

d-spacings

APPENDIX 1

LATTICE GEOMETRY

A1-1 Plane spacings. The value of d , the distance between adjacent planes in the set (hkl) , may be found from the following equations.

Cubic:
$$\frac{1}{d^2} = \frac{h^2 + k^2 + l^2}{a^2} \quad \text{for aluminum}$$

Tetragonal:
$$\frac{1}{d^2} = \frac{h^2 + k^2}{a^2} + \frac{l^2}{c^2}$$

Hexagonal:
$$\frac{1}{d^2} = \frac{4}{3} \left(\frac{h^2 + hk + k^2}{a^2} \right) + \frac{l^2}{c^2} \quad \text{for graphite}$$

Rhombohedral:

$$\frac{1}{d^2} = \frac{(h^2 + k^2 + l^2) \sin^2 \alpha + 2(hk + kl + hl)(\cos^2 \alpha - \cos \alpha)}{a^2(1 - 3 \cos^2 \alpha + 2 \cos^3 \alpha)}$$

Orthorhombic:
$$\frac{1}{d^2} = \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}$$

Monoclinic:
$$\frac{1}{d^2} = \frac{1}{\sin^2 \beta} \left(\frac{h^2}{a^2} + \frac{k^2 \sin^2 \beta}{b^2} + \frac{l^2}{c^2} - \frac{2hl \cos \beta}{ac} \right)$$

Triclinic:
$$\frac{1}{d^2} = \frac{1}{V^2} (S_{11}h^2 + S_{22}k^2 + S_{33}l^2 + 2S_{12}hk + 2S_{23}kl + 2S_{13}hl)$$

In the equation for triclinic crystals

V = volume of unit cell (see below),

$$S_{11} = b^2c^2 \sin^2 \alpha,$$

$$S_{22} = a^2c^2 \sin^2 \beta,$$

$$S_{33} = a^2b^2 \sin^2 \gamma,$$

$$S_{12} = abc^2(\cos \alpha \cos \beta - \cos \gamma),$$

$$S_{23} = a^2bc(\cos \beta \cos \gamma - \cos \alpha),$$

$$S_{13} = ab^2c(\cos \gamma \cos \alpha - \cos \beta).$$

allowed fcc

allowed
hexagonal

APPENDIX 6

QUADRATIC FORMS OF MILLER INDICES

$h^2 + k^2 + l^2$	Cubic				Hexagonal	
	Simple	hkl			$h^2 + hk + k^2$	hk
Face-centered		Body-centered	Diamond			
1	100				1	10
2	110		110		2	
3	111	111		111	3	11
4	200	200	200		4	20
5	210				5	
6	211		211		6	
7					7	21
8	220	220	220	220	8	
9	300, 221				9	30
10	310		310		10	
11	311	311		311	11	
12	222	222	222		12	22
13	320				13	31
14	321		321		14	
15					15	
16	400	400	400	400	16	40
17	410, 322				17	
18	411, 330		411, 330		18	
19	331	331		331	19	32
20	420	420	420		20	
21	421				21	41
22	332		332		22	
23					23	
24	422	422	422	422	24	
25	500, 430				25	50
26	510, 431		510, 431		26	
27	511, 333	511, 333		511, 333	27	33
28					28	42
29	520, 432				29	
30	521		521		30	
31					31	51
32	440	440	440	440	32	
33	522, 441				33	
34	530, 433		530, 433		34	
35	531	531		531	35	
36	600, 442	600, 442	600, 442		36	60
37	610				37	43
38	611, 532		611, 532		38	
39					39	52
40	620	620	620	620	40	
41	621, 540, 443				41	
42	541		541		42	
43	533	533		533	43	61
44	622	622	622		44	
45	630, 542				45	
46	631		631		46	
47					47	
48	444	444	444	444	48	44
49	700, 632				49	70, 53

(cont.)

calculated d-spacings for aluminum

h	k	l	$h^2 + k^2 + l^2$	d(hkl) calculated
1	1	1	3	2.338
2	0	0	4	2.025
2	2	0	8	1.432
4	0	0	16	1.012
3	3	1	19	0.929
4	2	0	20	0.906

aluminum intensities

ReciprOgraph - Al

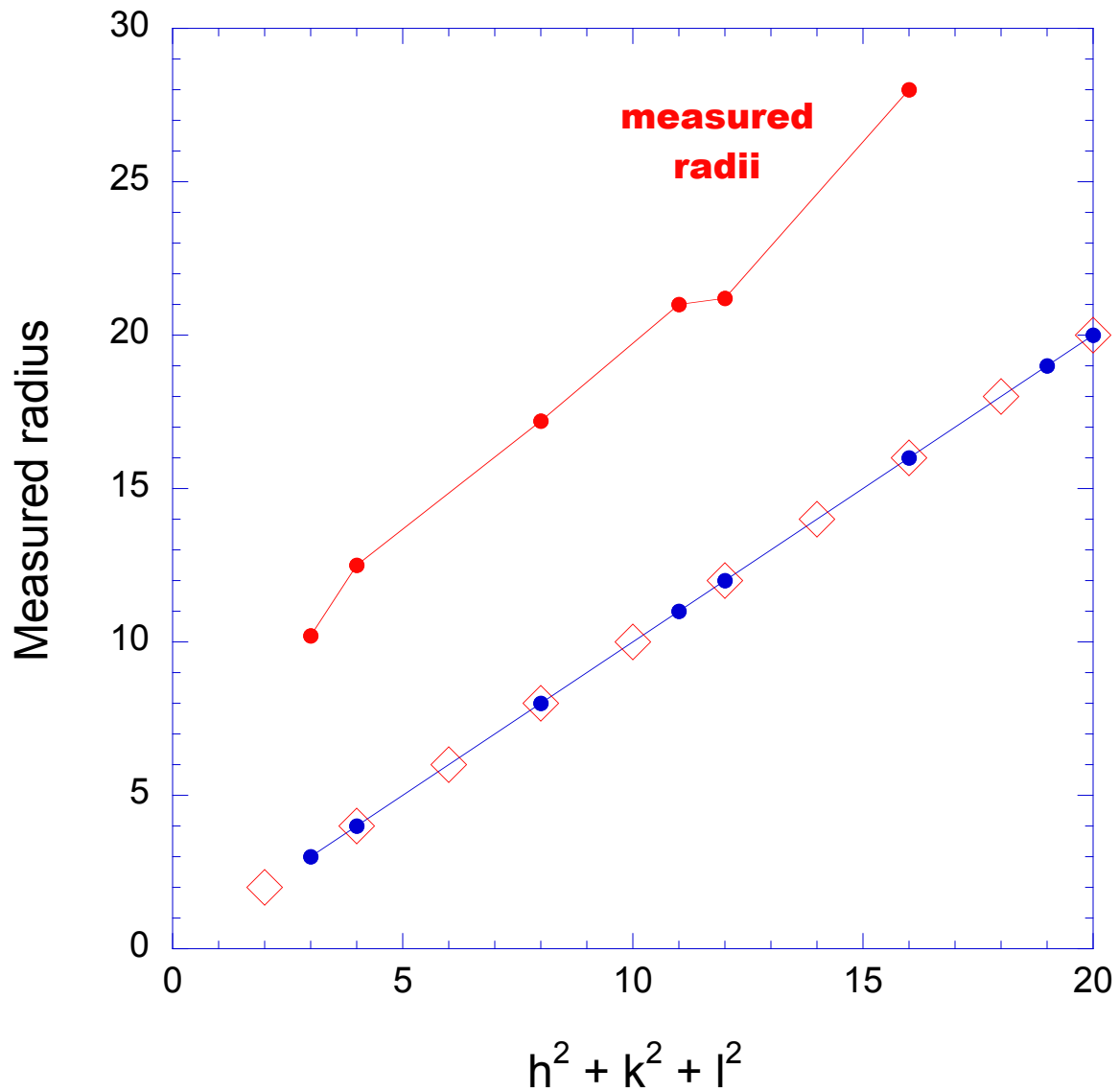
Single crystal

Powder diagram

Structure factors

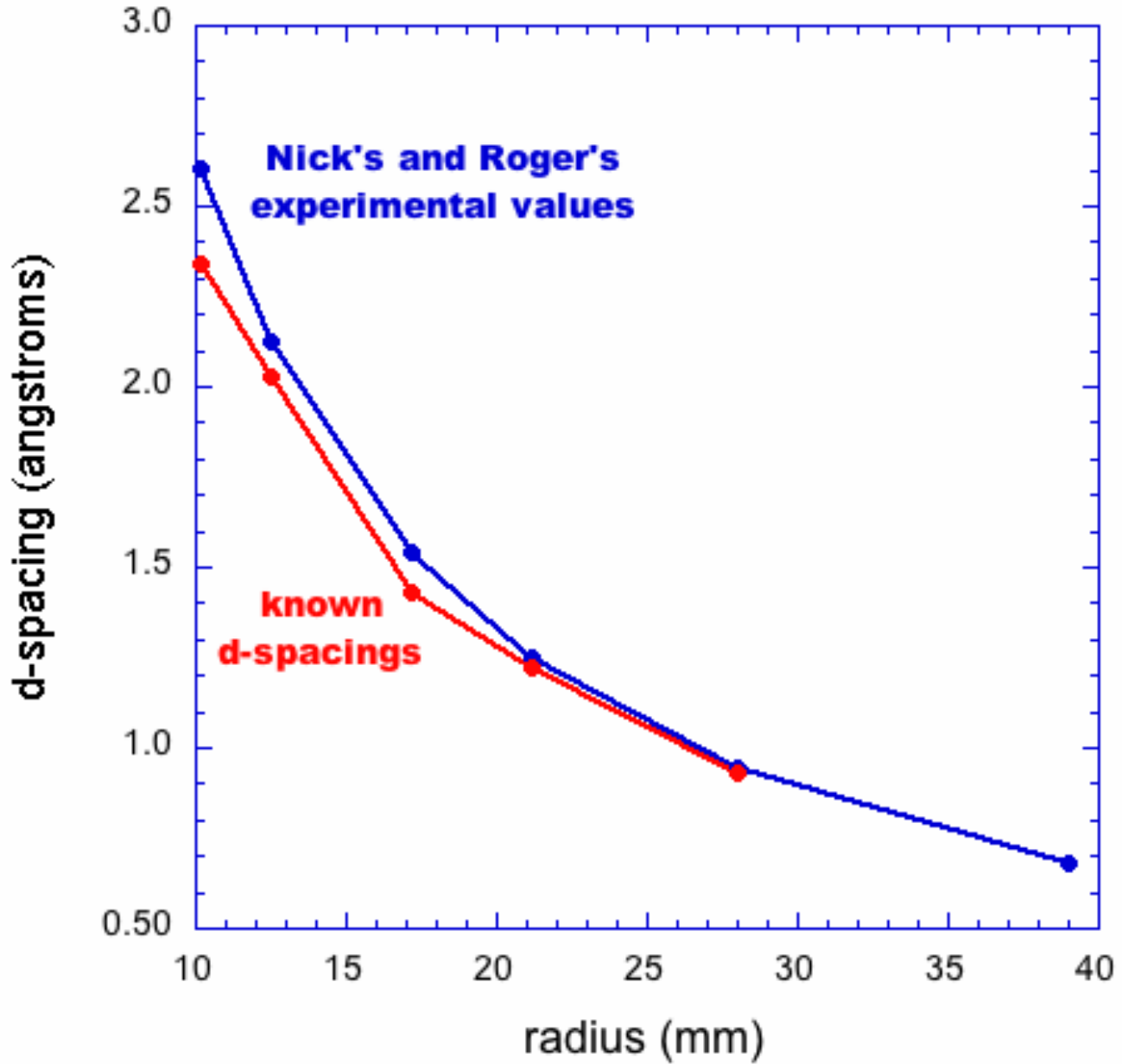
h	k	l	d(hkl)	2-Theta	F(re)	F(Im)	F ²	
3	3	3	0.7793	79.825	17.41	0.00	303.10	
3	3	1	0.9290	65.127	21.24	0.00	451.11	weak
3	3	-1	0.9290	65.127	21.24	0.00	451.11	
3	3	-3	0.7793	79.825	17.41	0.00	303.10	
3	1	3	0.9290	65.127	21.24	0.00	451.11	
3	1	1	1.2209	48.351	26.63	0.00	709.15	
3	1	-1	1.2209	48.351	26.63	0.00	709.15	
3	1	-3	0.9290	65.127	21.24	0.00	451.11	
3	-1	3	0.9290	65.127	21.24	0.00	451.11	
3	-1	1	1.2209	48.351	26.63	0.00	709.15	
3	-1	-1	1.2209	48.351	26.63	0.00	709.15	
3	-1	-3	0.9290	65.127	21.24	0.00	451.11	
3	-3	3	0.7793	79.825	17.41	0.00	303.10	
3	-3	1	0.9290	65.127	21.24	0.00	451.11	
3	-3	-1	0.9290	65.127	21.24	0.00	451.11	
3	-3	-3	0.7793	79.825	17.41	0.00	303.10	
2	2	2	1.1689	50.649	25.84	0.00	667.89	
2	2	0	1.4316	40.883	29.27	0.00	856.51	strong
2	2	-2	1.1689	50.649	25.84	0.00	667.89	
2	0	2	1.4316	40.883	29.27	0.00	856.51	strong
2	0	0	2.0246	28.595	34.04	0.00	1158.43	strong
2	0	-2	1.4316	40.883	29.27	0.00	856.51	
2	-2	2	1.1689	50.649	25.84	0.00	667.89	
2	-2	0	1.4316	40.883	29.27	0.00	856.51	
2	-2	-2	1.1689	50.649	25.84	0.00	667.89	
1	3	3	0.9290	65.127	21.24	0.00	451.11	
1	3	1	1.2209	48.351	26.63	0.00	709.15	
1	3	-1	1.2209	48.351	26.63	0.00	709.15	
1	3	-3	0.9290	65.127	21.24	0.00	451.11	
1	1	3	1.2209	48.351	26.63	0.00	709.15	
1	1	1	2.3378	24.699	35.82	0.00	1283.19	strong
1	1	-1	2.3378	24.699	35.82	0.00	1283.19	
1	1	-3	1.2209	48.351	26.63	0.00	709.15	
1	-1	3	1.2209	48.351	26.63	0.00	709.15	
1	-1	1	2.3378	24.699	35.82	0.00	1283.19	
1	-1	-1	2.3378	24.699	35.82	0.00	1283.19	
1	-1	-3	1.2209	48.351	26.63	0.00	709.15	
1	-3	3	0.9290	65.127	21.24	0.00	451.11	
1	-3	1	1.2209	48.351	26.63	0.00	709.15	
1	-3	-1	1.2209	48.351	26.63	0.00	709.15	
1	-3	-3	0.9290	65.127	21.24	0.00	451.11	
0	2	2	1.4316	40.883	29.27	0.00	856.51	
0	2	0	2.0246	28.595	34.04	0.00	1158.43	
0	2	-2	1.4316	40.883	29.27	0.00	856.51	
0	0	2	2.0246	28.595	34.04	0.00	1158.43	
0	0	0	2.0246	28.595	34.04	0.00	1158.43	
0	0	-2	2.0246	28.595	34.04	0.00	1158.43	
0	-2	2	1.4316	40.883	29.27	0.00	856.51	
0	-2	0	2.0246	28.595	34.04	0.00	1158.43	
0	-2	-2	1.4316	40.883	29.27	0.00	856.51	
-1	3	3	0.9290	65.127	21.24	0.00	451.11	
-1	3	1	1.2209	48.351	26.63	0.00	709.15	
-1	3	-1	1.2209	48.351	26.63	0.00	709.15	
-1	3	-3	0.9290	65.127	21.24	0.00	451.11	
-1	1	3	1.2209	48.351	26.63	0.00	709.15	
-1	1	1	2.3378	24.699	35.82	0.00	1283.19	
-1	1	-1	2.3378	24.699	35.82	0.00	1283.19	
-1	1	-3	1.2209	48.351	26.63	0.00	709.15	
-1	-1	3	1.2209	48.351	26.63	0.00	709.15	
-1	-1	1	2.3378	24.699	35.82	0.00	1283.19	
-1	-1	-1	2.3378	24.699	35.82	0.00	1283.19	
-1	-1	-3	1.2209	48.351	26.63	0.00	709.15	
-1	-3	3	0.9290	65.127	21.24	0.00	451.11	
-1	-3	1	1.2209	48.351	26.63	0.00	709.15	
-1	-3	-1	1.2209	48.351	26.63	0.00	709.15	
-1	-3	-3	0.9290	65.127	21.24	0.00	451.11	
-2	2	2	1.1689	50.649	25.84	0.00	667.89	
-2	2	0	1.4316	40.883	29.27	0.00	856.51	
-2	2	-2	1.1689	50.649	25.84	0.00	667.89	
-2	0	2	1.4316	40.883	29.27	0.00	856.51	
-2	0	0	2.0246	28.595	34.04	0.00	1158.43	
-2	0	-2	1.4316	40.883	29.27	0.00	856.51	
-2	-2	2	1.1689	50.649	25.84	0.00	667.89	
-2	-2	0	1.4316	40.883	29.27	0.00	856.51	
-2	-2	-2	1.1689	50.649	25.84	0.00	667.89	
-3	3	3	0.7793	79.825	17.41	0.00	303.10	
-3	3	1	0.9290	65.127	21.24	0.00	451.11	
-3	3	-1	0.9290	65.127	21.24	0.00	451.11	
-3	3	-3	0.7793	79.825	17.41	0.00	303.10	
-3	1	3	0.9290	65.127	21.24	0.00	451.11	

allowed FCC reflections = blue dots
allowed BCC reflections = red diamonds
measured reflections = red dots

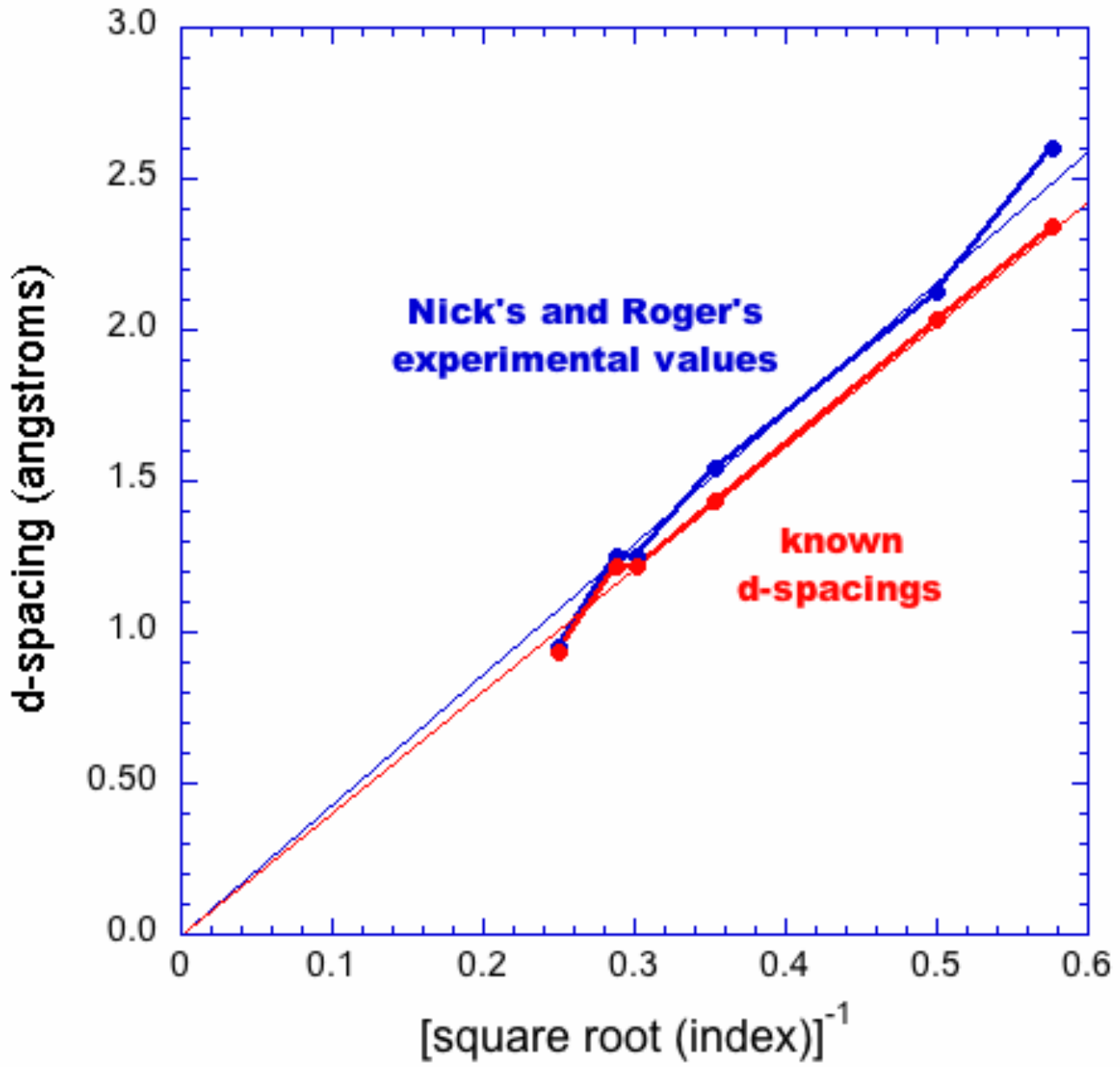


aluminum

d-spacing versus radius



aluminum



calculated d-spacings for graphite

h	k	$h^2 + hk + k^2$	d(hkl) calculated
1	0	1	2.139
1	1	3	1.235
2	0	4	1.070
2	1	7	0.809
3	0	9	0.713
2	2	12	0.618
3	1	13	0.593

For small angles α ($\cos 10^\circ = 0.985$) can put

$$\sin 2\alpha \approx 2 \sin \alpha \quad (6)$$

so that for small angles θ we obtain

$$\sin \alpha = \sin 2\theta \approx 2 \sin \theta \quad (6a)$$

With this approximation we obtain

$$r = \frac{2R}{d} \cdot n \cdot \lambda \quad (7)$$

The two inner interference rings occur through reflection from the lattice planes of spacing d_1 and d_2 (Fig. 4), for $n = 1$ in (7).

The wavelength is calculated from the anode voltage in accordance with (3):

$\frac{U_A}{\text{kV}}$	$\frac{\lambda}{\text{pm}}$
4.00	19.4
4.50	18.3
5.00	17.3
5.50	16.5
6.50	15.2
7.00	14.7
7.40	14.3

Applying the regression lines expressed by

$$Y = AX + B$$

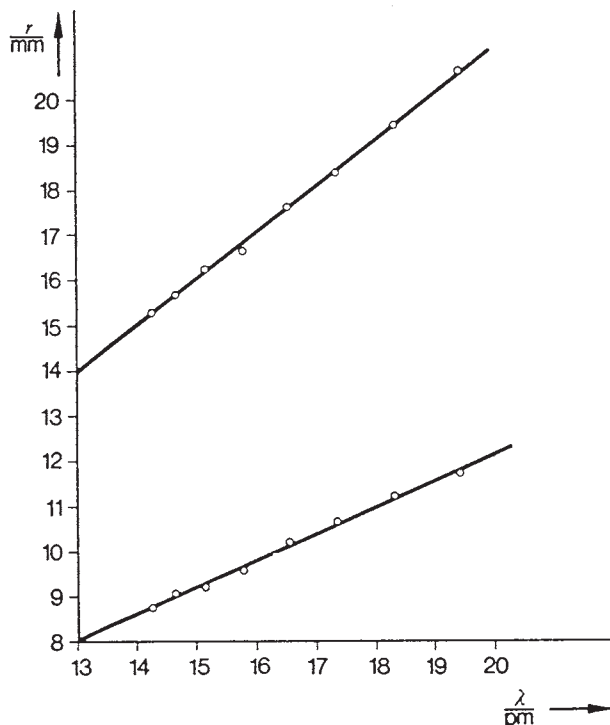


Fig. 5: Radii of the first two interference rings as a function of the wavelength of the electrons.

to the measured values from Fig. 5 gives a slopes

$$A_1 = 0.62 (2) \cdot 10^9$$

$$A_2 = 1.03 (2) \cdot 10^9$$

and the lattice constants

$$d_1 = 211 \text{ pm}$$

$$d_2 = 126 \text{ pm}$$

in accordance with (7),

$$\frac{T_i}{\lambda} = A_i = \frac{2R}{d_i} \quad \text{and}$$

$$d_i = \frac{2R}{A_i} .$$

Notes

- The intensity of higher order interference rings is much lower than that of first order rings. Thus, for example, the second order ring of d_1 is difficult to identify and the expected fourth order ring of d_1 simply cannot be seen. The third order ring of d_1 is easy to see because graphite always has two lattice planes together, spaced apart by a distance of $d_1/3$. (Fig. 6)

In the sixth ring, the first order of ring of d_4 clearly coincides with the second order one of d_2 .

Radii (mm) calculated according to (4) for the interference rings to be expected when $U_A = 7 \text{ kV}$:

	$n = 1$	$n = 2$	$n = 3$	$n = 4$
d_1	8.9	17.7	26.1	34.1
d_2	15.4	29.9		
d_3	23.2			
d_4	31.0			
d_5	38.5			

d-spacings

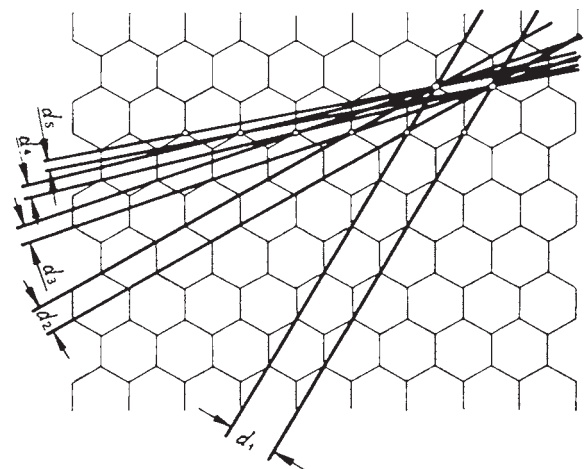
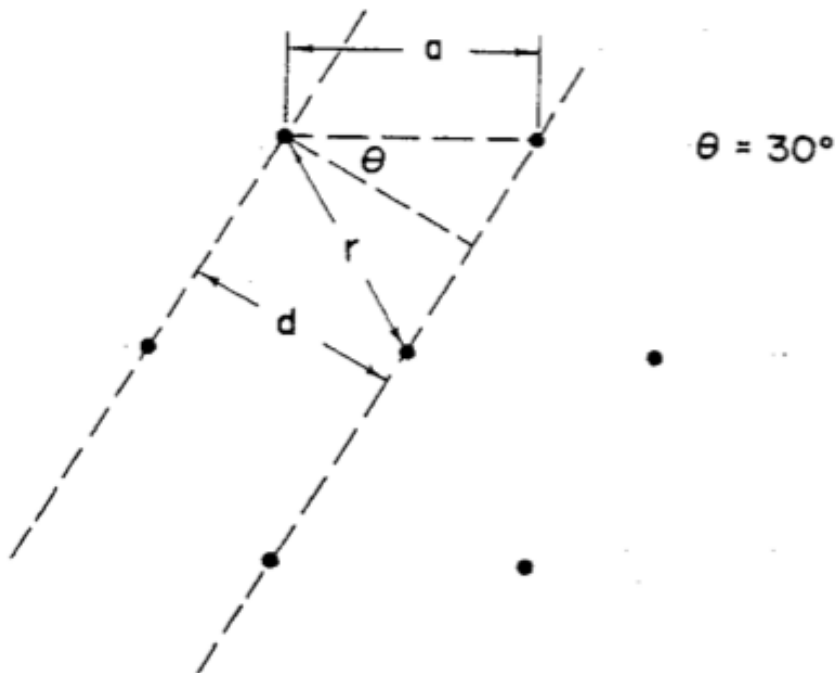


Fig. 6: Interplanar spacing in graphite

$d_1 = 213 \text{ pm}$	$d_2 = 123 \text{ pm}$	$d_3 = 80.5 \text{ pm}$
$d_4 = 59.1 \text{ pm}$	$d_5 = 46.5 \text{ pm}$	

from the 1, 2, square root of 3 triangle

$d = a \text{ times (the square root of 3) over 2}$



1. $\lambda = \sqrt{\frac{150}{V}}$
2. $d = \frac{\lambda D}{r}$
3. $a = \frac{\lambda D}{r \cos \theta}$

$$d = a \cos(30 \text{ degrees})$$

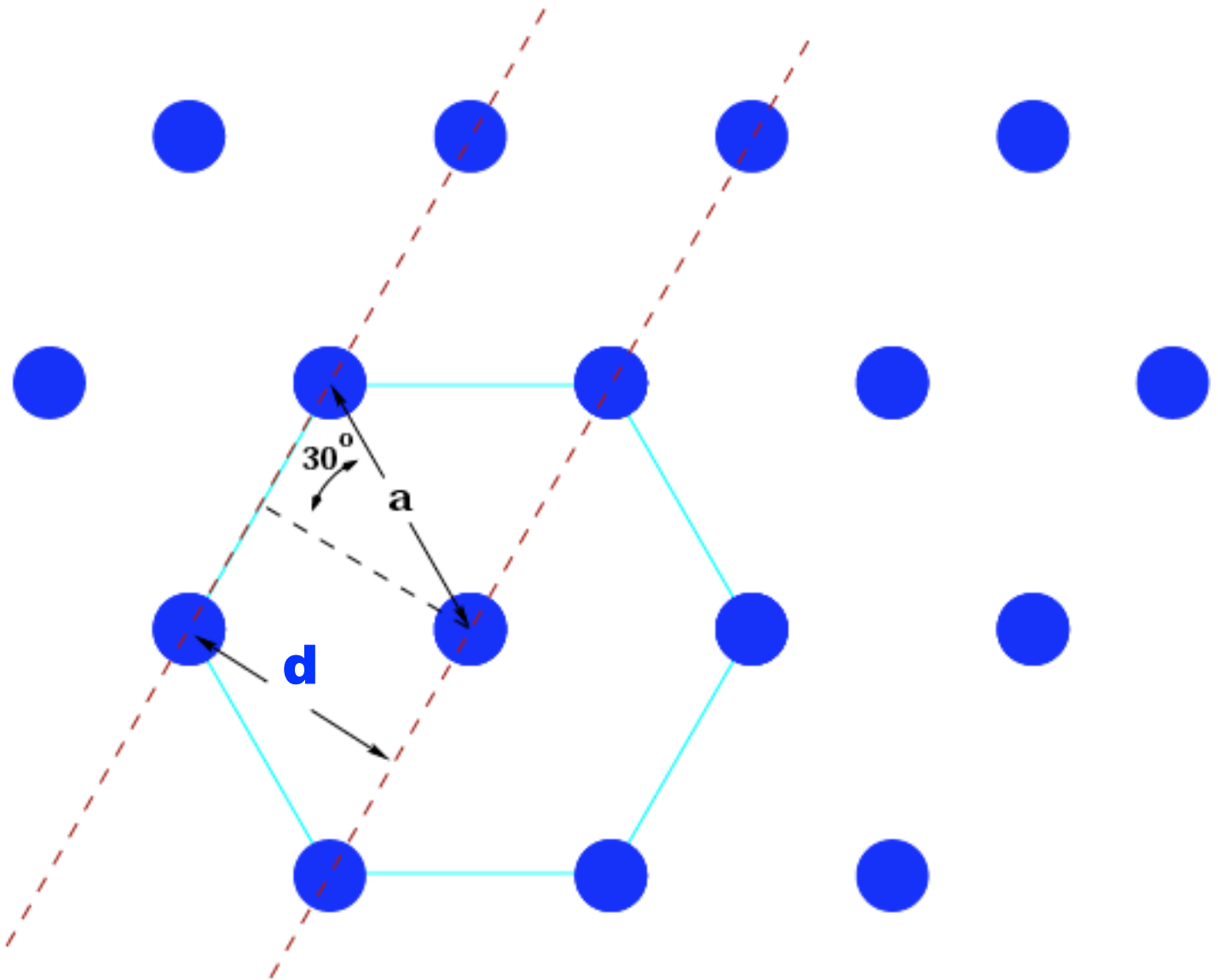


Figure 9 Lattice Plane Spacing of the Fundamental Lattice Planes with the Widest Spacing for Hexagonal Crystal Structures

graphite intensities

ReciprOgraph - C

Single crystal		Powder diagram		Structure factors			
h	k	l	d(hkl)	2-Theta	F(re)	F(Im)	F ²
2	1	2	0.7866	156.801	-1.50	0.00	2.24
2	1	1	0.8028	147.363	-2.62	0.00	6.84
2	1	0	0.8085	144.729	1.52	0.00	2.30
2	1	-1	0.8028	147.363	2.62	0.00	6.84
2	1	-2	0.7866	156.801	-1.50	0.00	2.24
2	0	2	1.0203	98.087	-1.70	0.00	2.90
2	0	1	1.0566	93.649	3.01	0.00	9.07
2	0	0	1.0695	92.175	1.75	0.00	3.07
2	0	-1	1.0566	93.649	-3.01	0.00	9.07
2	0	-2	1.0203	98.087	-1.70	0.00	2.90
2	-1	2	1.1608	83.176	-7.39	0.00	54.58
2	-1	0	1.2350	77.201	7.72	0.00	59.61
2	-1	-2	1.1608	83.176	-7.39	0.00	54.58
2	-2	2	1.0203	98.087	-1.71	0.00	2.91
2	-2	1	1.0566	93.649	-3.01	0.00	9.09
2	-2	0	1.0695	92.175	1.75	0.00	3.08
2	-2	-1	1.0566	93.649	3.01	0.00	9.09
2	-2	-2	1.0203	98.087	-1.71	0.00	2.91
1	2	2	0.7866	156.801	-1.50	0.00	2.24
1	2	1	0.8028	147.363	2.62	0.00	6.84
1	2	0	0.8085	144.729	1.52	0.00	2.30
1	2	-1	0.8028	147.363	-2.62	0.00	6.84
1	2	-2	0.7866	156.801	-1.50	0.00	2.24
1	1	2	1.1608	83.176	-7.39	0.00	54.58
1	1	0	1.2350	77.201	7.72	0.00	59.61
1	1	-2	1.1608	83.176	-7.39	0.00	54.58
1	0	2	1.8106	50.372	-2.69	0.00	7.26
1	0	1	2.0405	44.371	-5.20	0.00	27.06
1	0	0	2.1391	42.225	3.13	0.00	9.81
1	0	-1	2.0405	44.371	5.20	0.00	27.06
1	0	-2	1.8106	50.372	-2.69	0.00	7.26
1	-1	2	1.8106	50.372	-2.69	0.00	7.24
1	-1	1	2.0405	44.371	5.20	0.00	27.04
1	-1	0	2.1391	42.225	3.13	0.00	9.79
1	-1	-1	2.0405	44.371	-5.20	0.00	27.04
1	-1	-2	1.8106	50.372	-2.69	0.00	7.24
1	-2	2	1.1608	83.176	-7.39	0.00	54.58
1	-2	0	1.2350	77.201	7.72	0.00	59.61
1	-2	-2	1.1608	83.176	-7.39	0.00	54.58
0	2	2	1.0203	98.087	-1.70	0.00	2.90
0	2	1	1.0566	93.649	-3.01	0.00	9.07
0	2	0	1.0695	92.175	1.75	0.00	3.07
0	2	-1	1.0566	93.649	3.01	0.00	9.07
0	2	-2	1.0203	98.087	-1.70	0.00	2.90
0	1	2	1.8106	50.372	-2.69	0.00	7.26
0	1	1	2.0405	44.371	5.20	0.00	27.06
0	1	0	2.1391	42.225	3.13	0.00	9.81
0	1	-1	2.0405	44.371	-5.20	0.00	27.06
0	1	-2	1.8106	50.372	-2.69	0.00	7.26
0	0	2	3.4000	26.196	-17.43	0.00	303.82
0	0	0	0.0000	0.000	24.00	0.00	575.85

Calculated d-spacings and intensities for graphite

3. Experimental Technique

a. Apparatus

The electron diffraction tube is a small cathode ray tube (CRT) similar to that in a small (old-fashioned) TV set. The electrons pass through a target that consists of graphite, only a few molecular layers thick, vapor-deposited on a micromesh nickel grid. The target is crystalline in tiny regions, so a "powder" diffraction pattern results, seen as a pair of rings around a central spot on the luminescent screen. See diagram below. The distance between the target and phosphor screen is $L = 13.5$ cm.

$$\tan(2\theta) = r / L$$

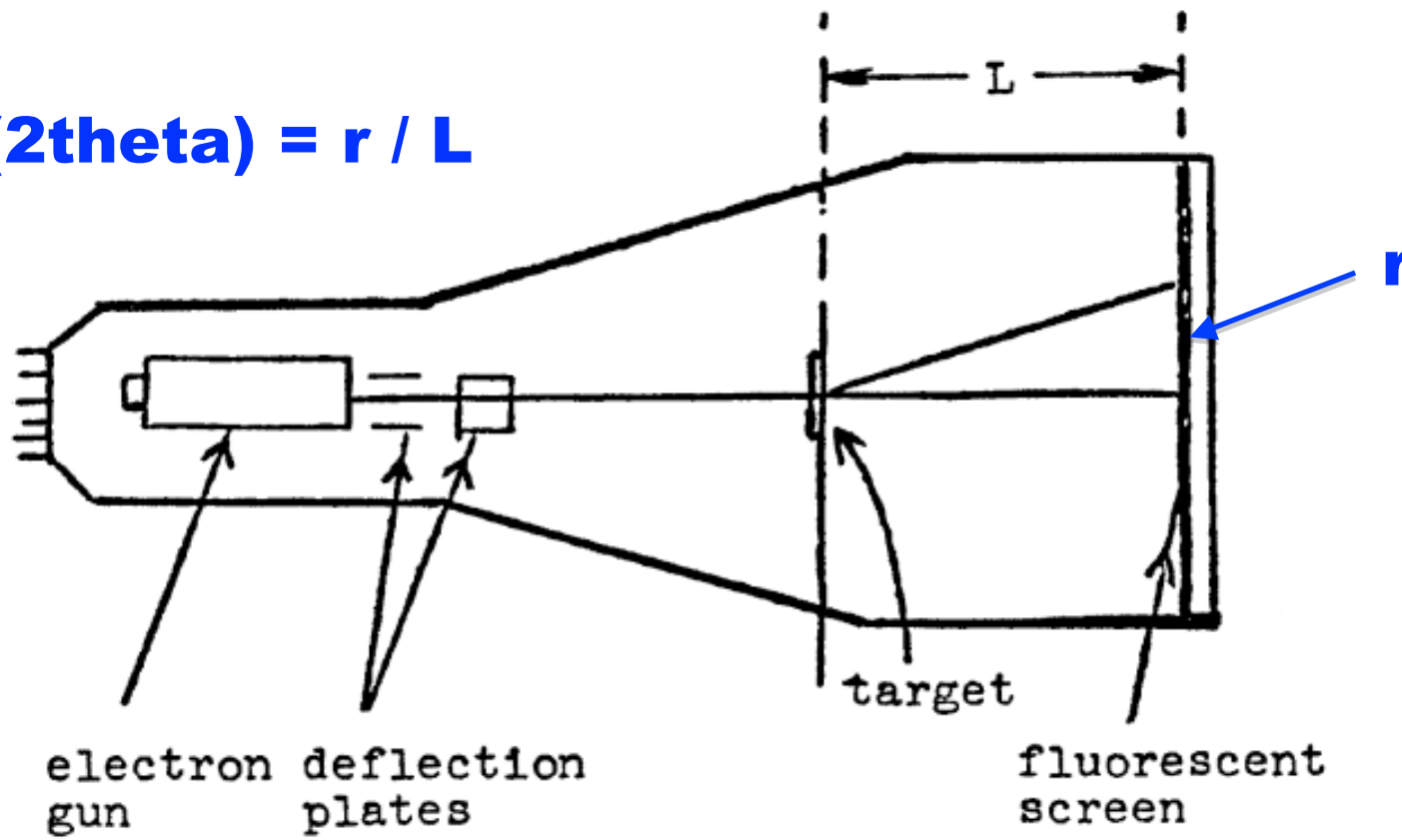


Figure 1 Schematic of the CRT tube

$$\tan(2\theta) = r / D$$

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

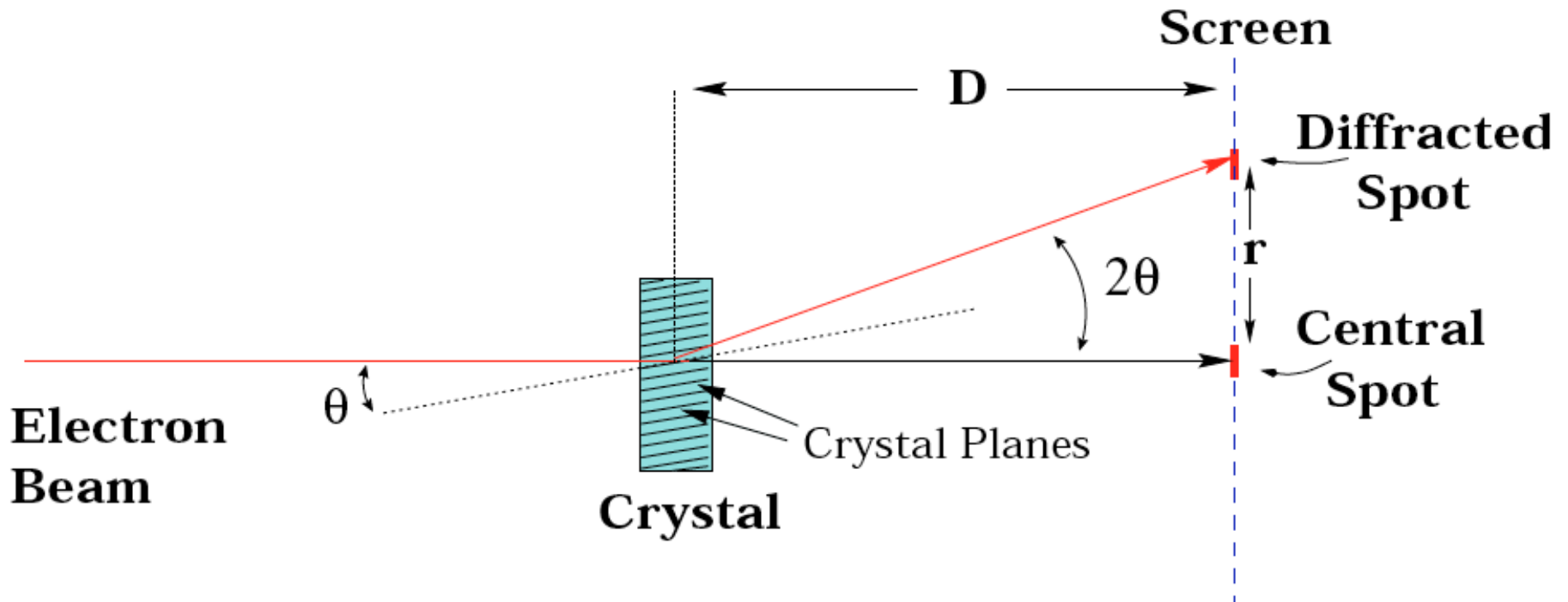
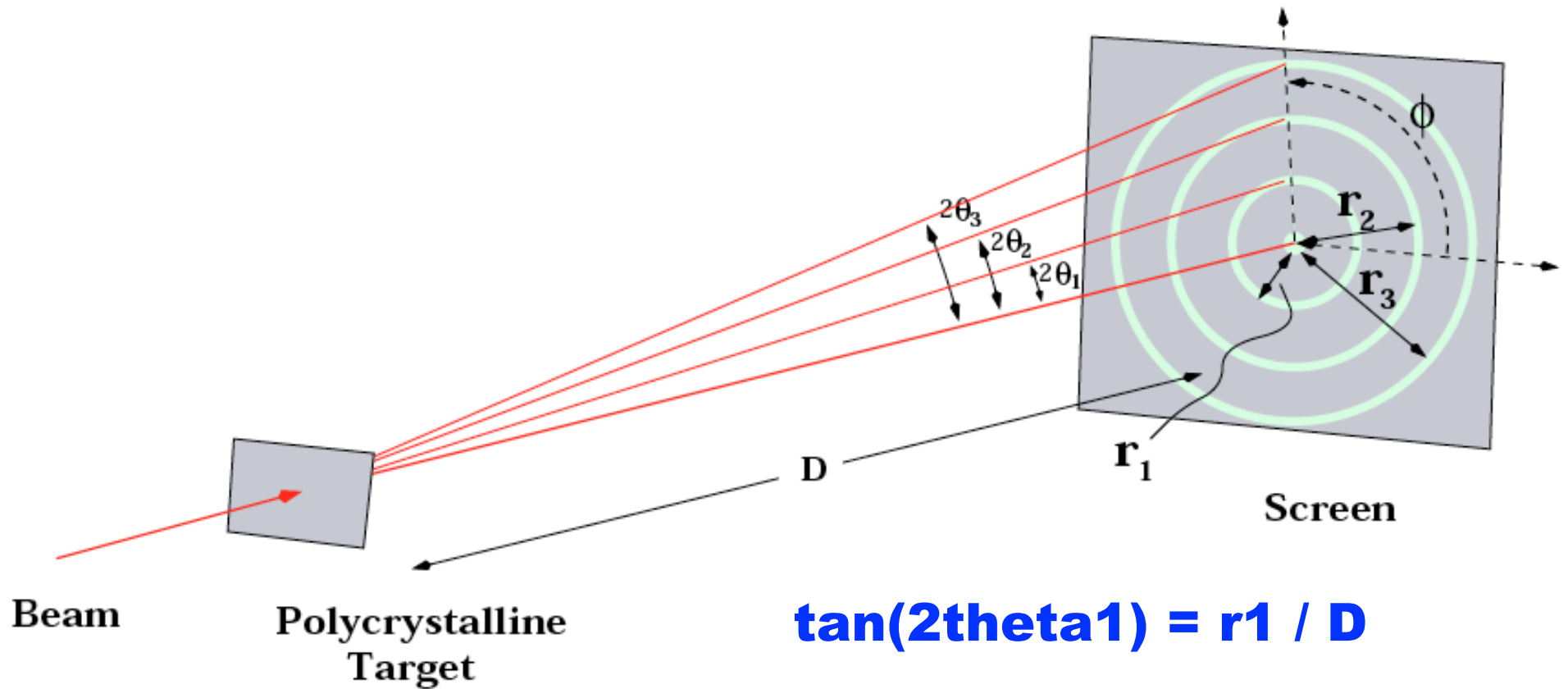


Figure 7 Crystal Diffraction Geometry

The total angle of a diffraction maxima due to reflection off of a particular crystal lattice plane is twice the angle of incidence on that plane. This angle may be approximated as the distance of the diffraction spot from the undiffracted beam over the distance between the imaging screen and the crystal, i.e. $q \approx 1/2 r/D$.

Multiple diffraction rings



$$\tan(2\theta_1) = r_1 / D$$

$$\tan(2\theta_2) = r_2 / D$$

$$\tan(2\theta_3) = r_3 / D$$

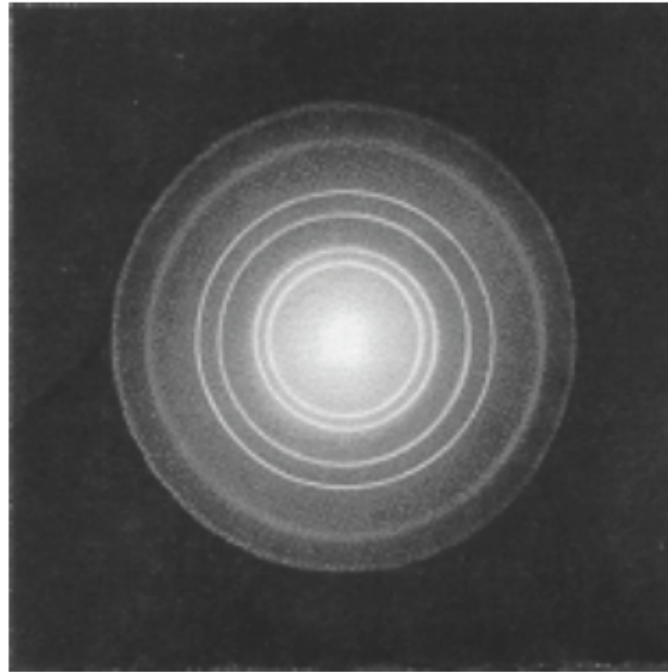
single crystals => diffraction peaks

powder => diffraction rings

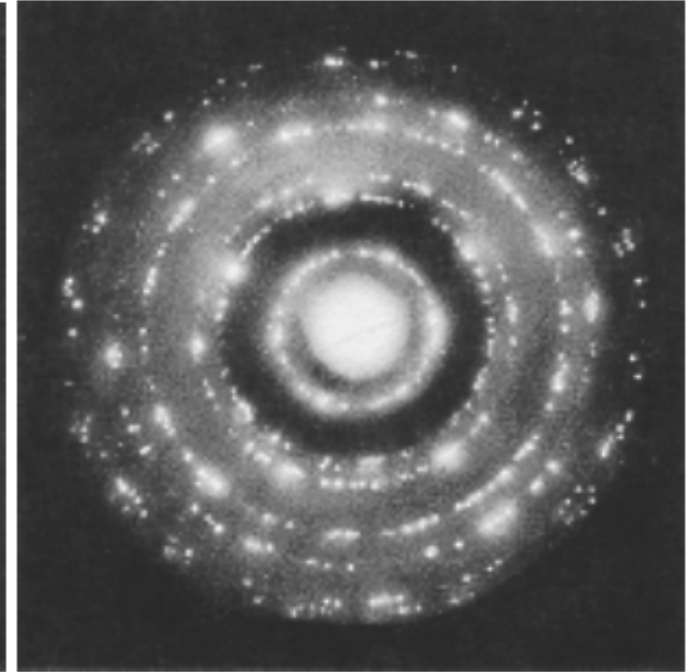
multiple crystals => spotted rings



graphene
also graphite
single crystal

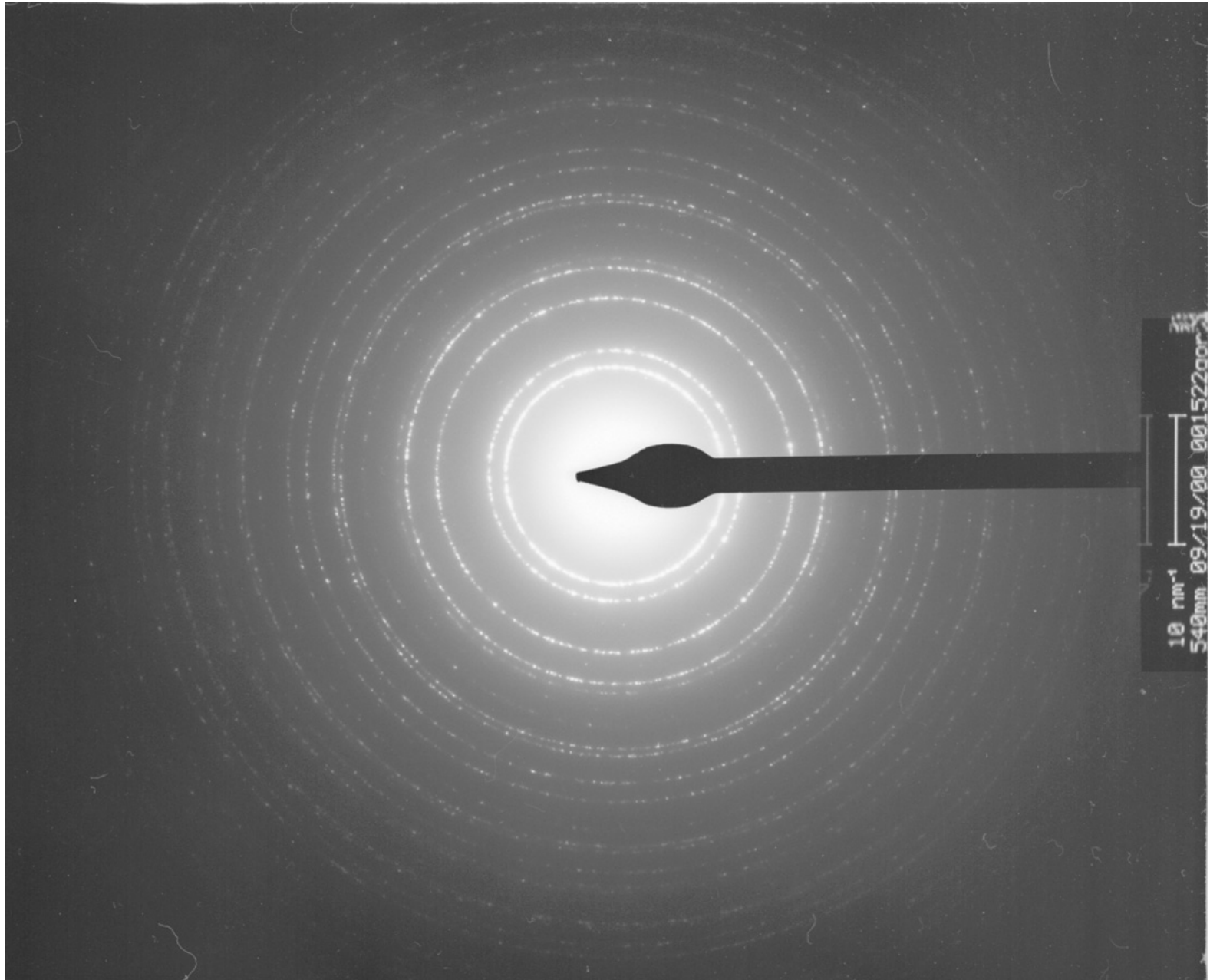


fcc aluminum
polycrystalline
also powder

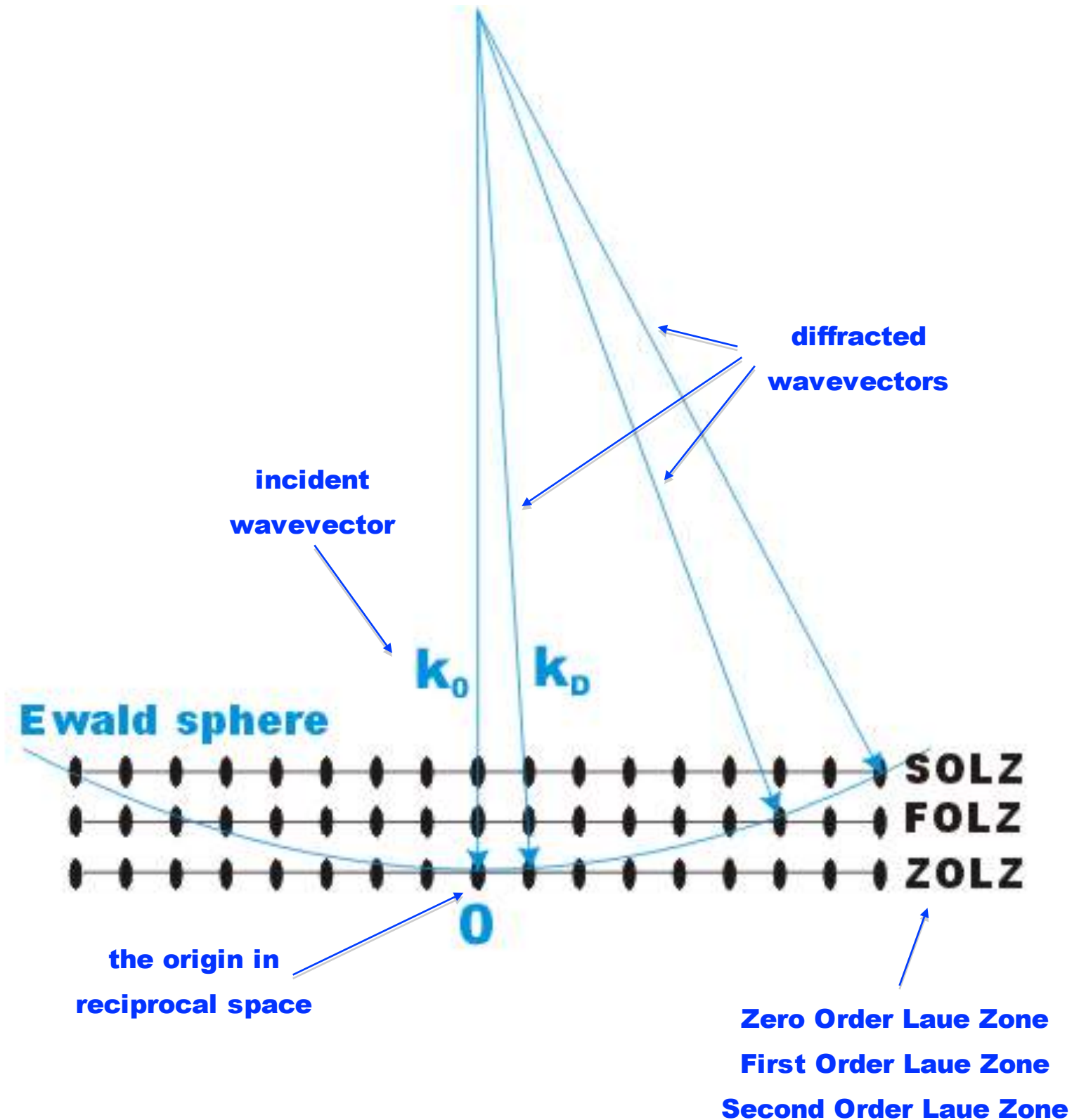


graphite
pyrolytic

Aluminum diffraction rings

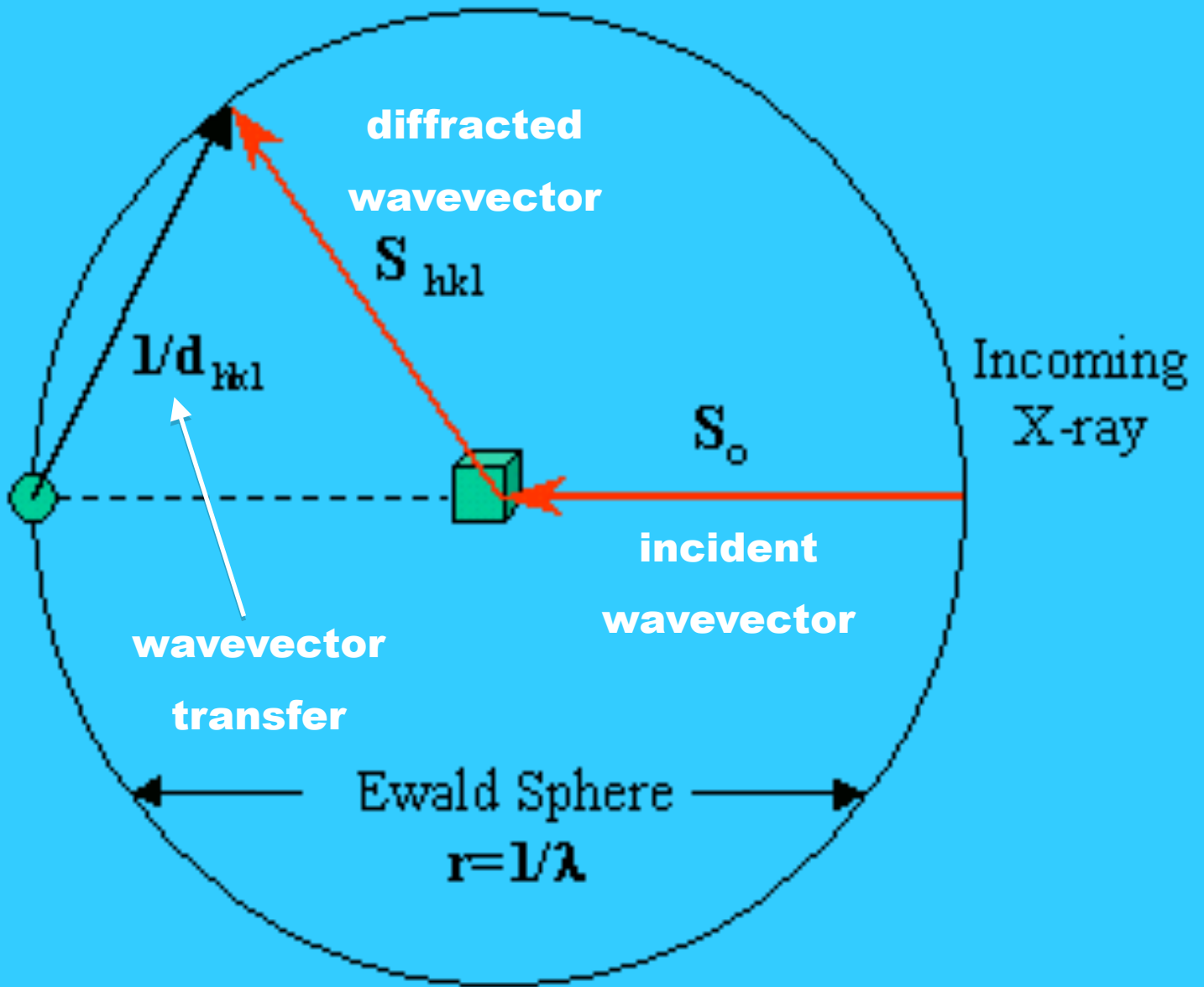


For our electron and optical diffraction experiments the wavelength is small compared to the lattice constant. Consequently, the wavevector $k = 2\pi / \lambda$ is much longer than the reciprocal lattice spacing $2\pi / a$ and the Ewald Sphere cuts through many reciprocal lattice points



In our experiments, we only see ZOLZ peaks

Ewald sphere geometry for x-ray diffraction



In contrast to electron and optical diffraction where there are many Bragg peaks on the Ewald sphere, in x-ray diffraction there is usually only one Bragg peak on the Ewald sphere