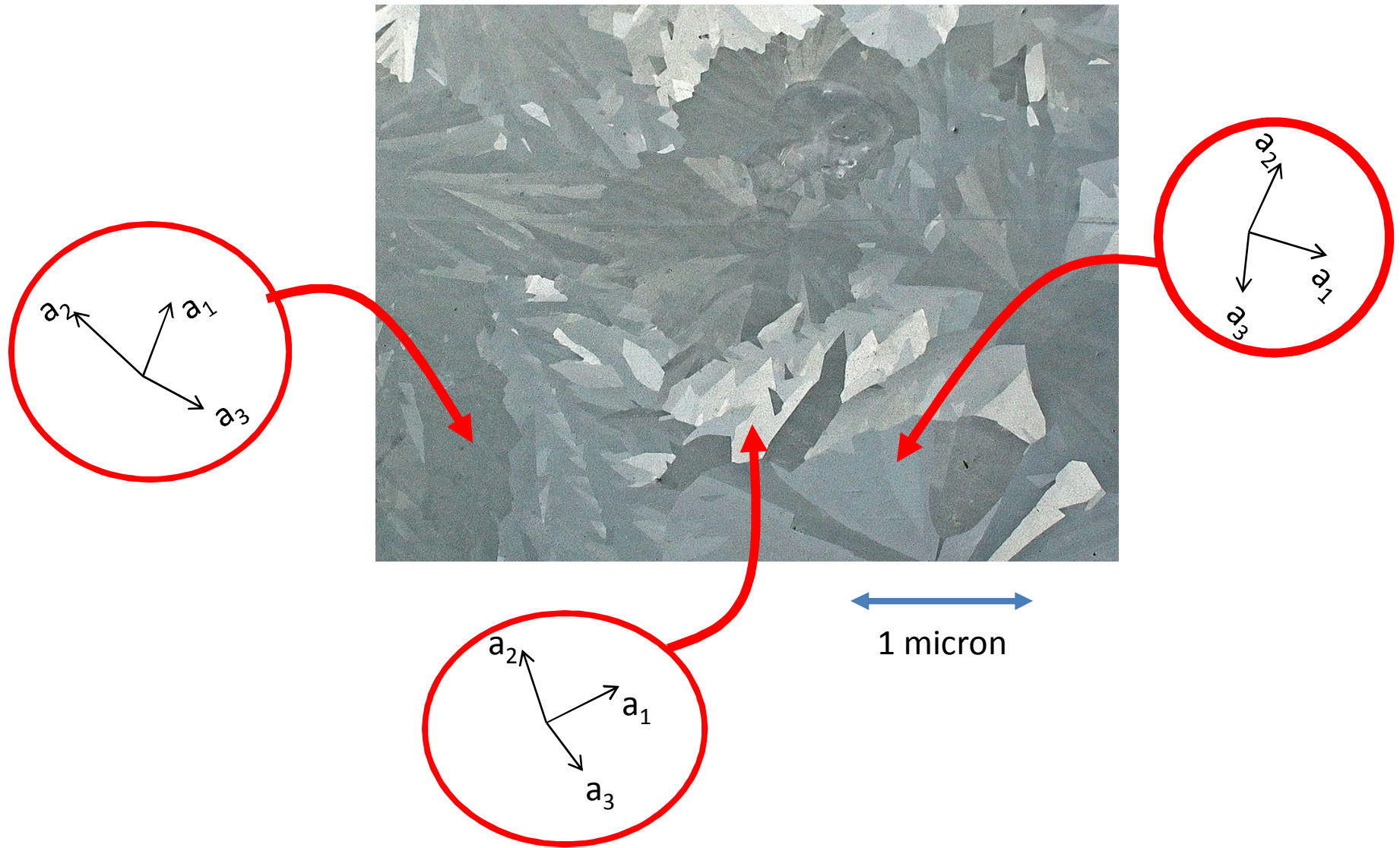
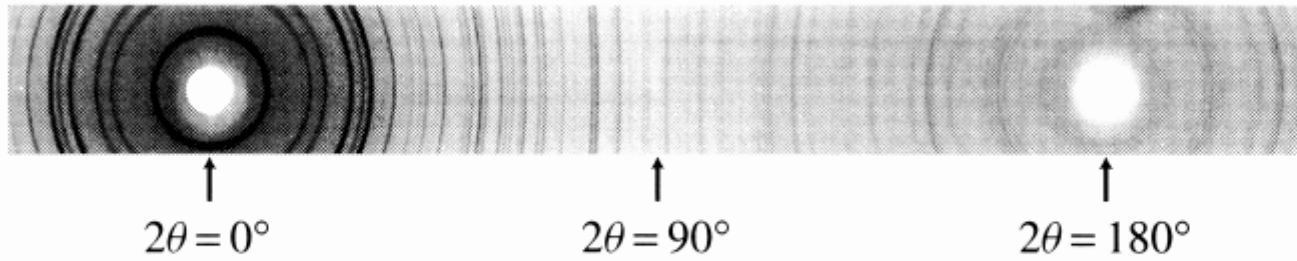


Nice single crystals (NaCl)

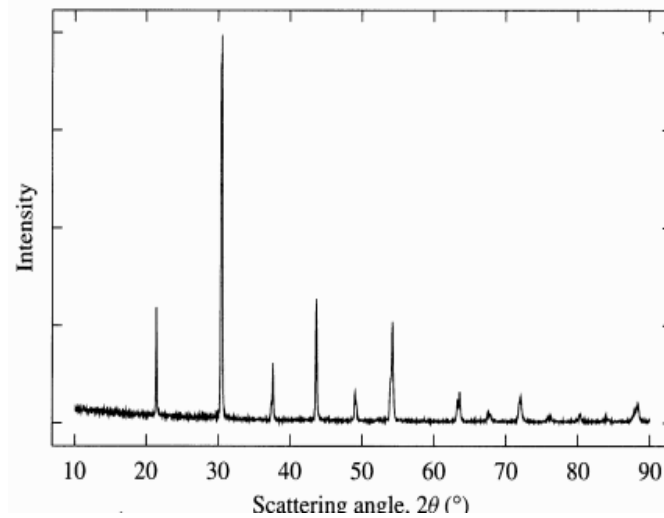
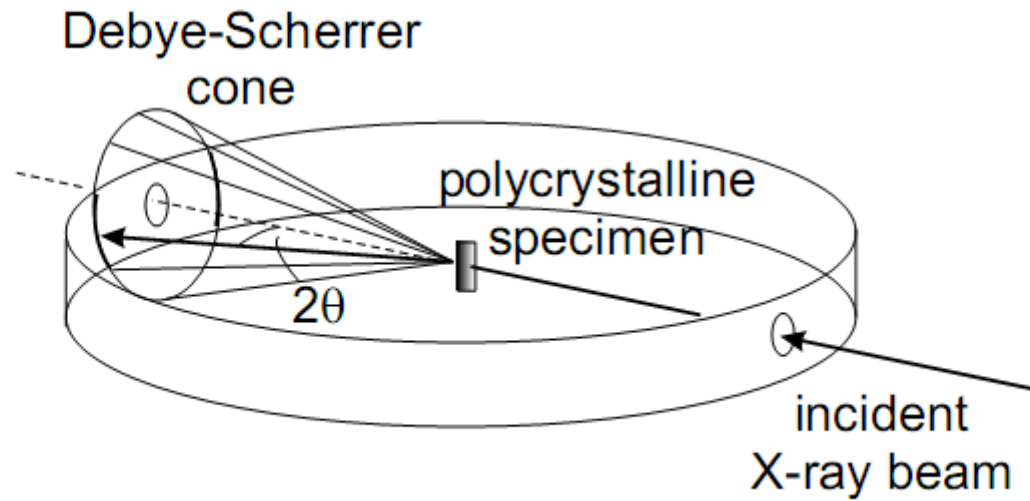




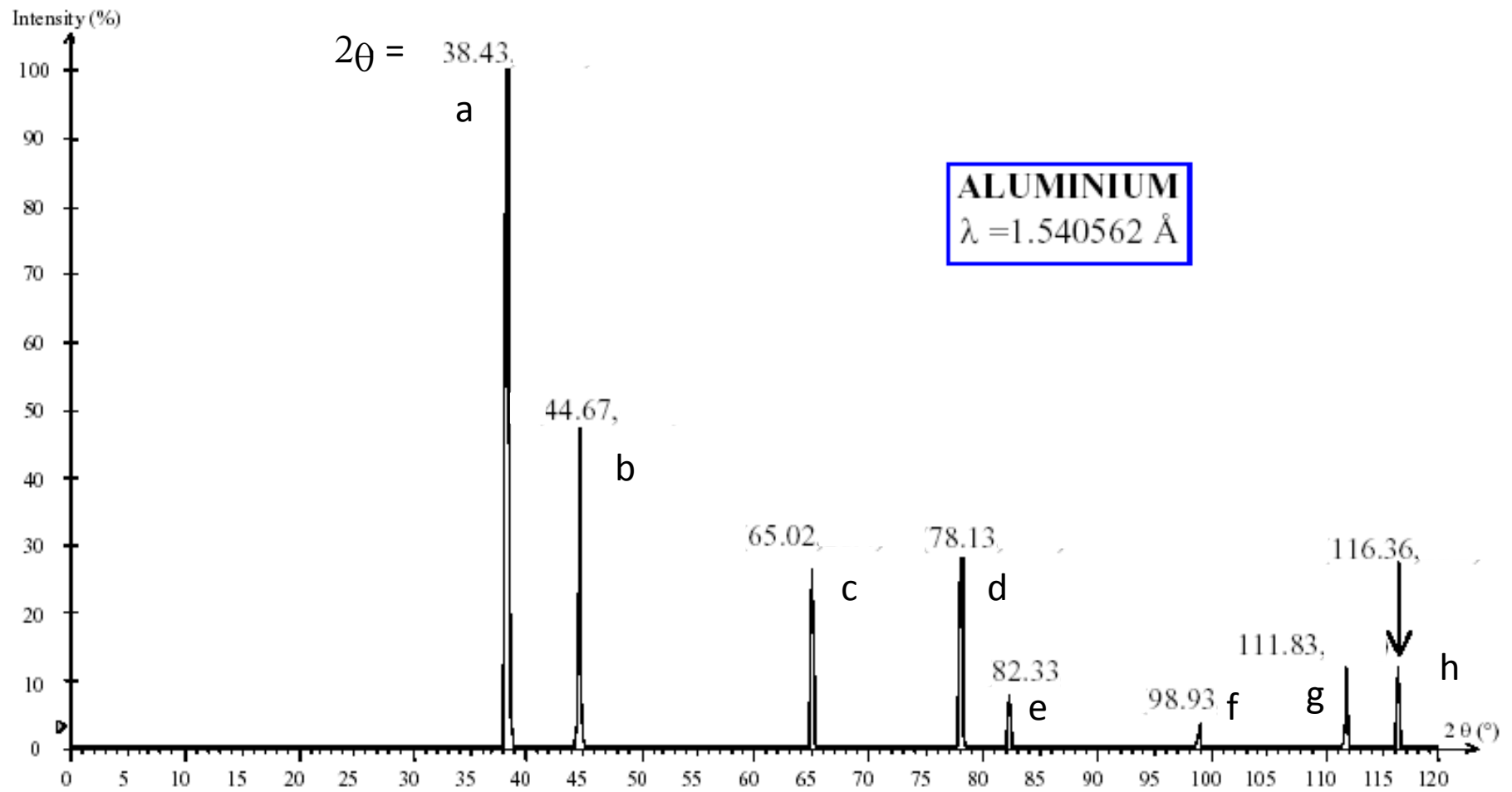
Polycrystalline Material



X-ray diffraction rings recorded on a photographic film



Consider the following XRD pattern for Aluminum, which was collected using $\text{CuK}\alpha$ radiation.



Scattering
Selection Rules

P = Primitive (simple) cubic
I = BCC
F = FCC

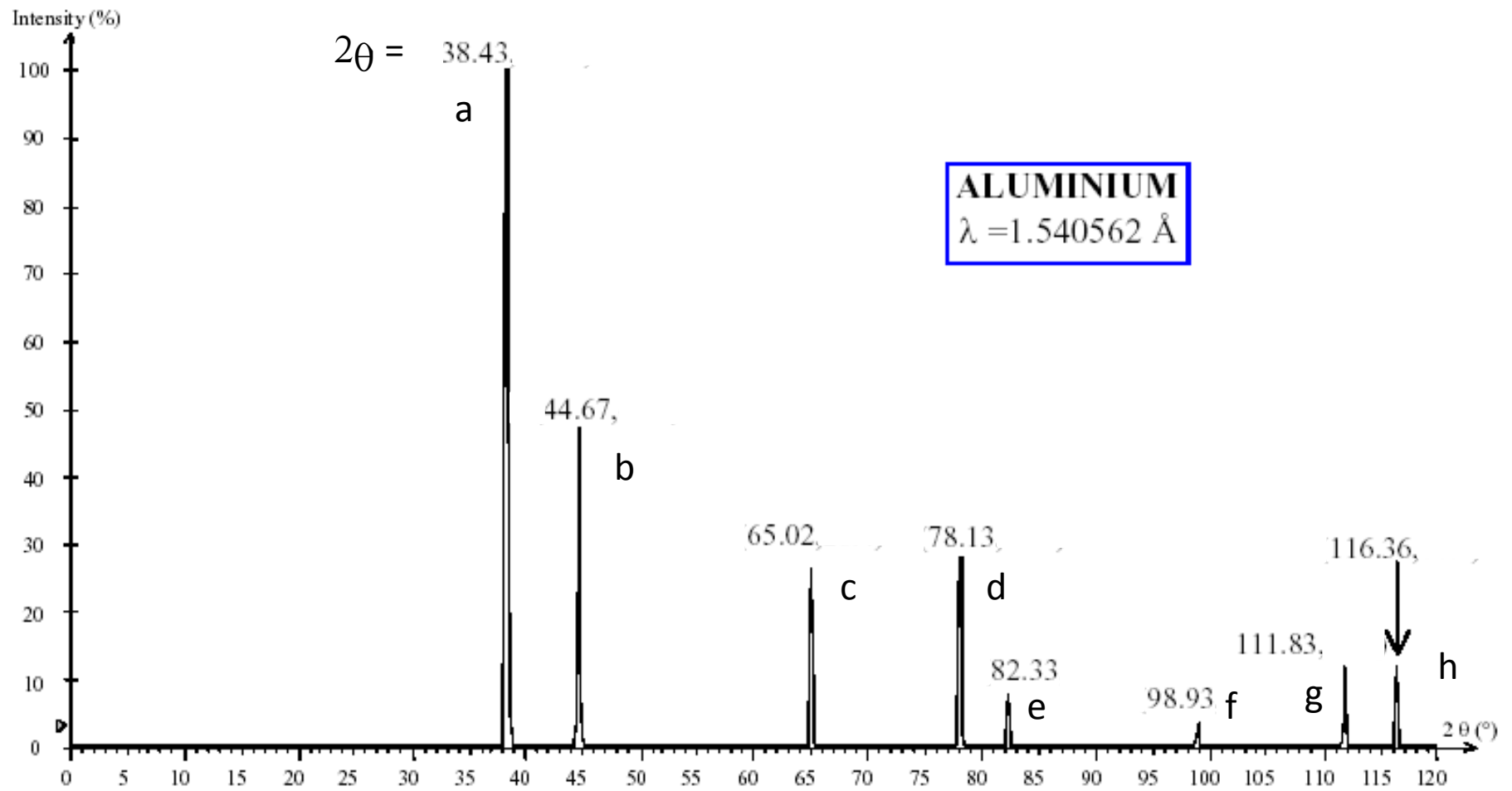
All hkl
 $h+k+l = \text{even}$
 h,k,l all even or all odd

$\{hkl\}$	$N=h^2+k^2+l^2$	P	I	F
100	1	*		
110	2	*	*	
111	3	*		*
200	4	*	*	*
210	5	*		
211	6	*	*	
---	7			
220	8	*	*	*
221, 300	9	*		
310	10	*	*	
311	11	*		*
222	12	*	*	*
320	13	*		
321	14	*	*	
---	15			
400	16	*	*	*

Sequence of
N values

P: 1,2,3,4,5,6,8,9, (= all integers excluding 7, 15, 23,...)
I: 2,4,6,8,10,12,14 ... (= even integers excluding 28, 60...)
F: 3,4,8,11,12,16,19,20

Consider the following XRD pattern for Aluminum, which was collected using $\text{CuK}\alpha$ radiation.



$$a = d\sqrt{h^2 + k^2 + l^2}$$

$$a^2/d^2 = h^2 + k^2 + l^2$$

$$N = h^2 + k^2 + l^2$$

$$d = \frac{\lambda}{2 \sin \theta}$$

$$d_a^2/d^2$$

$$3d^2/d_a^2$$

$$N$$

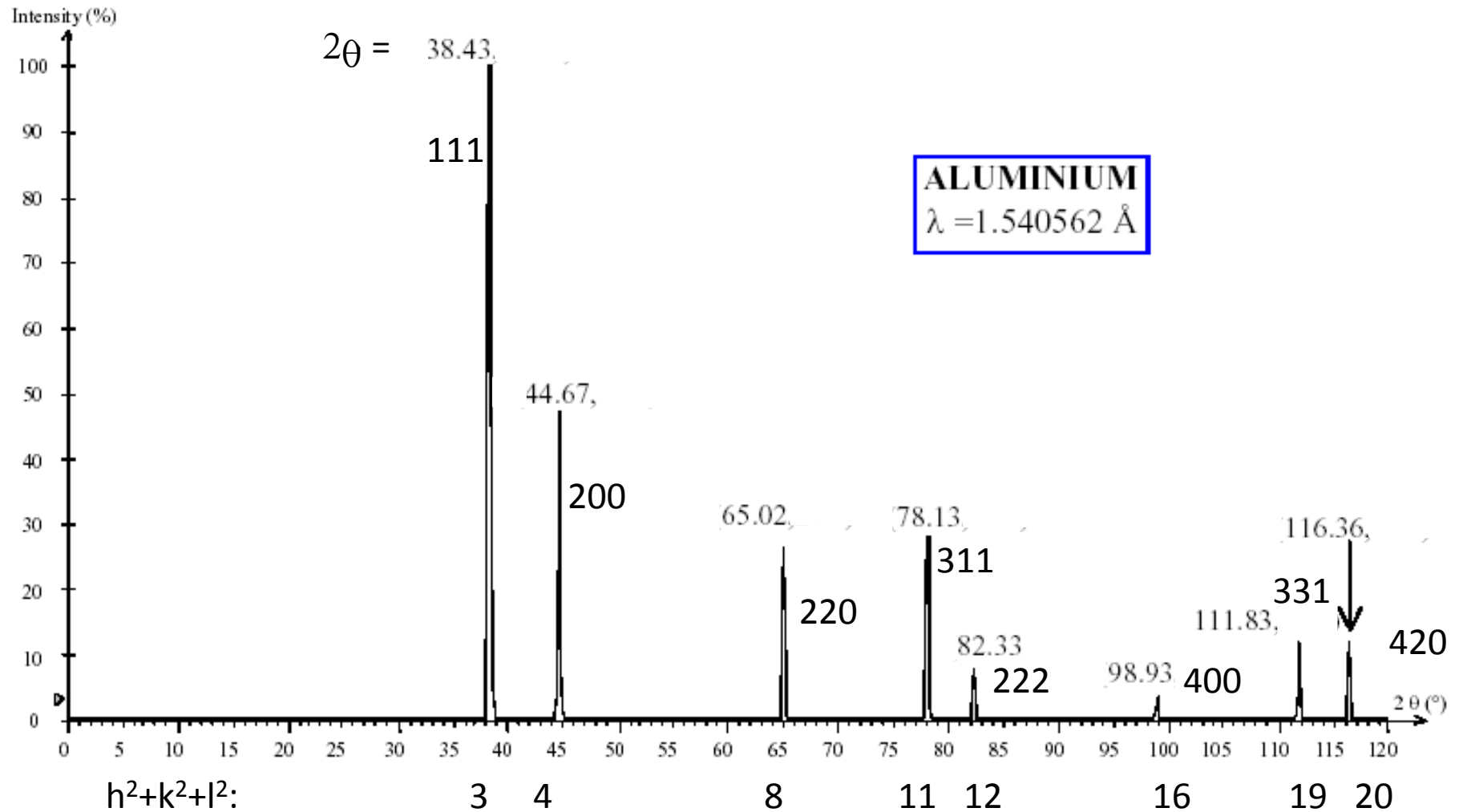
$$\{hkl\}$$

$$a$$

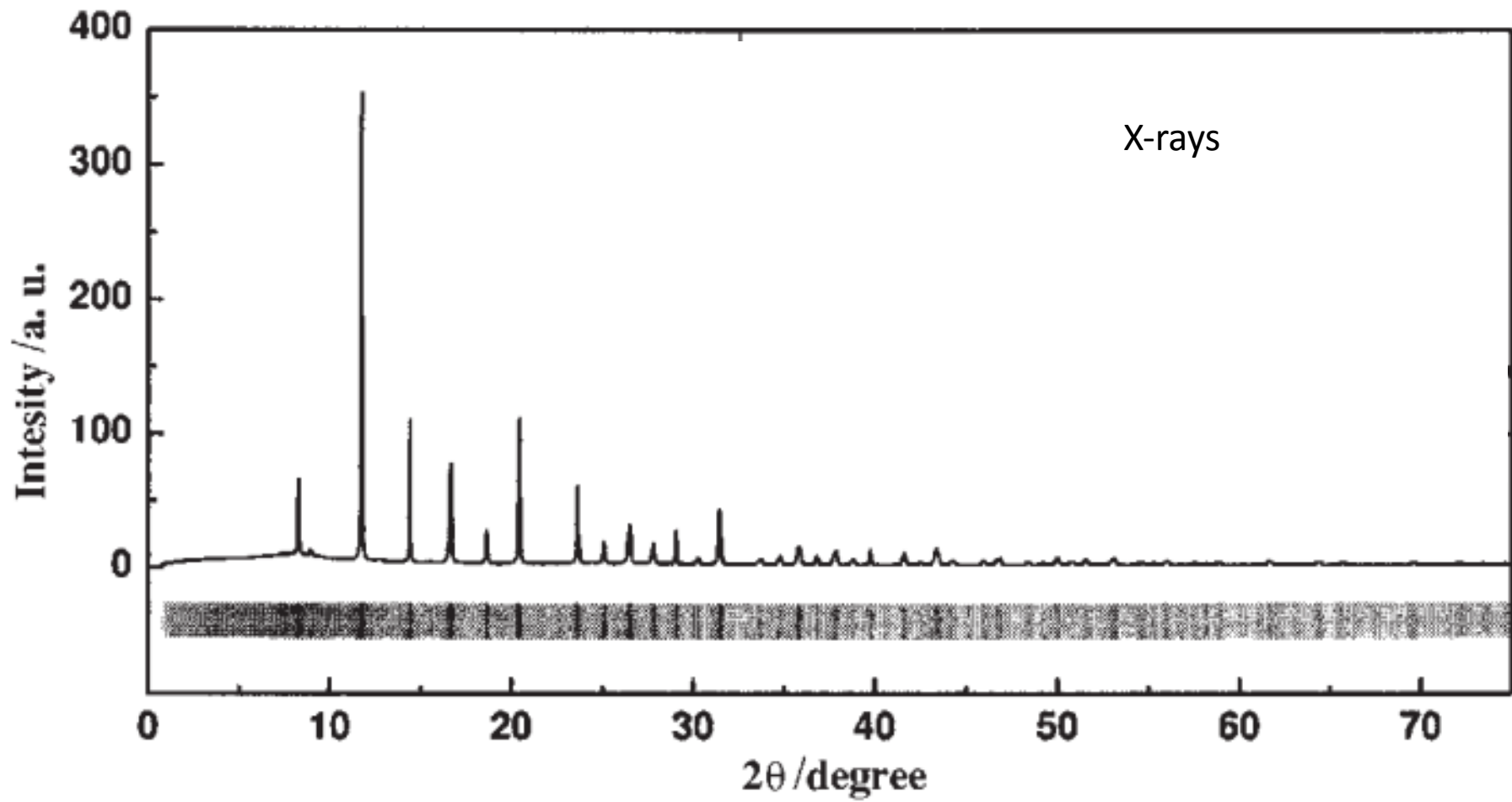
Peak	Angle 2θ	$d = \frac{\lambda}{2 \sin \theta}$	d_a^2/d^2	$3d^2/d_a^2$	N	$\{hkl\}$	a
a	38.43	2.3405Å	1.0000	3.0000	3	111	4.0538Å
b	44.67	2.0269Å	1.3333	3.9999	4	200	4.0539Å
c	65.02	1.4332Å	2.6667	8.0002	8	220	4.0538Å
d	78.13	1.2223Å	3.6666	10.9999	11	311	4.0538Å
e	82.33	1.1702Å	4.0000	12.0001	12	222	4.0538Å
f	98.93	1.0135Å	5.3327	15.9980	16	400	4.0541Å
g	111.83	0.9301Å	6.3327	18.9980	19	331	4.0540Å
h	116.36	0.9065Å	6.6657	19.9972	20	420	4.0541Å

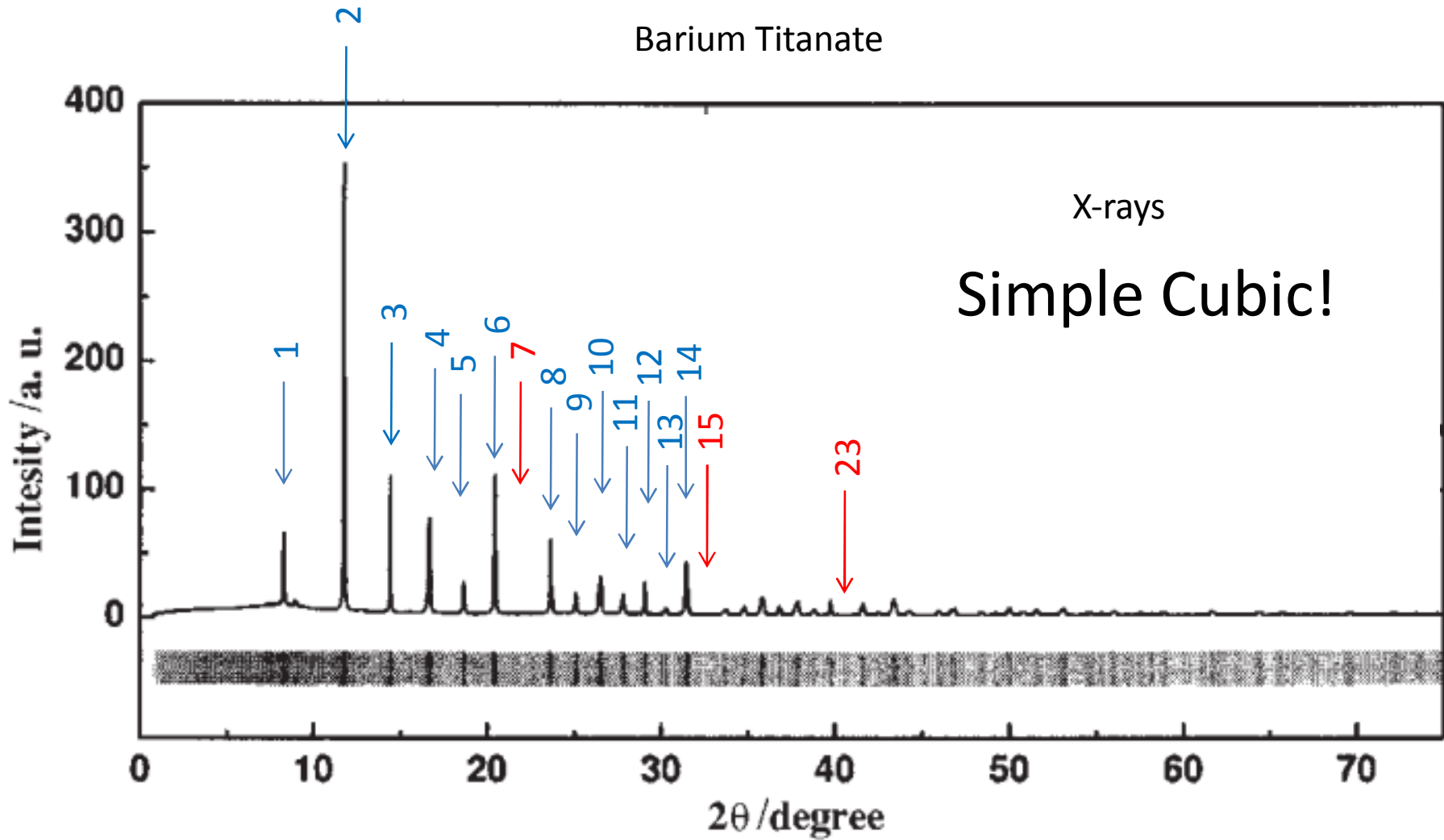
FCC! : h,k,l all even or all odd : N = 3,4,8,11,12 ...

Consider the following XRD pattern for Aluminum, which was collected using $\text{CuK}\alpha$ radiation.

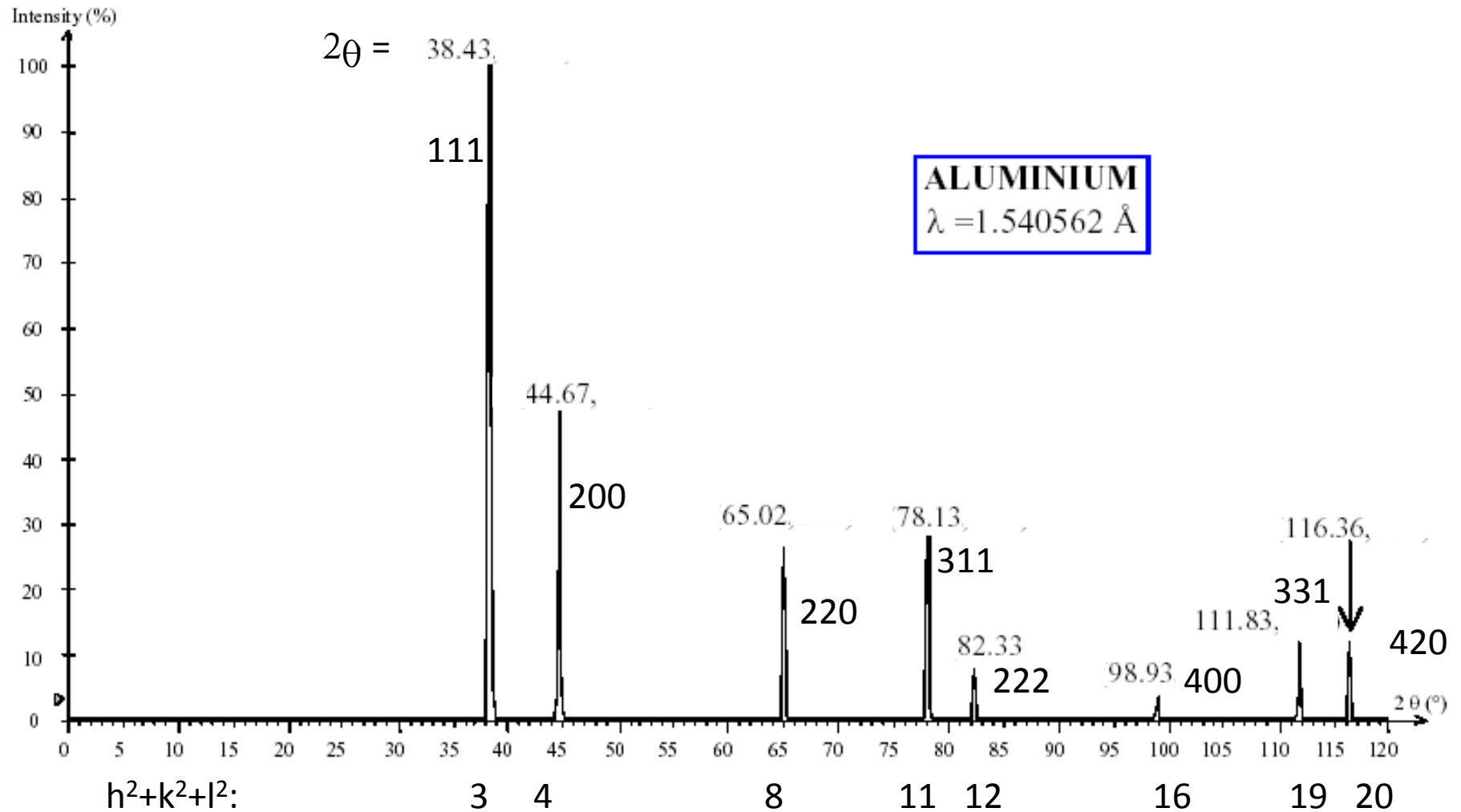


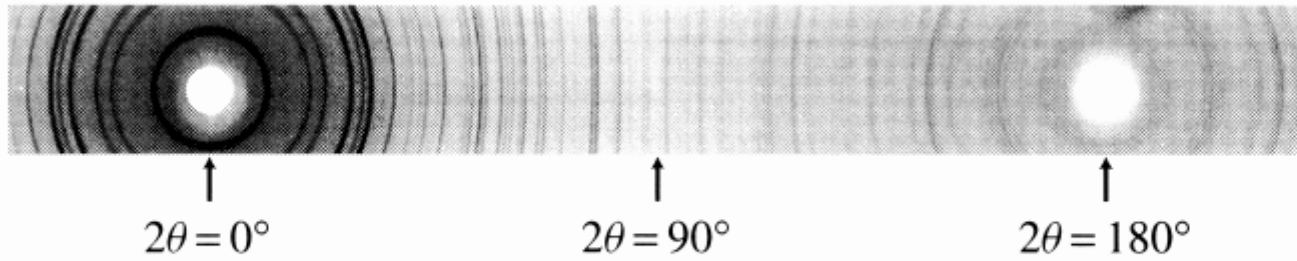
Barium Titanate



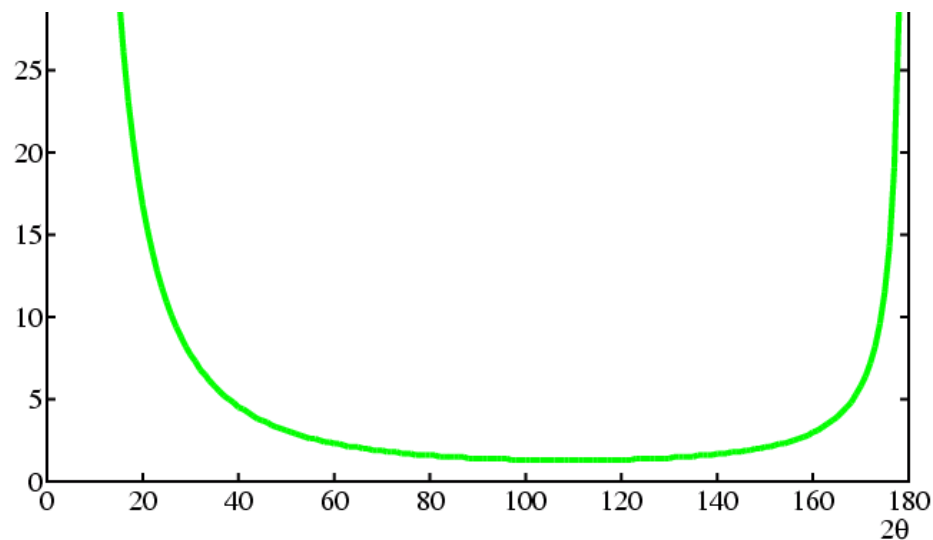
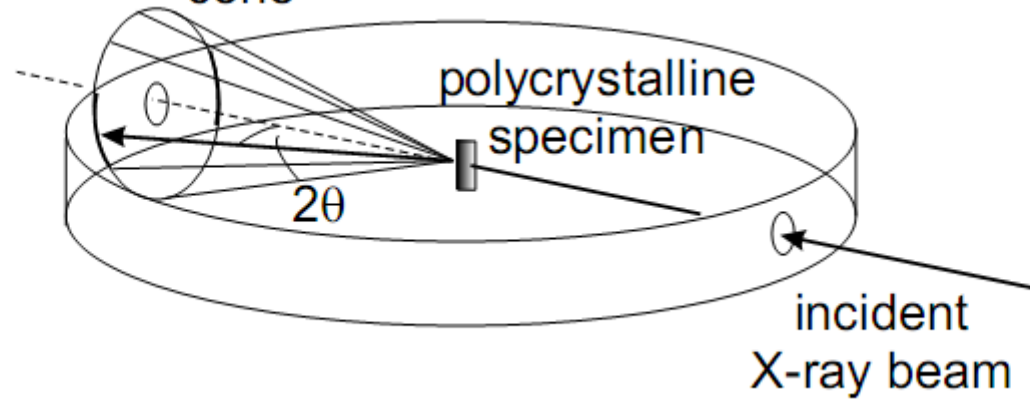


Consider the following XRD pattern for Aluminum, which was collected using $\text{CuK}\alpha$ radiation.



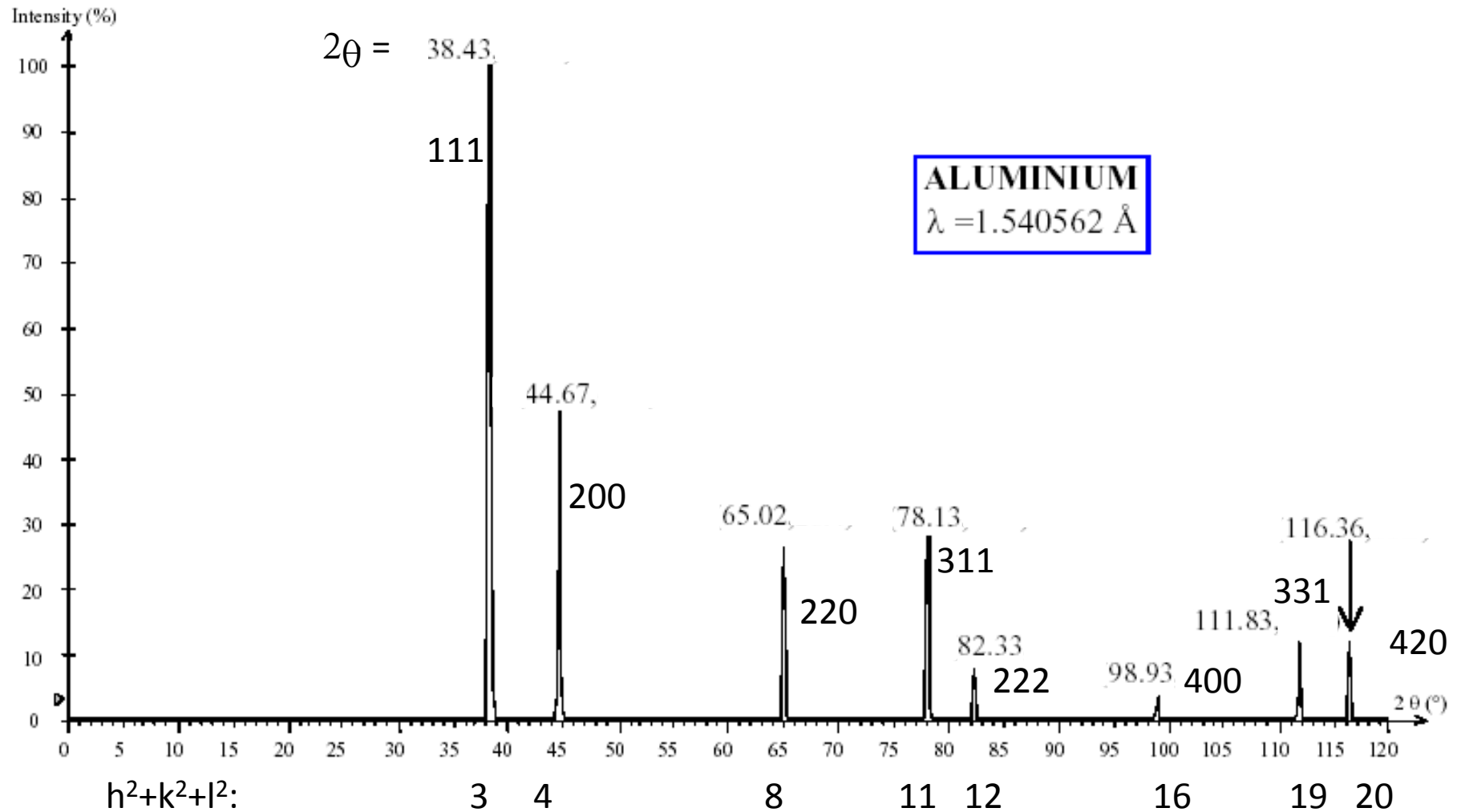


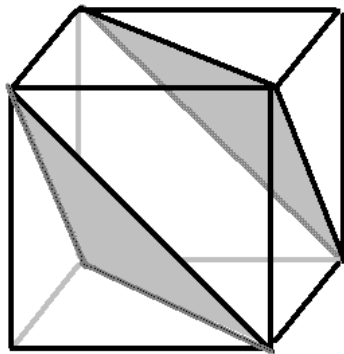
Debye-Scherrer
cone



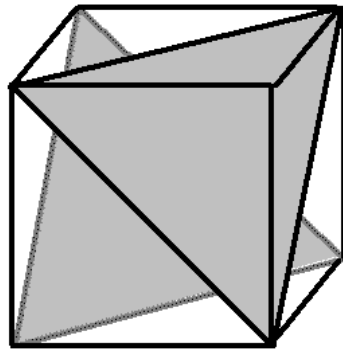
Geometric Lorentz Factor

Consider the following XRD pattern for Aluminum, which was collected using $\text{CuK}\alpha$ radiation.

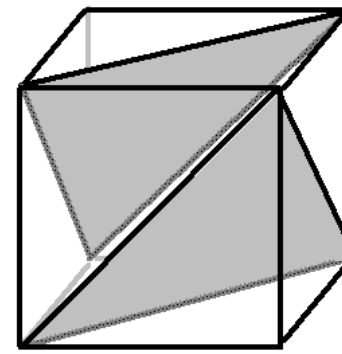




(111)



(1 $\bar{1}$ 1)



($\bar{1}$ 11)

Three of the 8 possible families of lattice planes in the $\{111\}$ class.

All of these faces show the same spacing between lattice planes.

In a powder experiment all of these scatter at the same angle

Intensity of scattering is weighted by the multiplicity

Scattering
Selection Rules

P = Primitive (simple) cubic
I = BCC
F = FCC

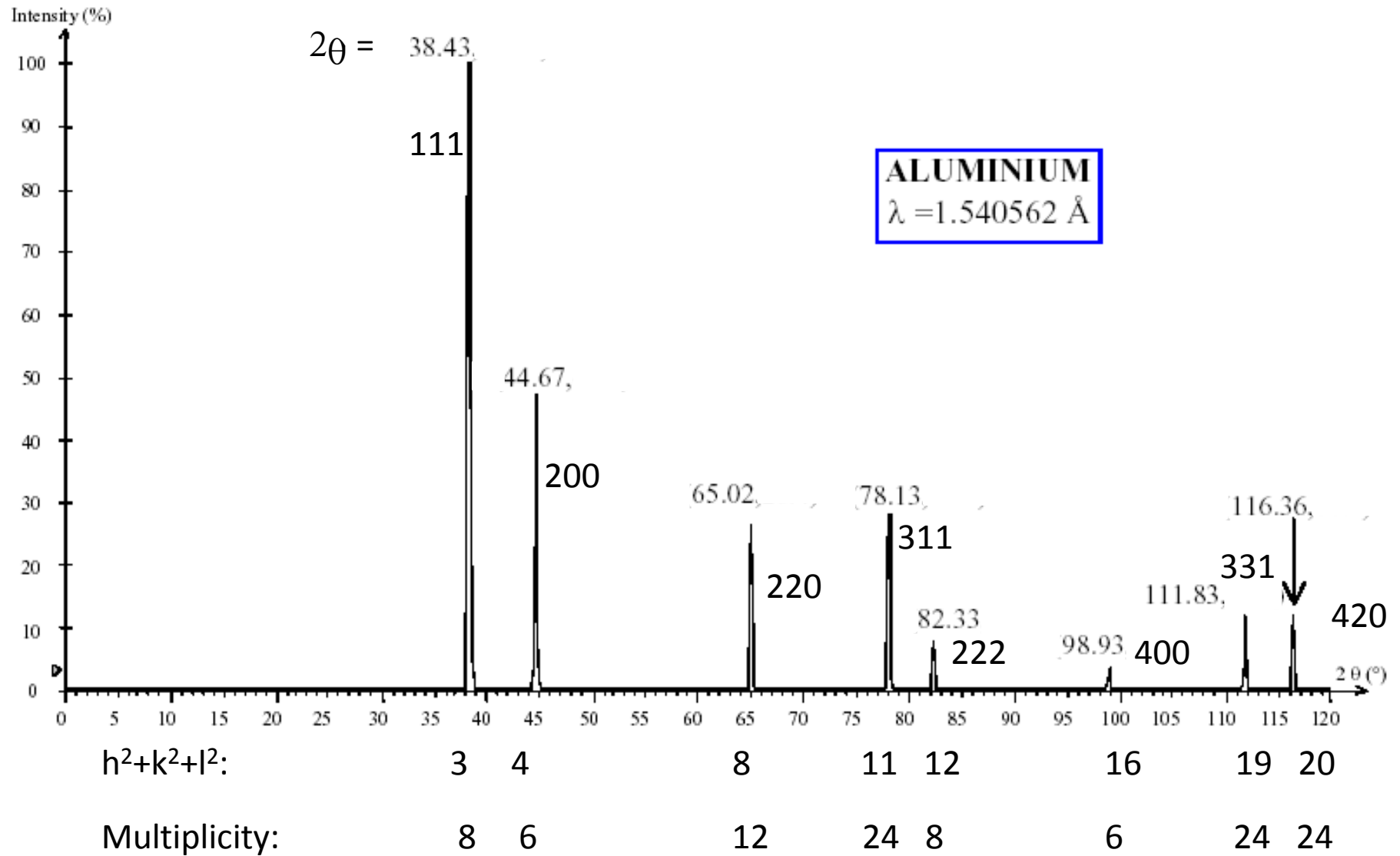
All hkl
 $h+k+l = \text{even}$
 h,k,l all even or all odd

$\{hkl\}$	$N=h^2+k^2+l^2$	Multiplicity	P	I	F
100	1	6	*		
110	2	12	*	*	
111	3	8	*		*
200	4	6	*	*	*
210	5	24	*		
211	6	24	*	*	
---	7	--			
220	8	12	*	*	*
221, 300	9	24+6	*		
310	10	24	*	*	
311	11	24	*		*
222	12	8	*	*	*
320	13	24	*		
321	14	48	*	*	
---	15	--			
400	16	6	*	*	*

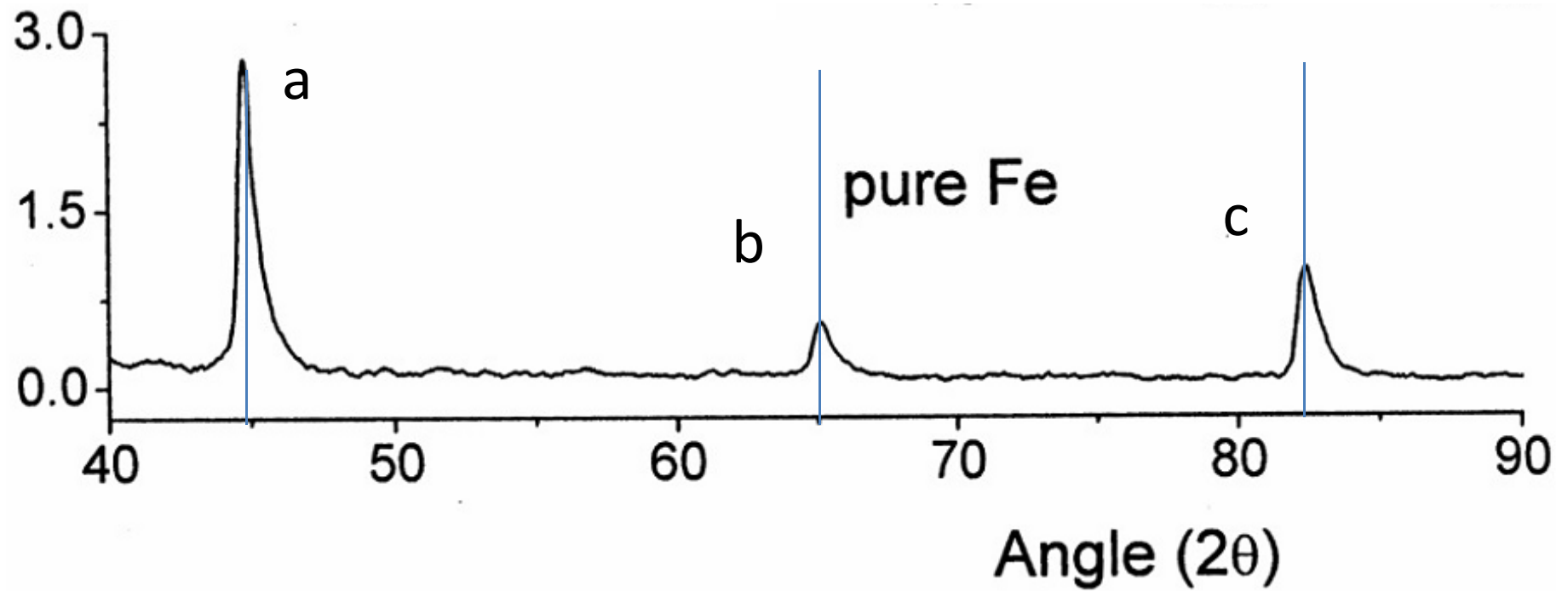
Sequence of
N values

P: 1,2,3,4,5,6,8,9, (= all integers excluding 7, 15, 23,...)
I: 2,4,6,8,10,12,14 ... (= even integers excluding 28, 60...)
F: 3,4,8,11,12,16,19,20

Consider the following XRD pattern for Aluminum, which was collected using $\text{CuK}\alpha$ radiation.



X-ray $\lambda=1.54$ Angstrom



$$a^2/d^2 = h^2 + k^2 + l^2$$

$$d = \frac{\lambda}{2 \sin \theta} \quad d_a^2/d^2$$

Peak	Angle 2θ	d	d_a^2/d^2
a	44.7	2.03Å	1.00
b	65.2	1.43Å	2.01
c	82.7	1.17Å	3.02

$$N = h^2 + k^2 + l^2$$

N = 1, 2, 3 Simple Cubic {hkl} = {100}, {110}, {111}

OR

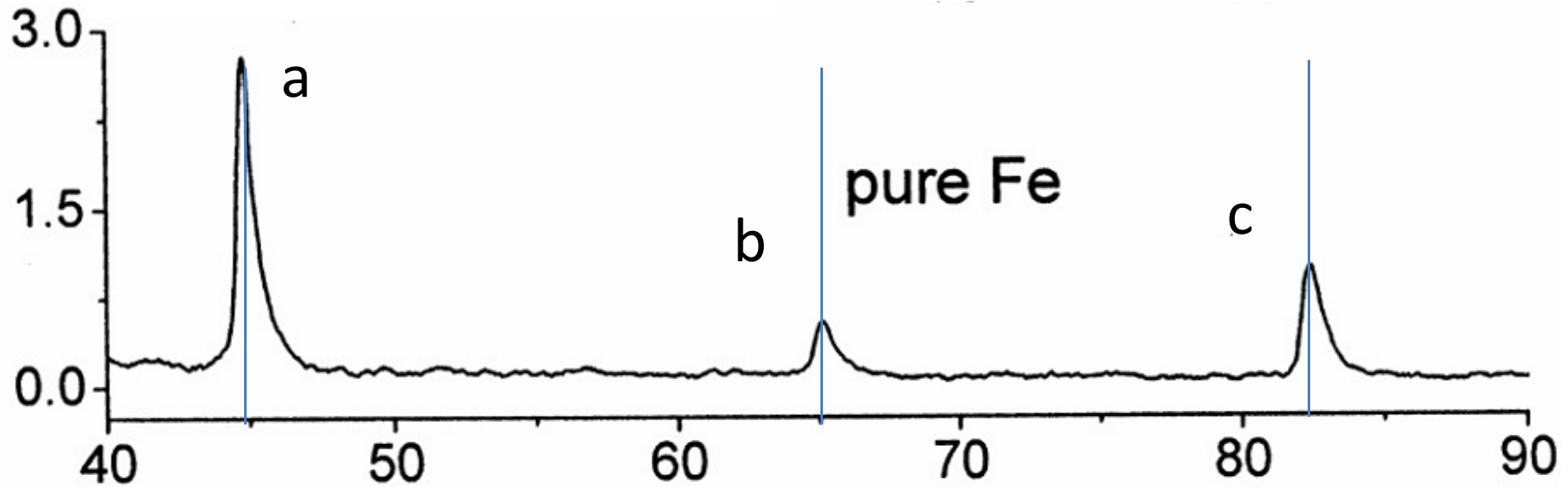
N = 2, 4, 6 BCC {hkl} = {110}, {200}, {211}

$$a = d\sqrt{h^2 + k^2 + l^2} = 2.03 \text{ \AA} \quad \text{if we choose simple cubic}$$

$$= 2.86 \text{ \AA} \quad \text{if we choose BCC}$$

Calculated Atomic Densities : $1/(2.03 \text{ \AA})^3$ for simple cubic vs $2/(2.86 \text{ \AA})^3$ for BCC

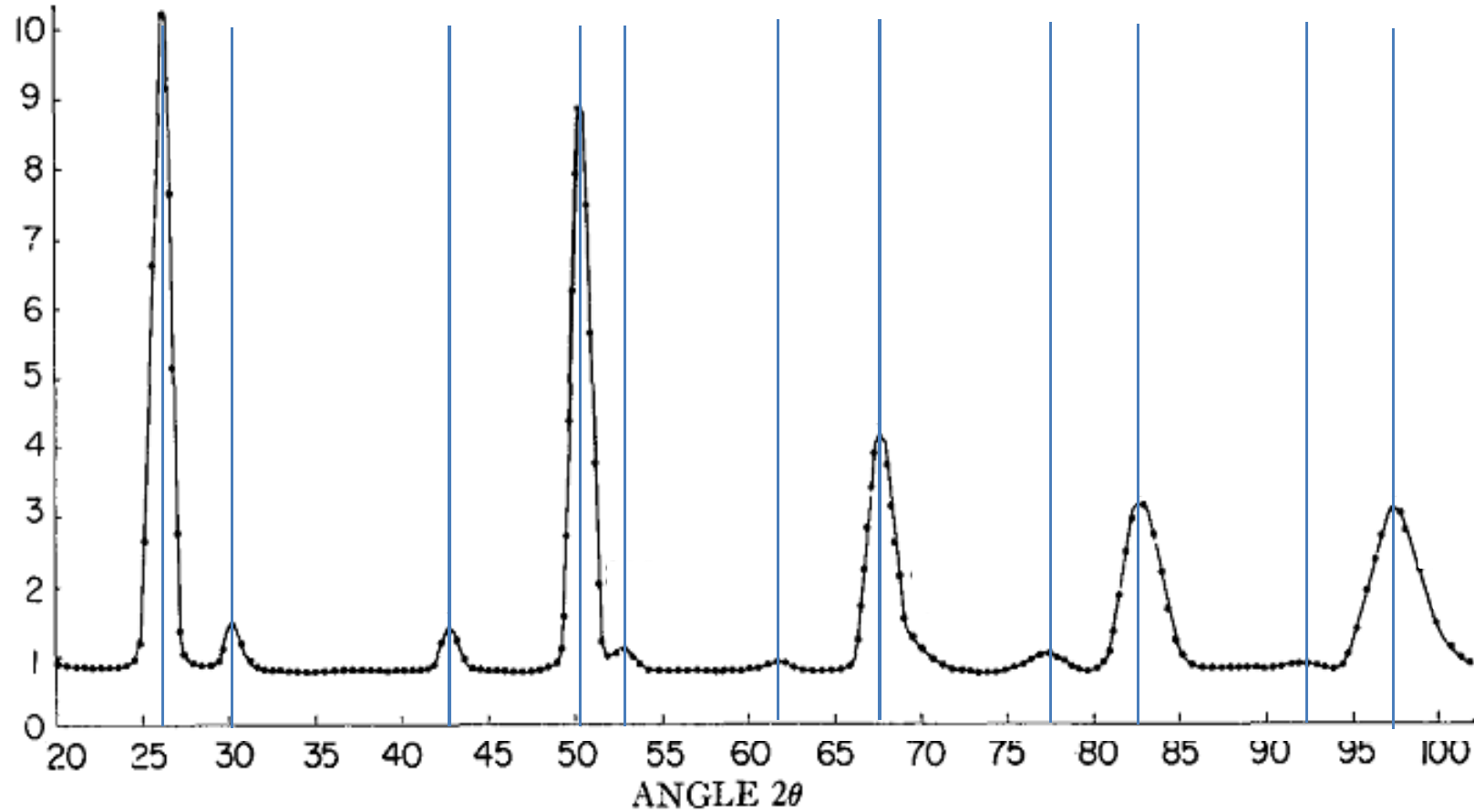
X-ray $\lambda=1.54$ Angstrom



Simple Cubic	{100}	{110}	{111}
Multiplicity	6	12	8
BCC	{110}	{200}	{211}
Multiplicity	12	6	24

Since form factor is decaying with increased angle (and additional geometric factors also decaying) , c having much more intensity than b is only consistent with BCC

$\lambda = 1.09$ Angstrom TiC neutron powder diffraction



Sidhu et al, J. Applied Physics, 30 1323 (1959).

$$a^2/d^2 = h^2 + k^2 + l^2$$

$$a = d\sqrt{h^2 + k^2 + l^2}$$

$$N = h^2 + k^2 + l^2$$



$$d = \frac{\lambda}{2 \sin \theta}$$

$$d_a^2/d^2$$

$$3d^2/d_a^2$$

$$N$$

$$\{hkl\}$$

$$a$$

Peak	Angle 2θ	$d = \frac{\lambda}{2 \sin \theta}$	d_a^2/d^2	$3d^2/d_a^2$	N	$\{hkl\}$	a
a	26	2.42Å	1.00	3.00	3	111	4.20Å
b	30.1	2.10Å	1.33	4.00	4	200	4.20Å
c	42.8	1.49Å	2.63	7.89	8	220	4.22Å
d	50.2	1.28Å	3.56	10.67	11	311	4.26Å
e	52.8	1.23Å	3.91	11.72	12	222	4.25Å
f	62.4	1.05Å	5.30	15.91	16	400	4.21Å
g	67.6	0.98Å	6.12	18.35	19	331	4.27Å
h	70	0.95Å	6.50	19.50	20	420	4.25Å

FCC! : h,k,l all even or all odd : N = 3,4,8,11,12 ...