó padrão:
60% GaN
40% Ga_2O_3



DRX de pó padrão:
70% GaN
30% Ga_2O_3

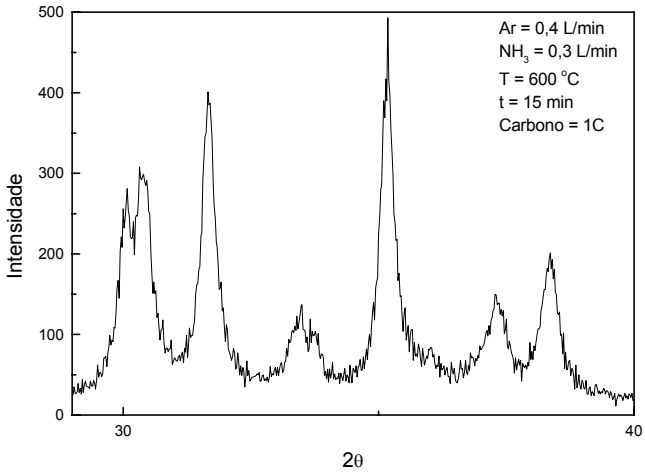


DRX de pó padrão:
80% GaN
20% Ga_2O_3

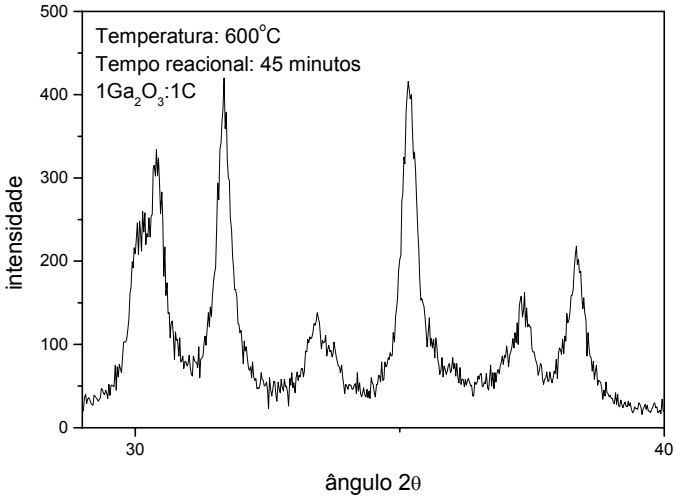


DRX do pó padrão
90% GaN
10% Ga_2O_3

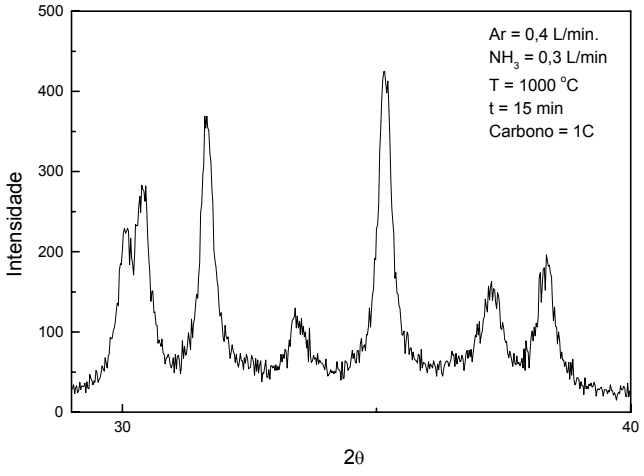
Resultados experimentais – DRX



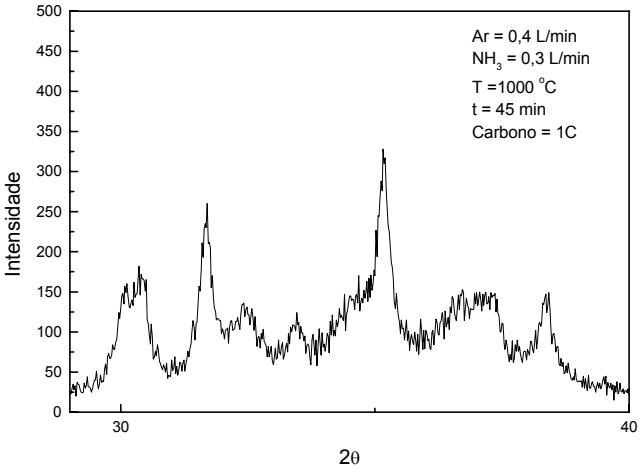
DRX de pó produzido na condição 00:
Temperatura: 600 °C
Tempo experimental : 15 minutos
$1Ga_2O_3$: 1C



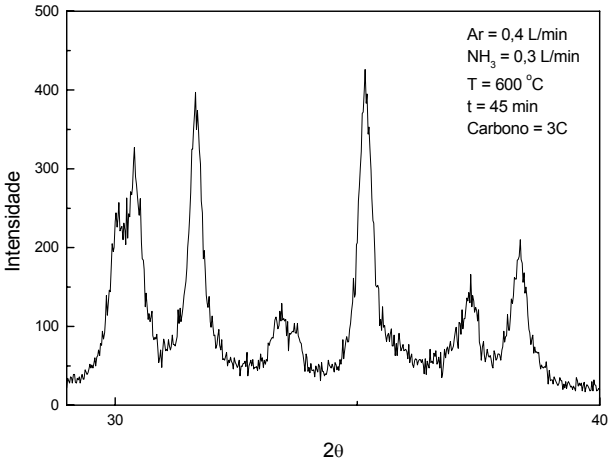
DRX de pó produzido na condição 01:
Temperatura: 600 °C
Tempo experimental : 45 minutos
$1Ga_2O_3$: 1C



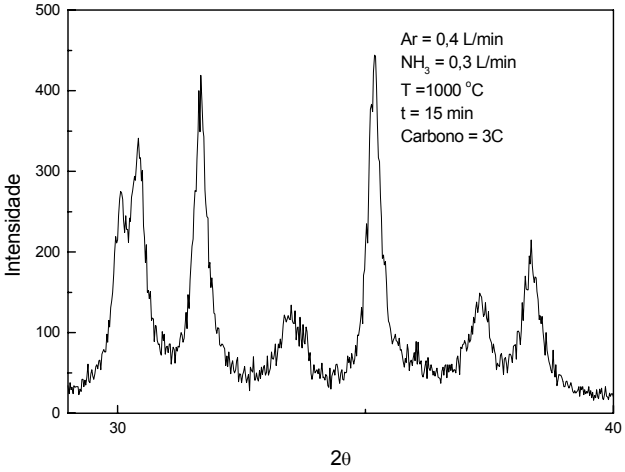
DRX de pó produzido na condição 02:
Temperatura: 1000 °C
Tempo experimental : 15 minutos
$1Ga_2O_3$: 1C



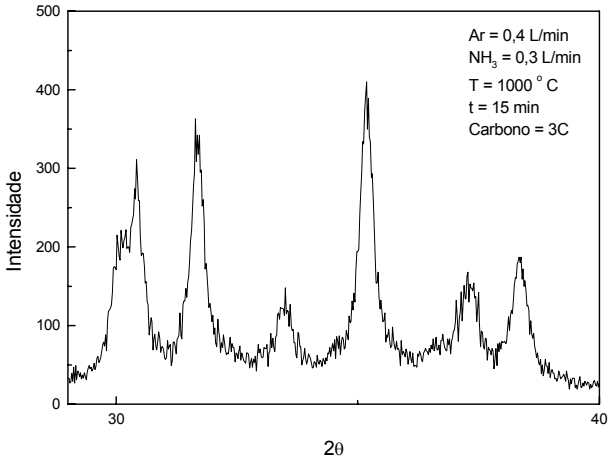
DRX de pó produzido na condição 03:
Temperatura: 1000 °C
Tempo experimental : 15 minutos
$1Ga_2O_3$: 1C



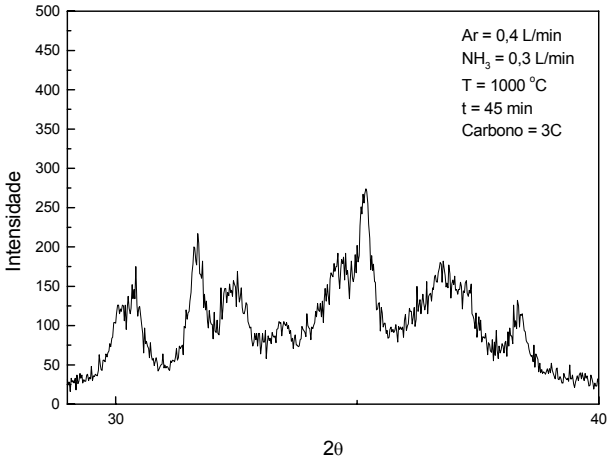
DRX de pó produzido na condição 04:
Temperatura: 600 °C
Tempo experimental : 15 minutos
$1Ga_2O_3$: 3C



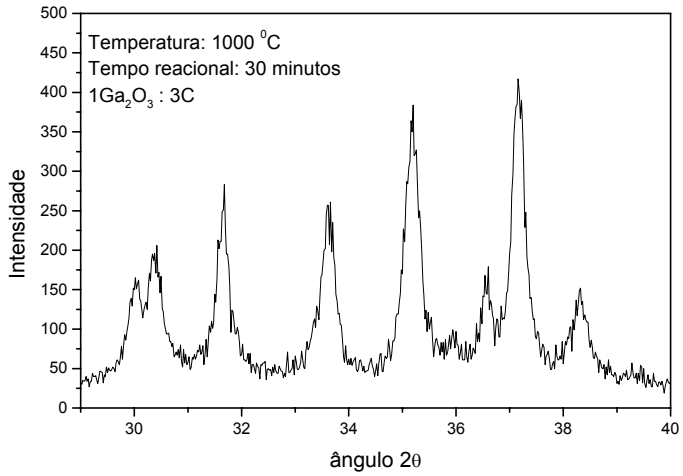
DRX de pó produzido na condição 05:
Temperatura: 600 °C
Tempo experimental : 15 minutos
$1Ga_2O_3$: 3C



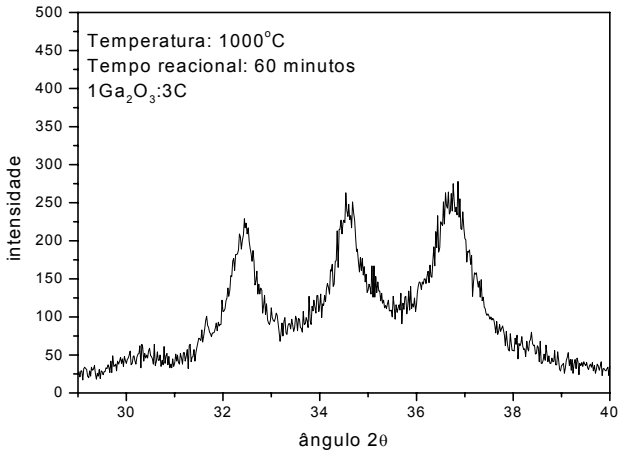
DRX de pó produzido na condição 06:
Temperatura: 1000 °C
Tempo experimental : 15 minutos
$1Ga_2O_3$: 3C



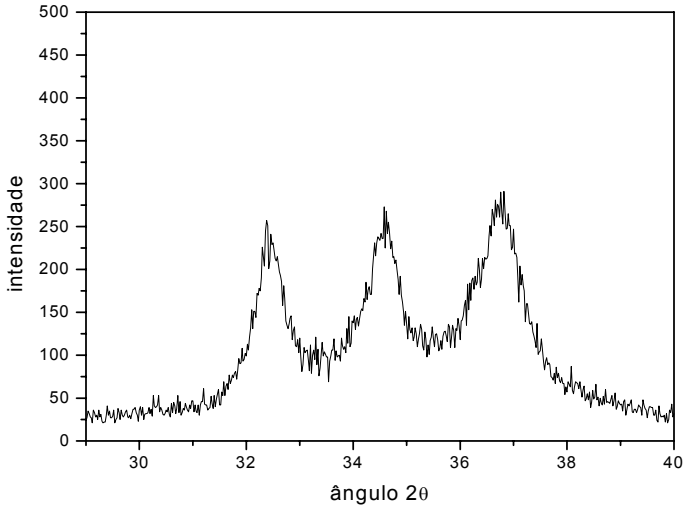
DRX de pó produzido na condição 07:
Temperatura: 1000 °C
Tempo experimental : 15 minutos
$1Ga_2O_3$: 3C



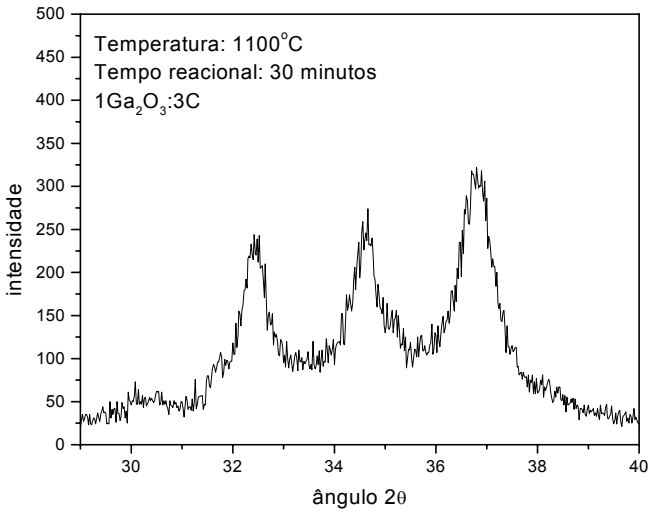
DRX de pó produzido na condição 09:
Temperatura: 1000 °C
Tempo experimental : 30 minutos
$1Ga_2O_3$: 3C



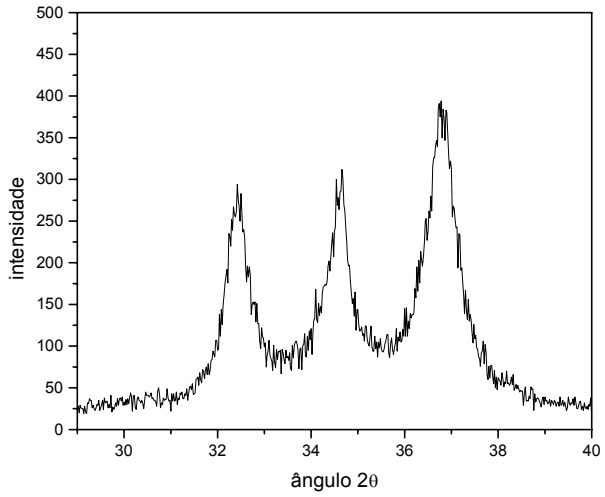
DRX de pó produzido na condição 10:
Temperatura: 1000 °C
Tempo experimental : 60 minutos
$1Ga_2O_3$: 3C



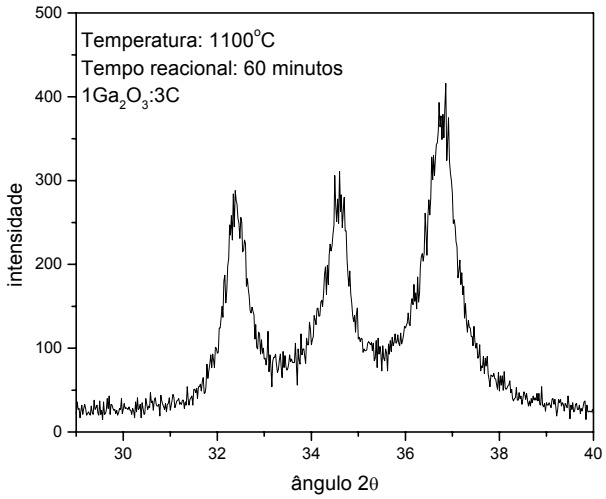
DRX de pó produzido na condição 11:
Temperatura: 1000 °C
Tempo experimental : 75 minutos
$1Ga_2O_3$: 3C



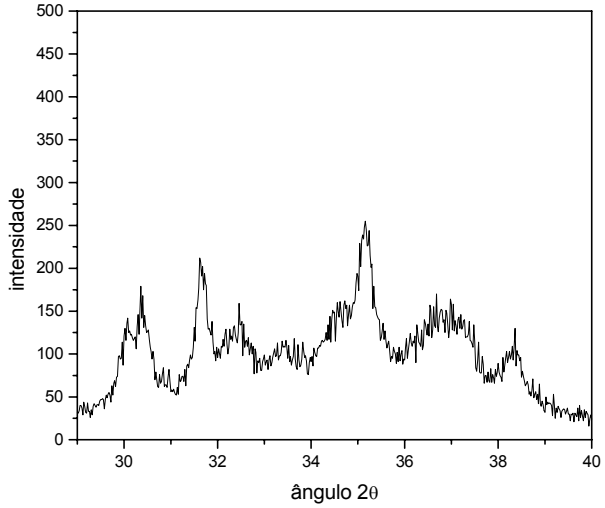
DRX de pó produzido na condição 12:
Temperatura: 1100 °C
Tempo experimental : 30 minutos
$1Ga_2O_3$: 3C



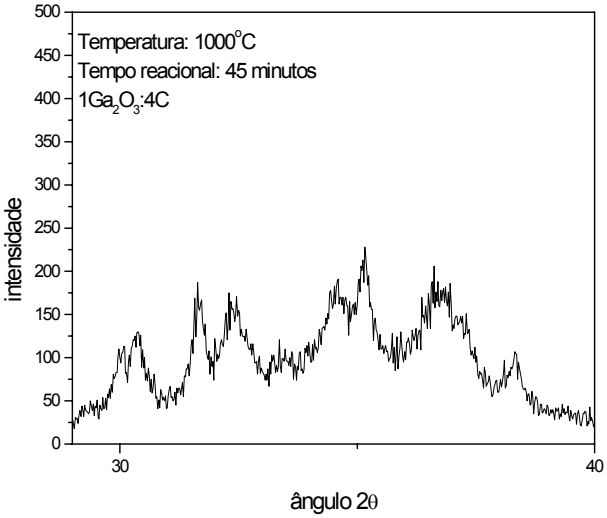
DRX de pó produzido na condição 13:
Temperatura: 1100 °C
Tempo experimental : 45 minutos
$1Ga_2O_3$: 3C



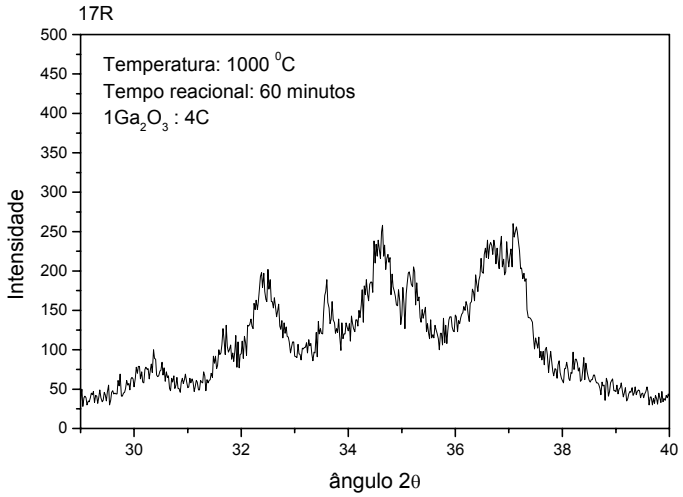
DRX de pó produzido na condição 14:
Temperatura: 1100 °C
Tempo experimental : 60 minutos
$1Ga_2O_3$: 3C



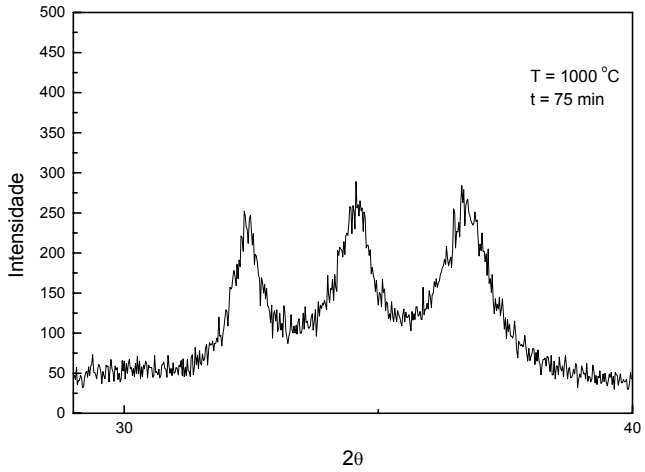
DRX de pó produzido na condição 15:
Temperatura: 1000 °C
Tempo experimental : 30 minutos
$1Ga_2O_3$: 4C



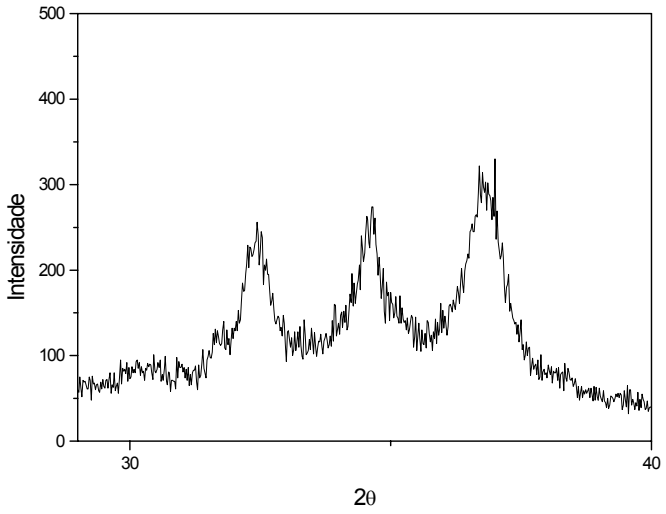
DRX de pó produzido na condição 16:
Temperatura: 1000 °C
Tempo experimental : 45 minutos
$1Ga_2O_3$: 4C



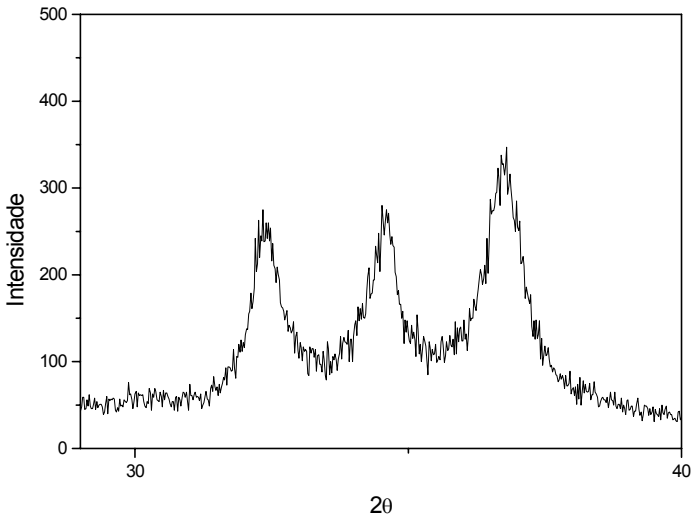
DRX de pó produzido na condição 17:
Temperatura: 1000 °C
Tempo experimental : 60 minutos
$1Ga_2O_3$: 4C



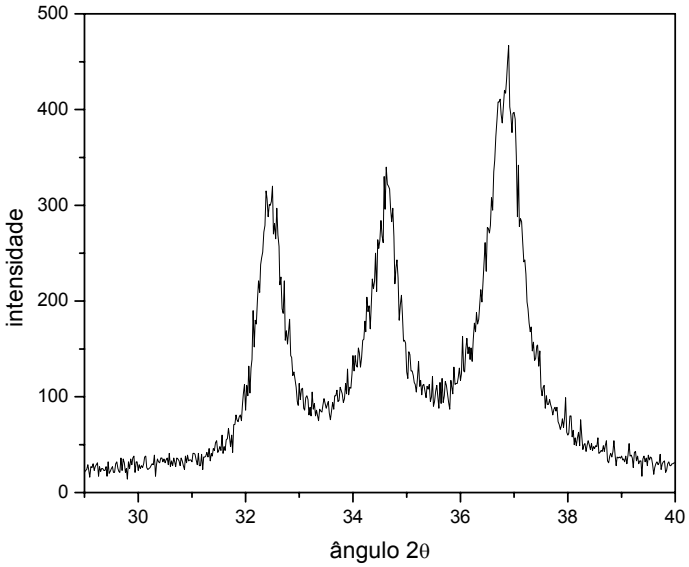
DRX de pó produzido na condição 18:
Temperatura: 1000 °C
Tempo experimental : 75 minutos
$1Ga_2O_3$: 4C



DRX de pó produzido na condição 19:
Temperatura: 1100 °C
Tempo experimental : 30 minutos
$1Ga_2O_3$: 4C



DRX de pó produzido na condição 20:
Temperatura: 1100 °C
Tempo experimental : 45 minutos
$1Ga_2O_3$: 4C



DRX de pó produzido na condição 21
Temperatura: 1100 ^{o}C
Tempo experimental : 60 minutos
1Ga_2O_3 : 4C