

Diffraction Peak Table

Crystal	Miller Index			2θ angle (deg)	Relative Intensity
	h	k	l		
Al(cub)	1	1	1	38.47	100
	2	0	0	44.74	47
AlN(hex-WZ) a=0.311nm c=0.4978nm	1	0	0	33.27	100
	0	0	2	36.08	64
	1	0	1	37.99	87
	1	0	2	49.89	30
	1	1	0	59.45	45
	0	1	2	25.62	65
Al ₂ O ₃ (trig->hex) a=0.4754nm c=1.299nm	1	0	4	35.20	100
	1	1	0	37.85	45
	1	1	3	43.43	94
	0	2	4	52.64	44
	1	1	6	57.58	82
	1	1	1	28.57	100
CeO ₂ (cub)	2	0	0	33.11	35
	2	2	0	47.53	97
	3	1	1	56.40	86
	2	2	2	59.15	16
	2	1	0	45.88	100
CoSi(cub)	2	1	1	50.46	90
	1	1	0	28.49	60
	1	1	1	34.88	50
	2	0	0	40.80	40
CoSi ₂ (cub)	2	2	0	47.92	100
	1	1	1	28.81	90
Cu(cub)	1	1	1	43.36	100
	2	0	0	50.50	48
HfO ₂ (mncl) a=0.512nm b=0.518nm c=0.529nm β=99.3deg	-1	1	1	28.34	100
	1	1	1	31.67	74
	0	0	2	34.36	25
	0	2	0	34.59	21
	2	0	0	35.52	21
	0	1	1	24.19	15
HfN(cub)	1	1	0	24.60	12
	1	1	1	33.14	100
	2	0	0	38.45	83
	2	2	0	55.51	75
HfO ₂ (ortho) a=0.331nm b=0.555nm c=0.646nm	0	1	2	32.05	100
	1	1	1	34.42	50
	1	0	1	30.27	40
	1	2	1	44.71	40
	1	0	3	50.49	25
Ir(cub)	1	1	1	40.66	100
	2	0	0	47.30	55
IrO ₂ (tet) a=0.450nm c=0.315nm	1	1	0	28.03	100
	1	0	1	34.70	88
	2	1	1	54.02	54
	2	0	0	40.06	25

Crystal	Miller Index			2θ angle (deg)	Relative Intensity
	h	k	l		
La ₂ O ₃ (hex) a=0.3938nm c=0.61361nm	1	0	0	26.13	24
	0	0	2	29.11	27
	1	0	1	29.98	100
	1	0	2	39.51	36
	1	1	0	46.10	56
	1	0	3	52.14	50
	1	1	2	55.45	50
	2	0	1	55.97	32
	2	0	0	42.91	100
	1	1	1	44.39	100
MgO(cub)	2	0	0	51.72	45
Ni(cub)	1	1	1	37.13	60
	2	0	0	43.13	100
NiO(cub)	2	2	0	62.64	53
NiSi(ortho) Pnma a=0.561nm b=0.333nm c=0.561nm	0	1	1	31.22	49
	2	0	0	31.91	23
	1	1	0	35.18	25
	1	0	2	35.79	15
	2	1	0	42.11	13
	1	1	2	45.25	69
	2	1	1	45.25	100
	2	0	2	45.75	31
	1	0	3	51.52	24
	3	0	1	51.52	19
NiSi ₂ (cub)	0	2	0	55.12	26
	1	1	1	28.60	59
	2	2	0	47.57	100
	3	1	1	56.45	26
Pt(cub)	1	1	1	39.76	100
	2	0	0	46.24	53
Si(cub)	1	1	1	28.44	100
	2	2	0	47.30	55
	3	1	1	56.12	30
Ta(cub) α-phase	1	1	0	38.47	100
	2	0	0	55.55	21
Ta(cub) β-phase a=1.0194nm c=0.5313nm	0	0	2	33.60	40
	4	1	0	36.28	80
	3	3	0	37.39	55
	2	0	2	38.20	55
	2	1	2	39.24	80
TaN(cub)	4	1	1	40.21	100
	3	3	1	41.18	65
	1	1	1	35.85	100
	2	0	0	41.60	80
Ti(hex) a=0.295nm c=0.4683nm	2	2	0	60.41	40
	1	0	0	35.09	25
	0	0	2	38.42	30
	1	0	1	40.17	100
Ti(cub)	1	0	2	53.00	13
	1	1	0	38.48	100
	2	0	0	55.54	12

CuKα (λ=0.15418nm)

Crystal	Miller Index			2θ angle (deg)	Relative Intensity
	h	k	l		
TiSi(ortho) a=0.3618nm b=0.6492nm c=0.4730nm	1	0	1	30.56	16
	0	0	2	36.12	25
	1	2	1	41.55	100
	0	2	2	45.98	20
	2	0	0	50.45	20
TiSi ₂ (ortho) (C54) a=0.8269nm b=0.8554nm c=0.4798nm	1	1	1	23.81	12
	2	2	0	30.05	10
	3	1	1	39.10	100
	0	4	0	42.23	43
	0	2	2	43.18	70
TiSi ₂ (ortho) (C49) a=0.3629nm b=1.376nm c=0.3605nm	3	3	1	49.73	45
	0	2	0	12.82	10
	0	2	1	27.95	20
	1	3	0	31.47	15
	0	6	0	39.31	80
WN(cub)	1	3	1	40.41	100
	1	5	0	41.18	15
	0	6	1	46.91	20
	2	0	0	50.37	35
	1	1	1	37.73	100
Y ₂ O ₃ (cub)	2	0	0	43.84	78
	2	2	0	63.73	63
	2	1	1	20.51	13
	2	2	2	29.16	100
ZnO(hex-WZ) a=0.3245nm c=0.5195nm	4	0	0	33.80	31
	4	4	0	48.55	58
	1	0	0	31.87	50
	0	0	2	34.53	40
	1	0	1	36.37	100
ZrO ₂ (cub)	1	0	2	47.69	25
	1	1	0	56.78	40
	1	0	3	63.07	35
	1	1	1	30.42	100
	2	0	0	35.27	23
ZrO ₂ (tet) a=0.364nm c=0.527nm	2	2	0	50.73	100
	3	1	1	60.31	64
	1	0	1	29.83	100
	0	0	2	34.02	10
	1	1	0	34.86	15
ZrO ₂ (mncl) a=0.515nm b=0.5217nm c=0.5317nm β=99.2deg	1	1	2	49.50	50
	2	0	0	50.12	30
	1	0	3	58.32	20
	2	1	1	59.43	40
	2	0	2	61.97	10
	0	1	1	24.06	15
	-1	1	1	28.19	100
	1	1	1	31.48	75
	0	0	2	34.17	25
	0	2	0	34.42	15
	2	0	0	35.31	20
	-2	1	1	40.74	20
	1	1	2	44.84	10
	-2	0	2	45.52	10

BRAGG'S LAW

$$2d \sin \theta = n\lambda$$

where :

d lattice spacing in nm

θ diffraction angle in degree

λ wavelength in nm

n order in integer