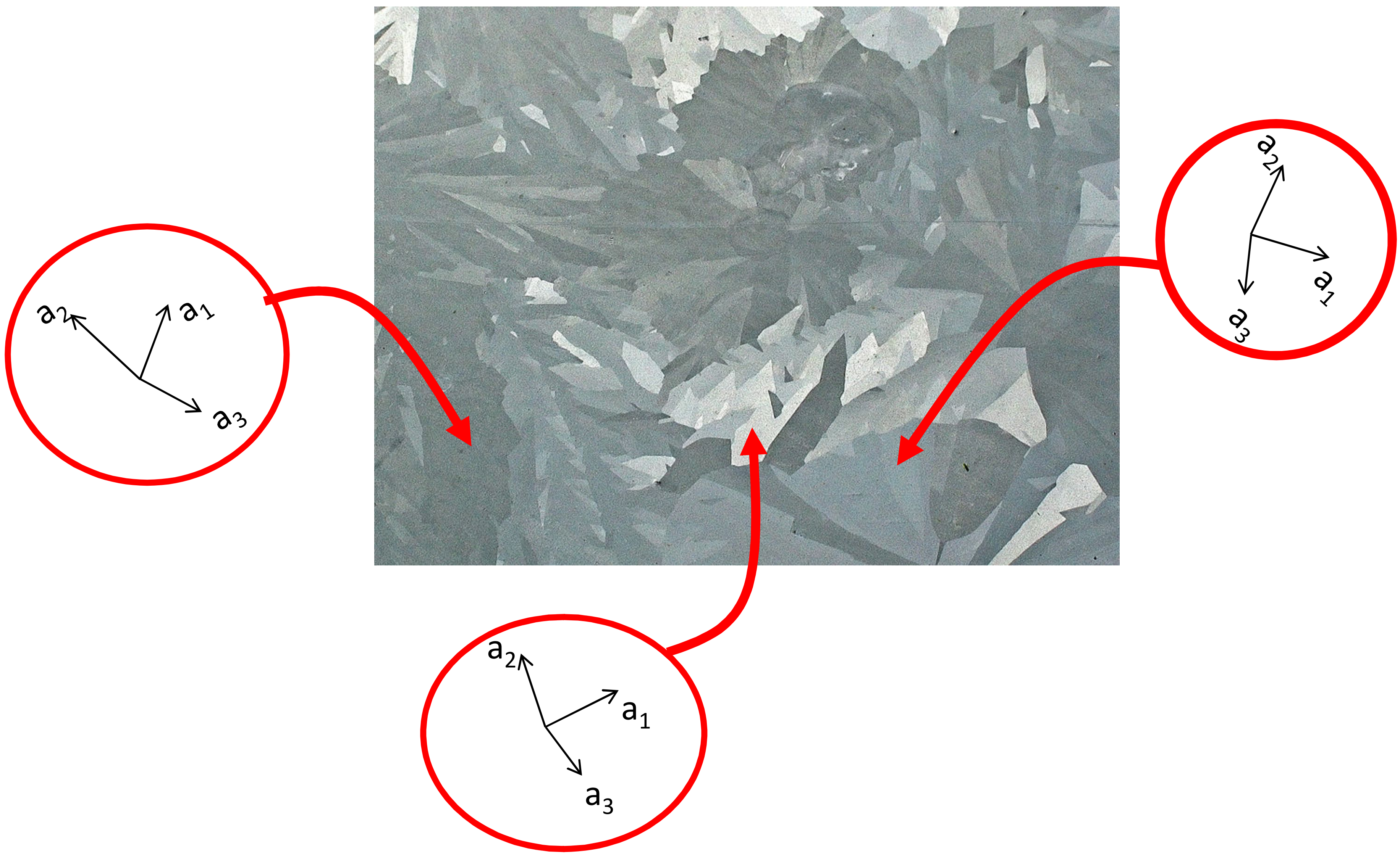
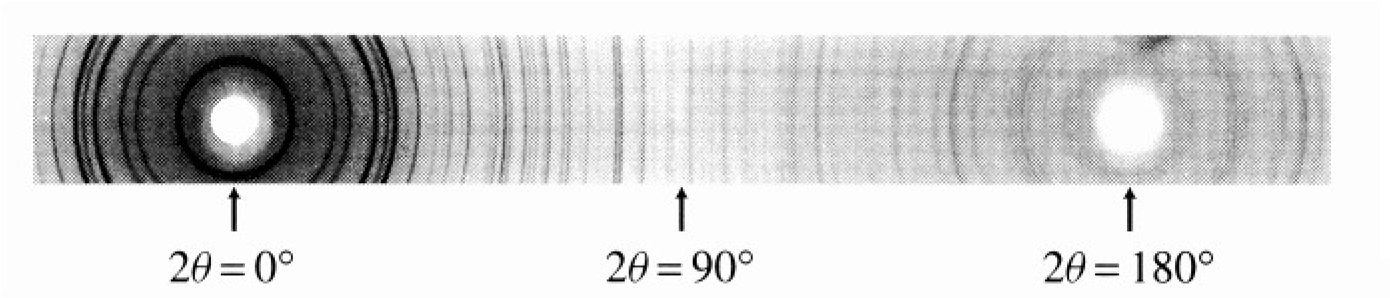
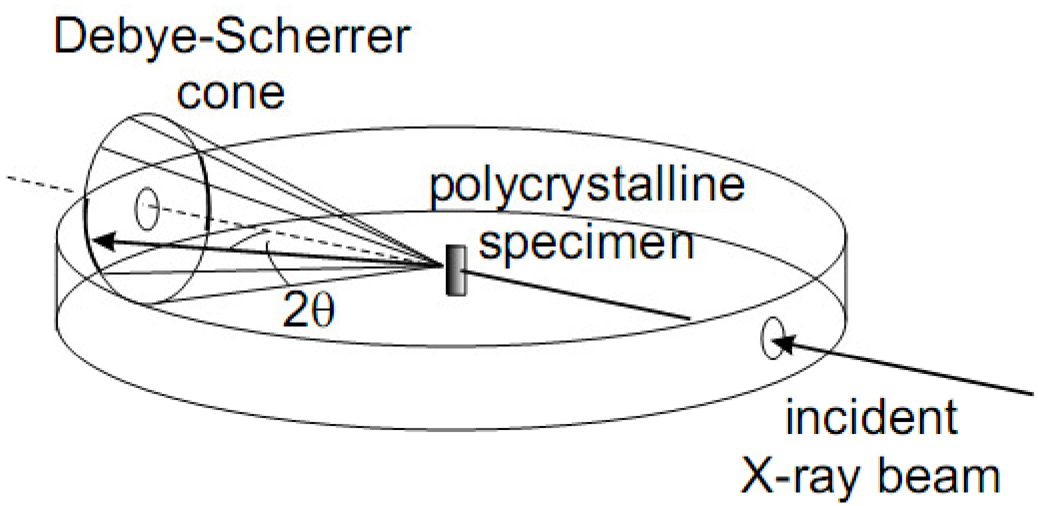
Slides
Condensed Matter Physics
Lecture 13



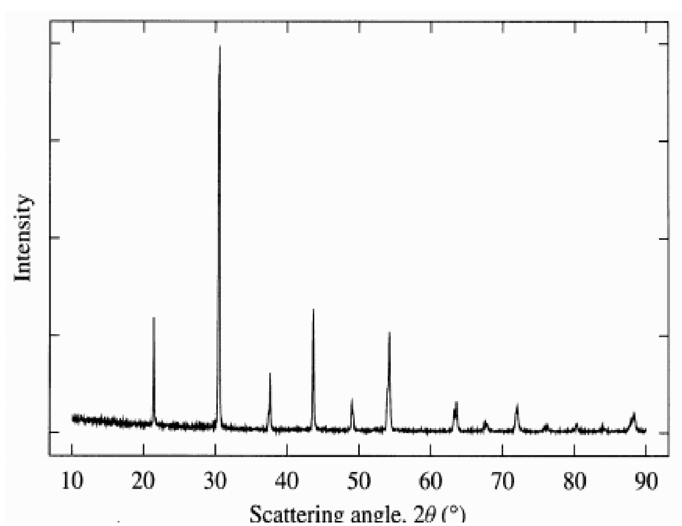
Polycrystalline Material



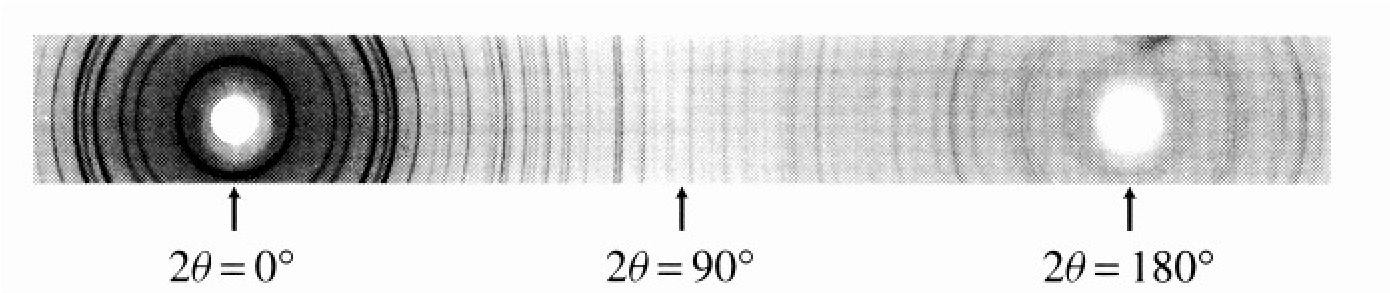
$2\theta = 0°$
$2\theta = 90°$
$2\theta = 180°$



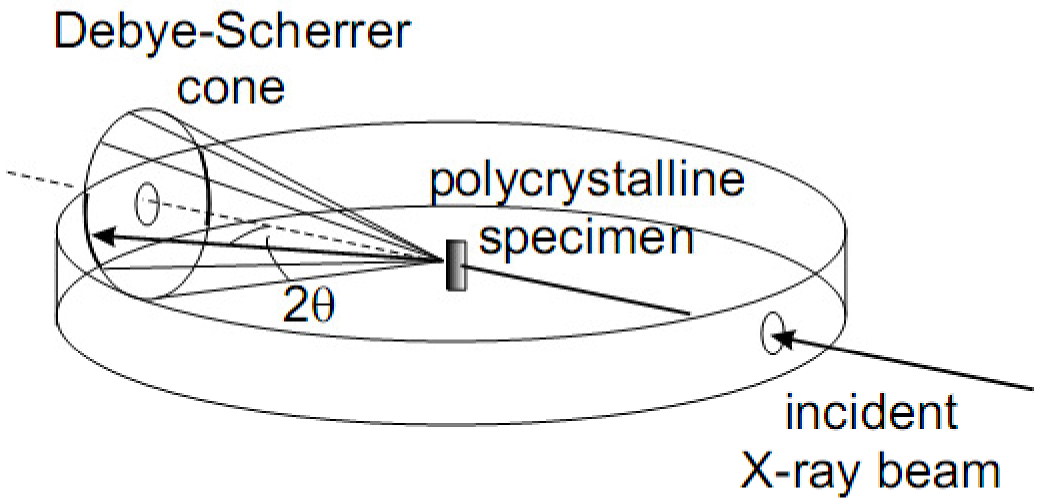
Debye-Scherrer cone
polycrystalline specimen
2θ
incident X-ray beam

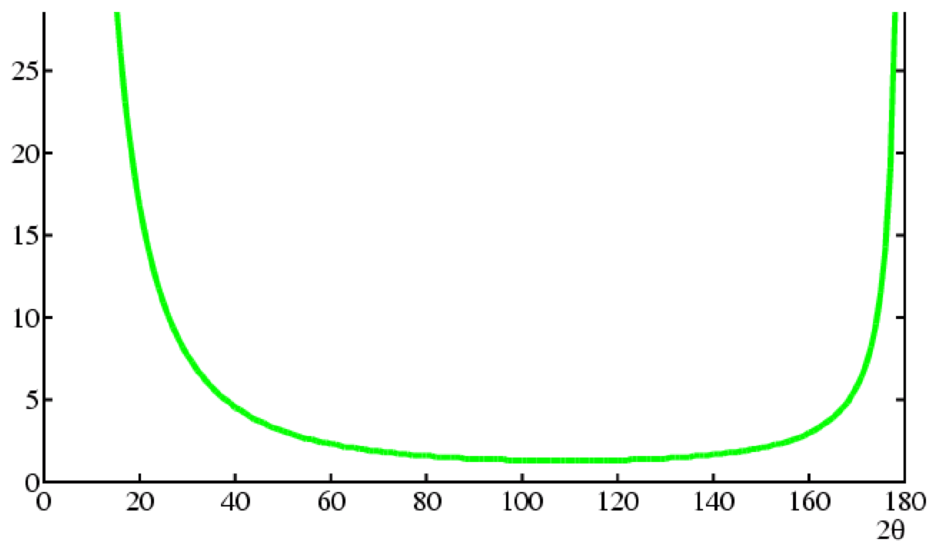


Intensity
10
20
30
40
50
60
70
80
90
Scattering angle, 2θ (°)



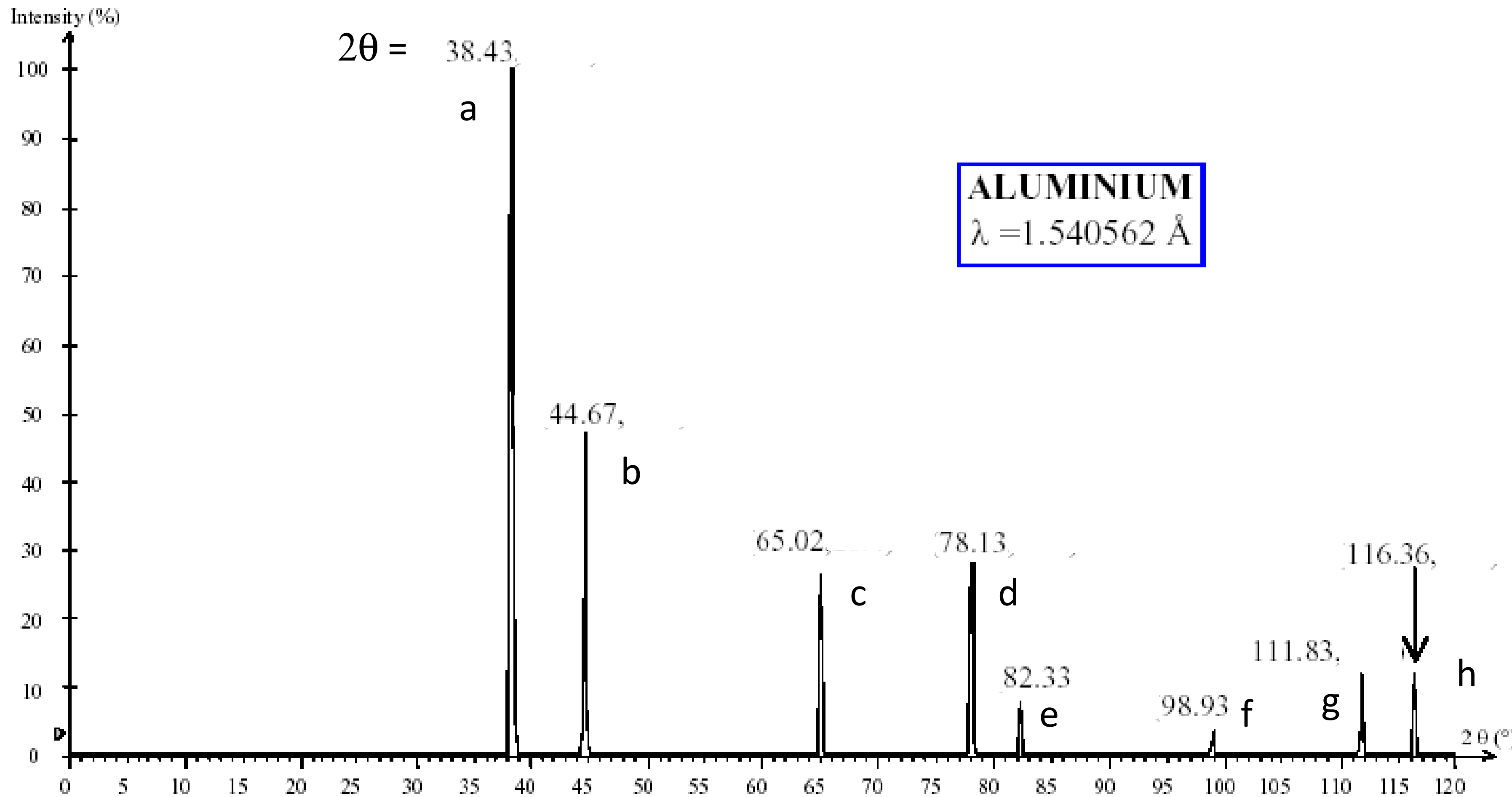
X-ray diffraction rings recorded on a photographic film





Geometric Lorentz Factor

Consider the following XRD pattern for Aluminum, which was collected using CuKα radiation.



Scattering Selection Rules

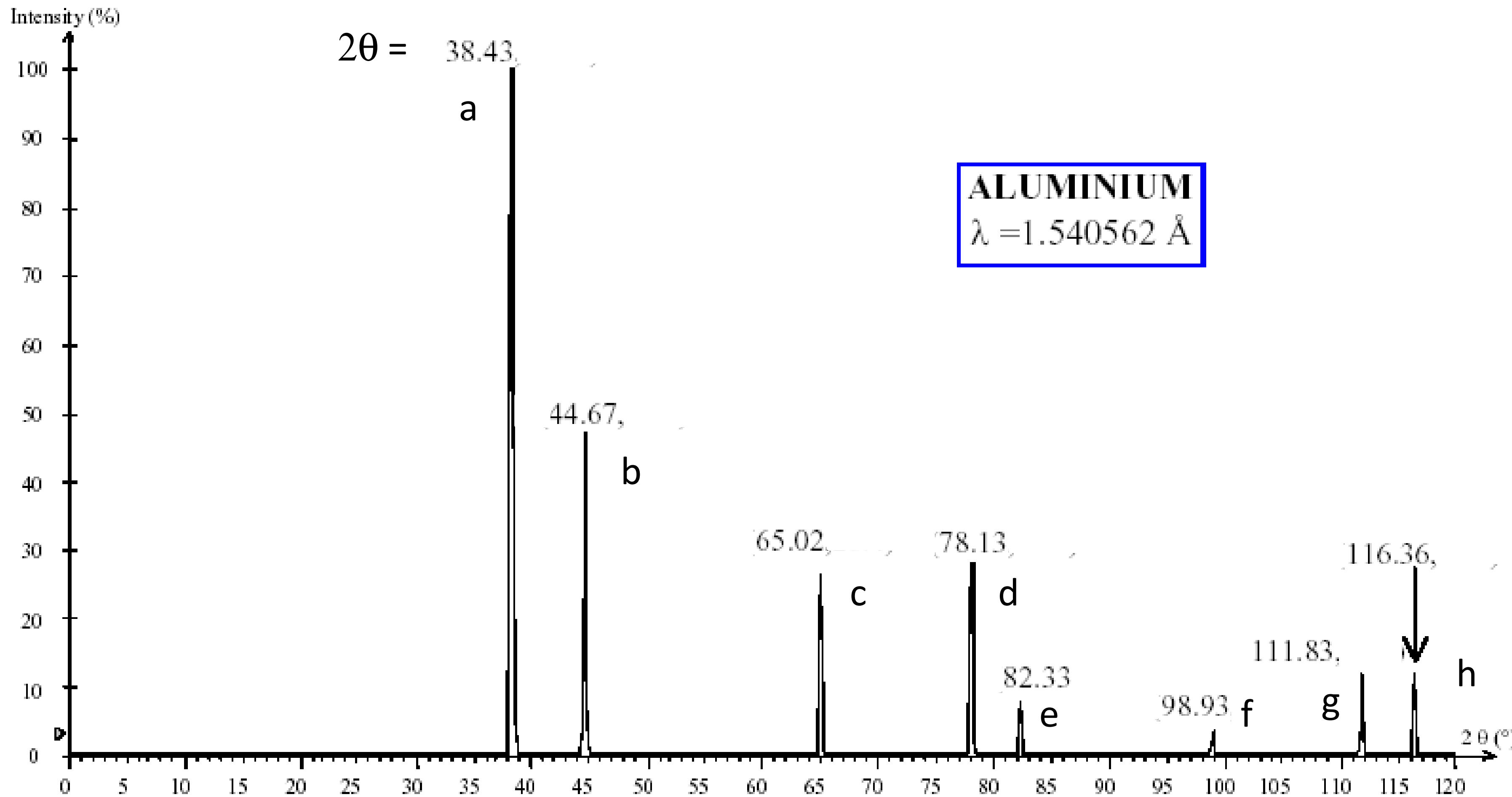
P = Primitive (simple) cubic — All *hkl*
I = BCC — $h+k+l$ = even
F= FCC — h,k,l all even or all odd

{*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 CuKα radiation.



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

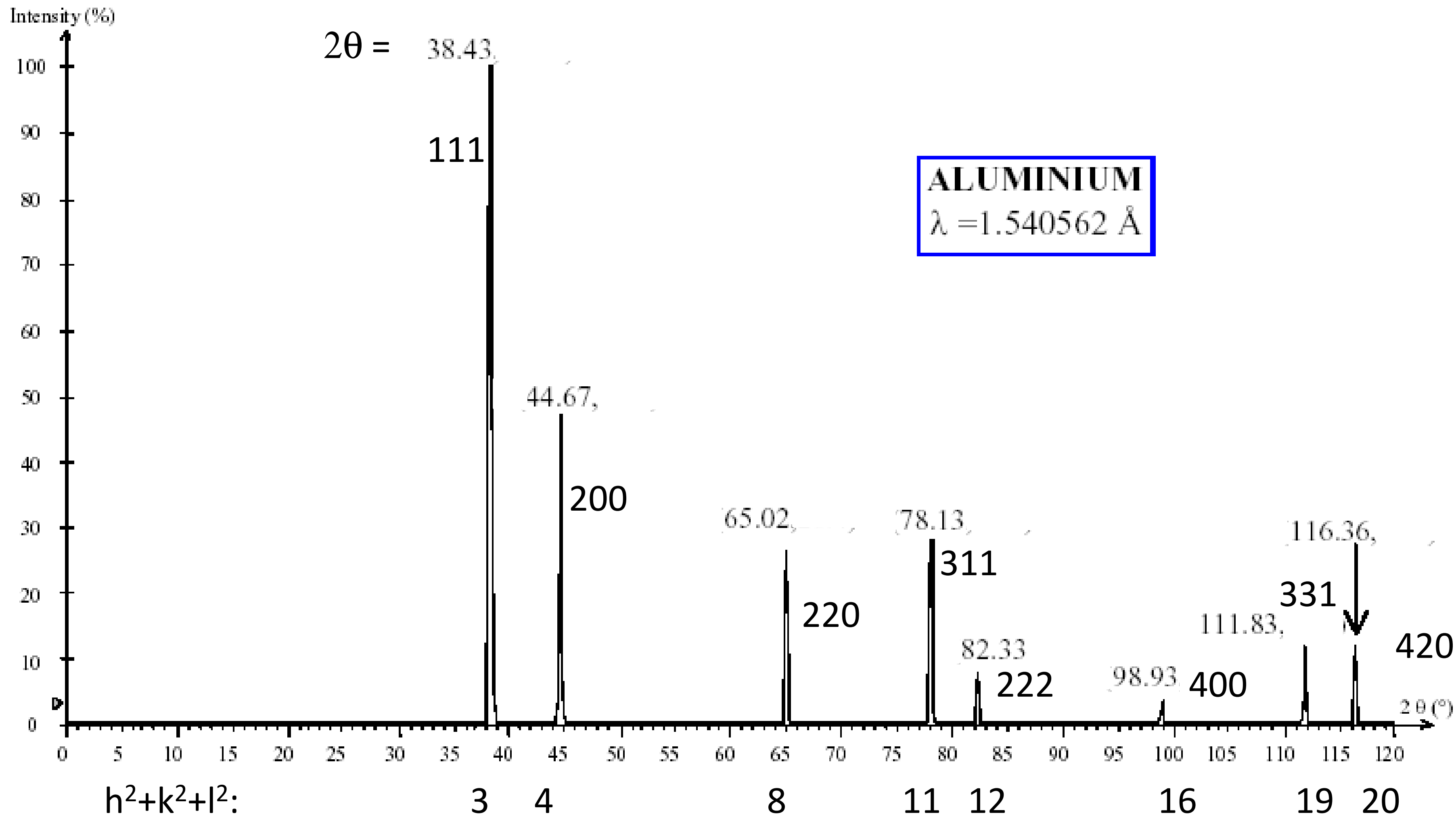
$$a^2/d^2 = h^2 + k^2 + l^2$$

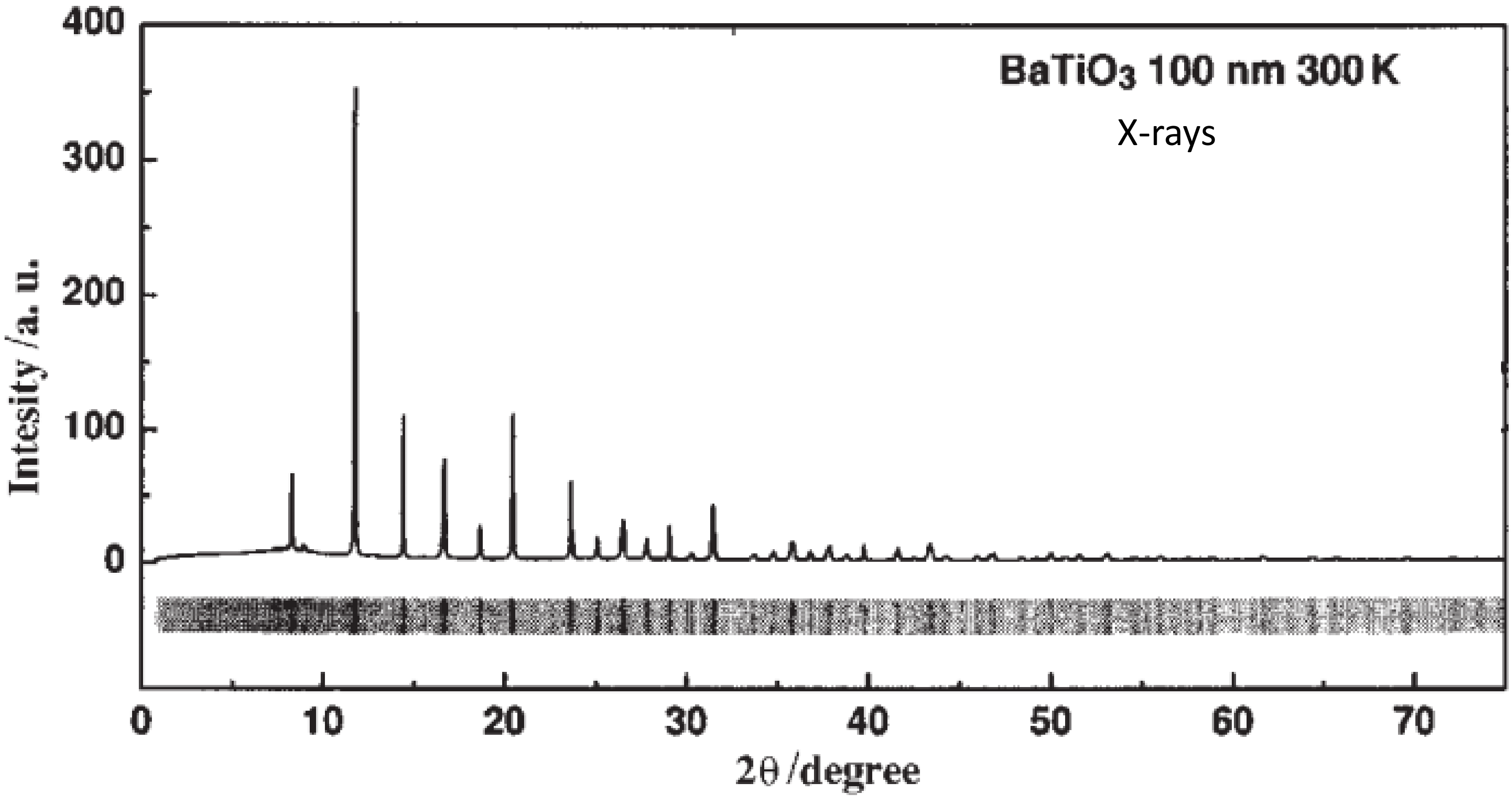
$$N = h^2 + k^2 + l^2$$

Peak	Angle 2θ	$d = \dfrac{\lambda}{2\sin\theta}$	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

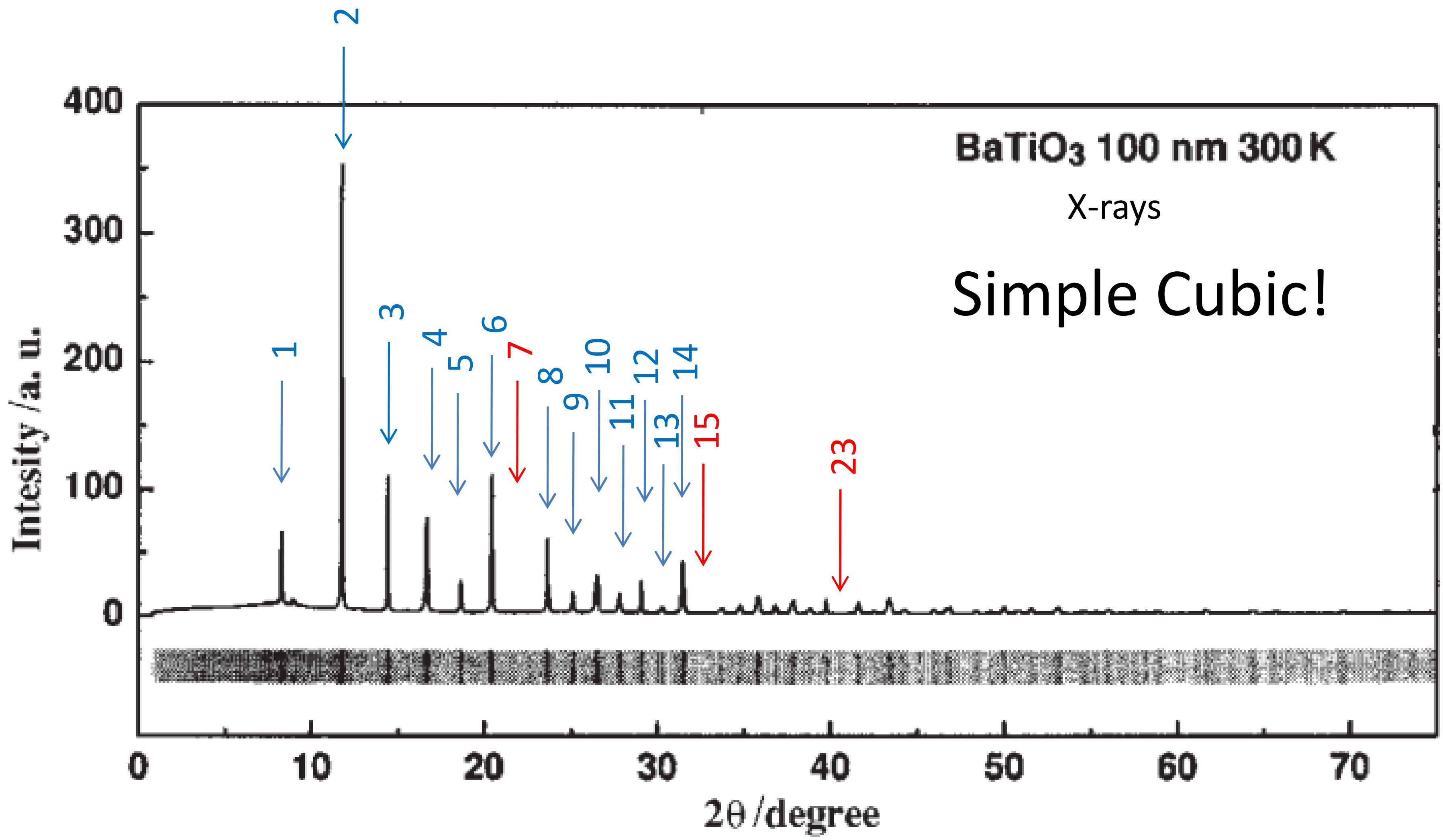
FCC! : h,k,l all even or all odd : N = 3,4,8,11,12 ...

Consider the following XRD pattern for Aluminum, which was collected using CuKα radiation.





Journal of Thermal Analysis and Calorimetry, Vol. 69 (2002) 933–938



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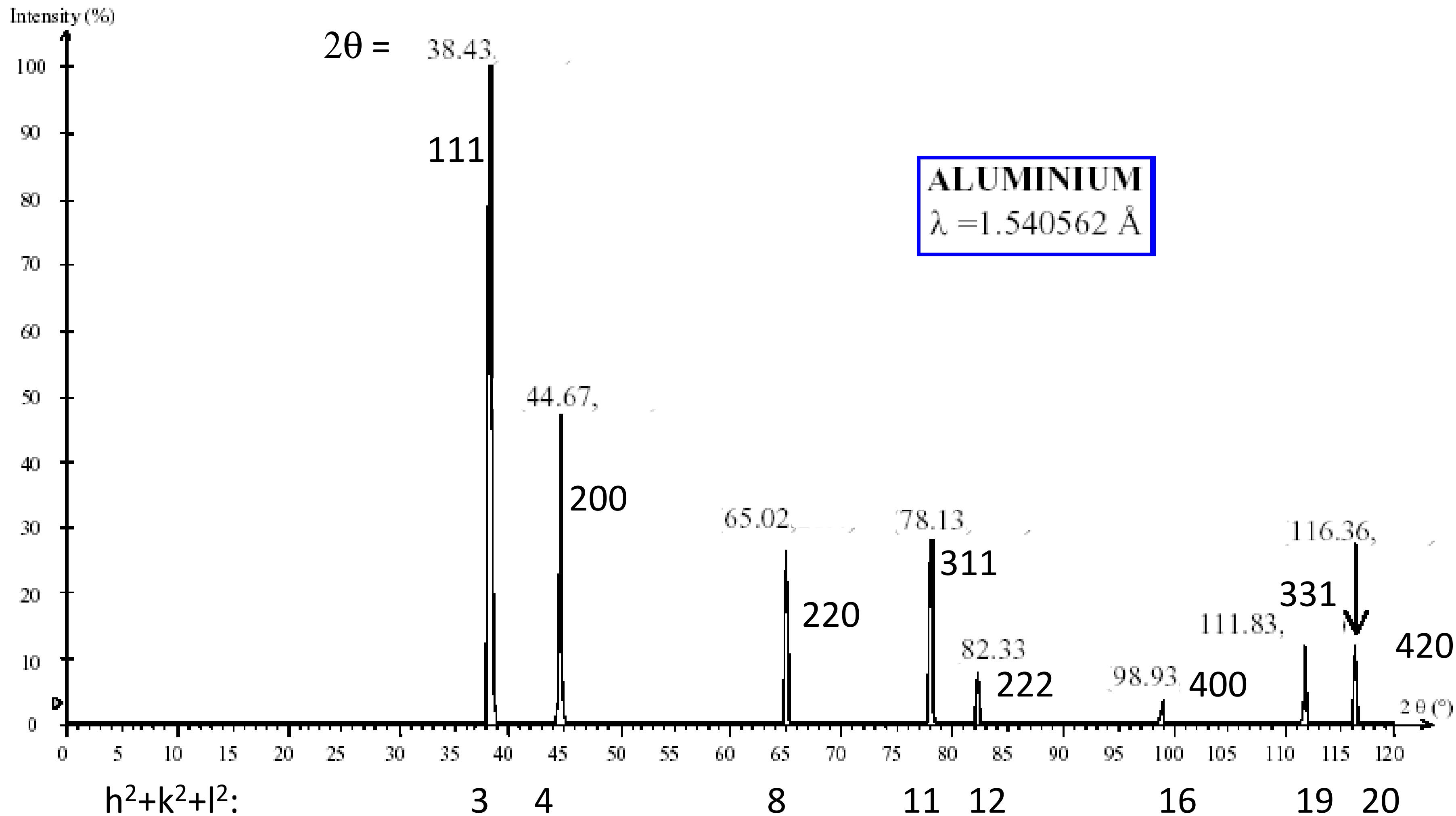
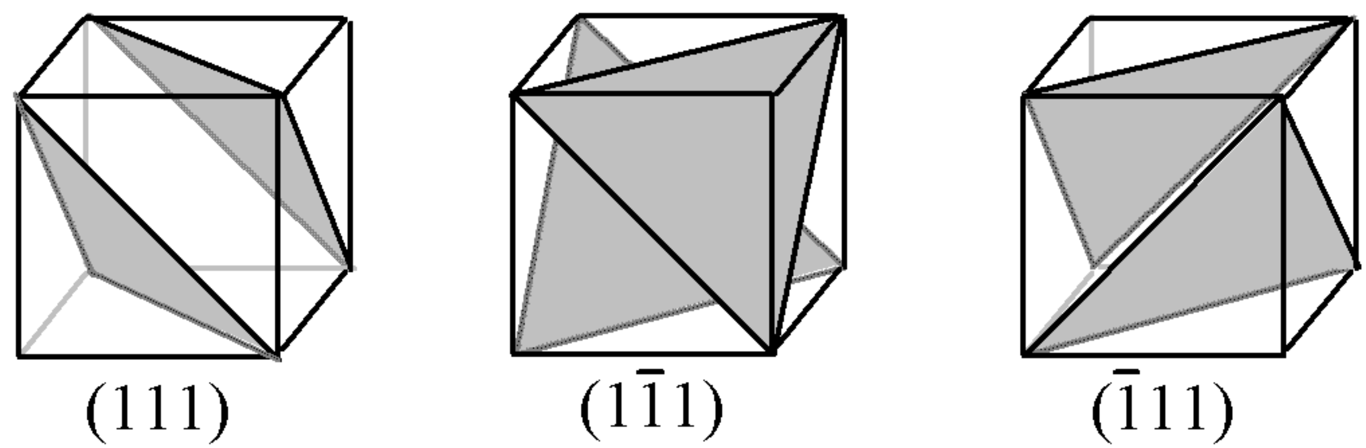




Three of the 8 possible families of lattice planes in the {111} class.

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

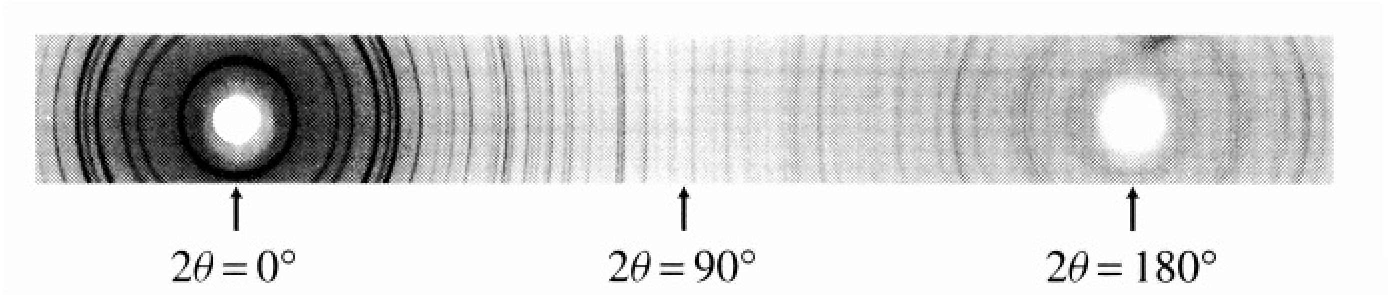
Scattering Selection Rules

P = Primitive (simple) cubic — All hkl
I = BCC — $h+k+l$ = even
F= FCC — h,k,l all even or all odd

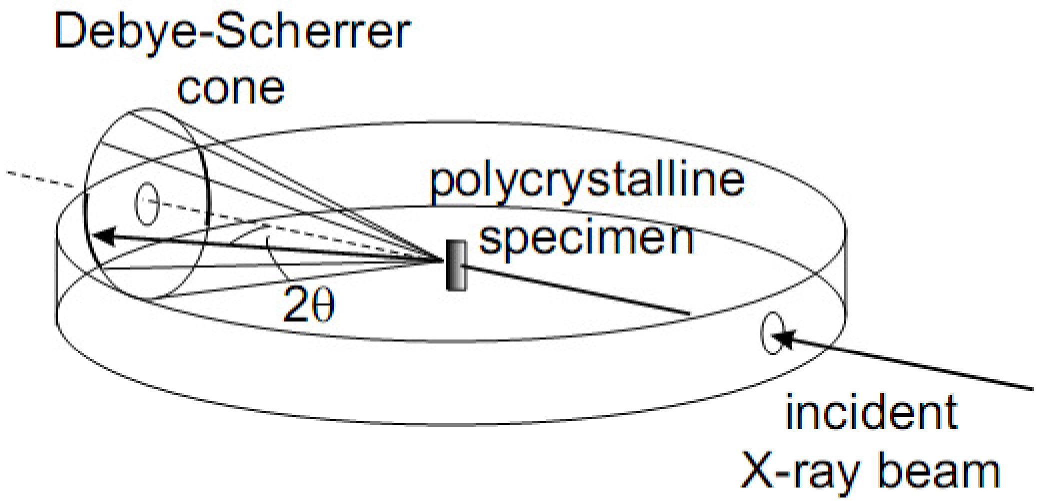
$\{hkl\}$	$N=h^2+k^2+l^2$	Multiplicity	P	I	F
100	1	6	*		
110	2	12	*	*	
111	3	8	*		*
200	4	6	*	*	*
210	5	24	*		
211	6	24	*	*	
---	7	--			
220	8	12	*	*	*
221 , 300	9	24+6	*		
310	10	24	*	*	
311	11	24	*		*
222	12	8	*	*	*
320	13	24	*		
321	14	48	*	*	
---	15	--			
400	16	6	*	*	*

Sequence of N values

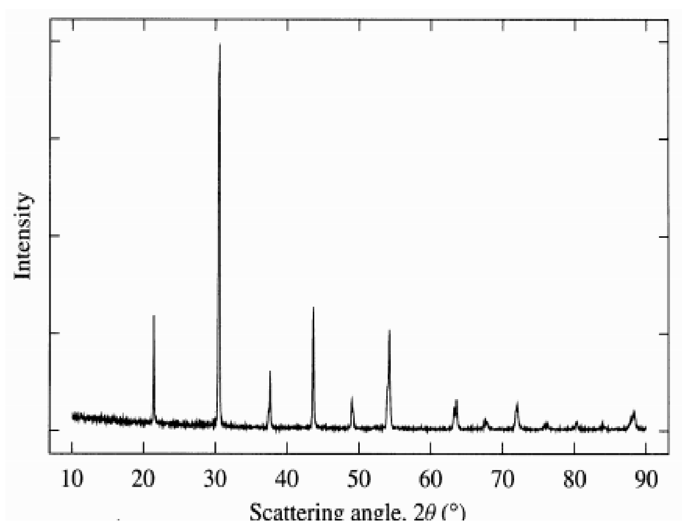
P: 1,2,3,4,5,6,8,9, ….. (= all integers excluding 7, 15, 23,…)
I : 2,4,6,8,10,12,14 … (= even integers excluding 28, 60…)
F: 3,4,8,11,12,16,19,20 ….



$2\theta = 0°$
$2\theta = 90°$
$2\theta = 180°$



Debye-Scherrer cone
polycrystalline specimen
2θ
incident X-ray beam



Intensity
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20
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40
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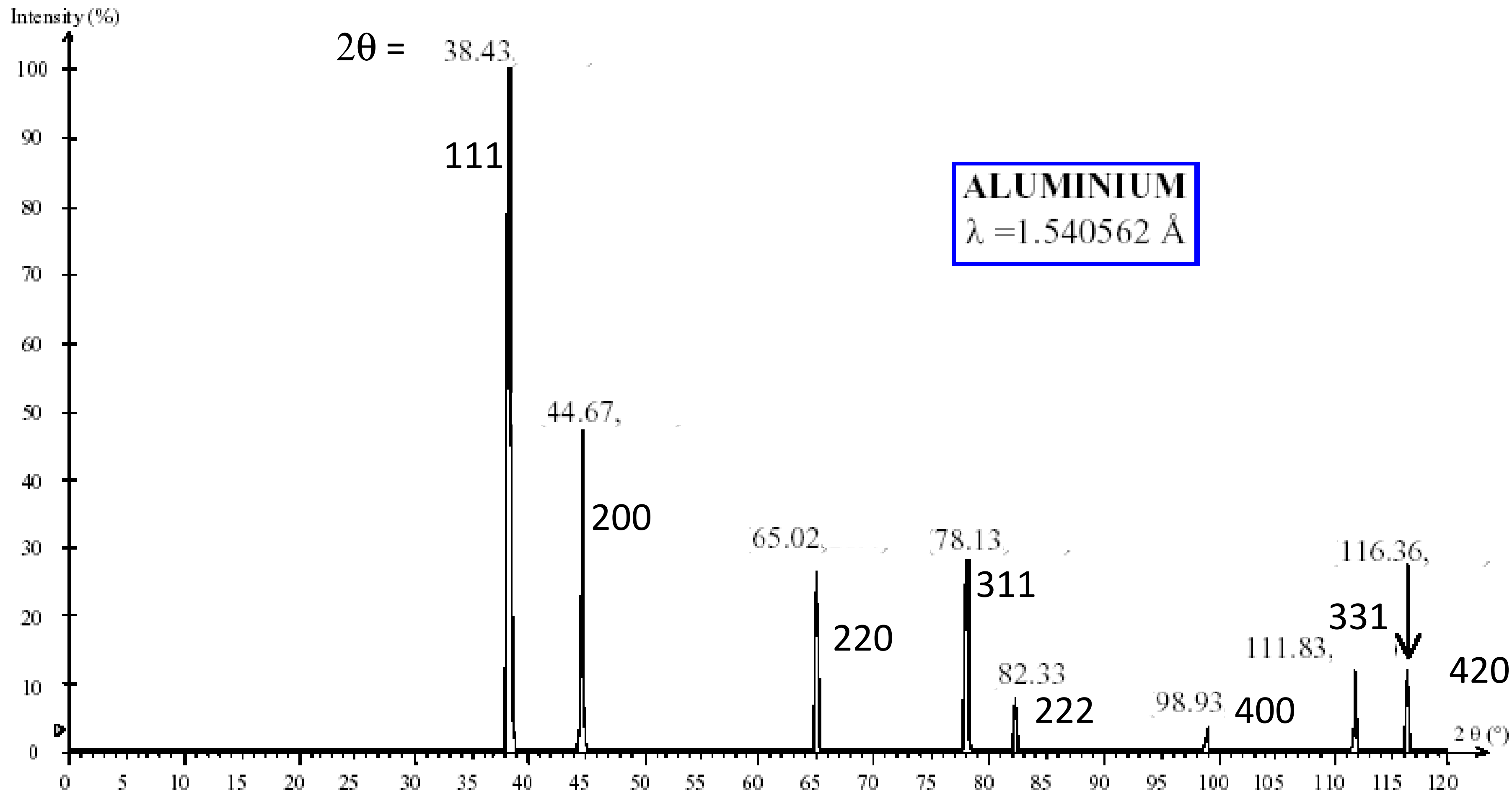
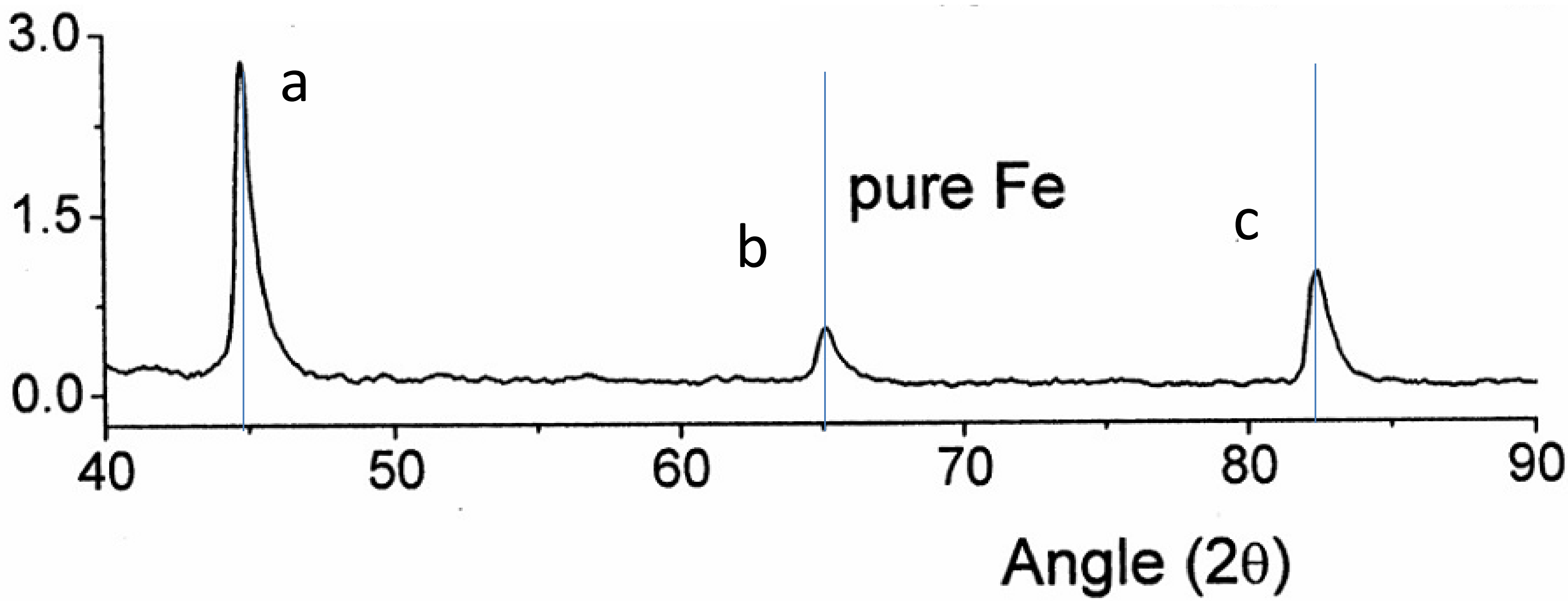
70
80
90
Scattering angle, 2θ (°)

Consider the following XRD pattern for Aluminum, which was collected using CuKα radiation.



$h^2+k^2+l^2$:	3	4	8	11	12	16	19	20
Multiplicity:	8	6	12	24	8	6	24	24

X-ray λ=1.54 Angstrom



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Vol. 45, October 2006, pp. 851-855

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

Peak Angle 2θ

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

$$d_a^2/d^2$$

a	44.7
b	65.2
c	82.7

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

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

OR

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

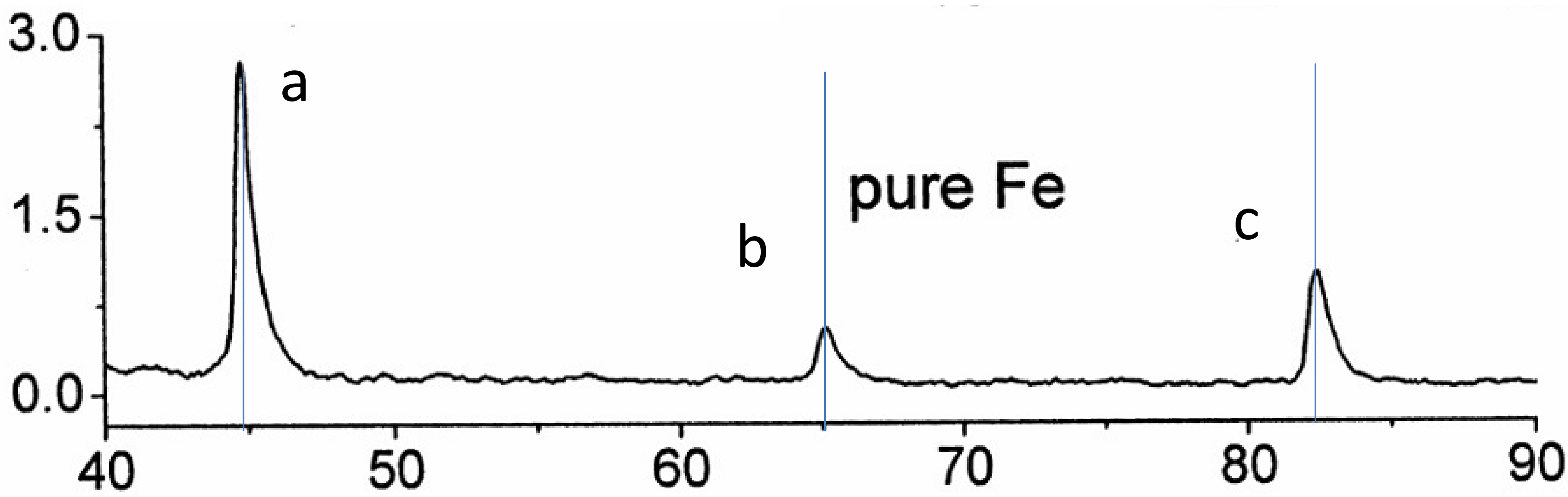
$$a = d\sqrt{h^2 + k^2 + l^2}$$

= 2.03 Å if we choose simple cubic

= 2.86 Å if we choose BCC

Calculated Atomic Densities : 1/(2.03 Å)^3 for simple cubic vs 2/(2.86 Å)^3 for BCC

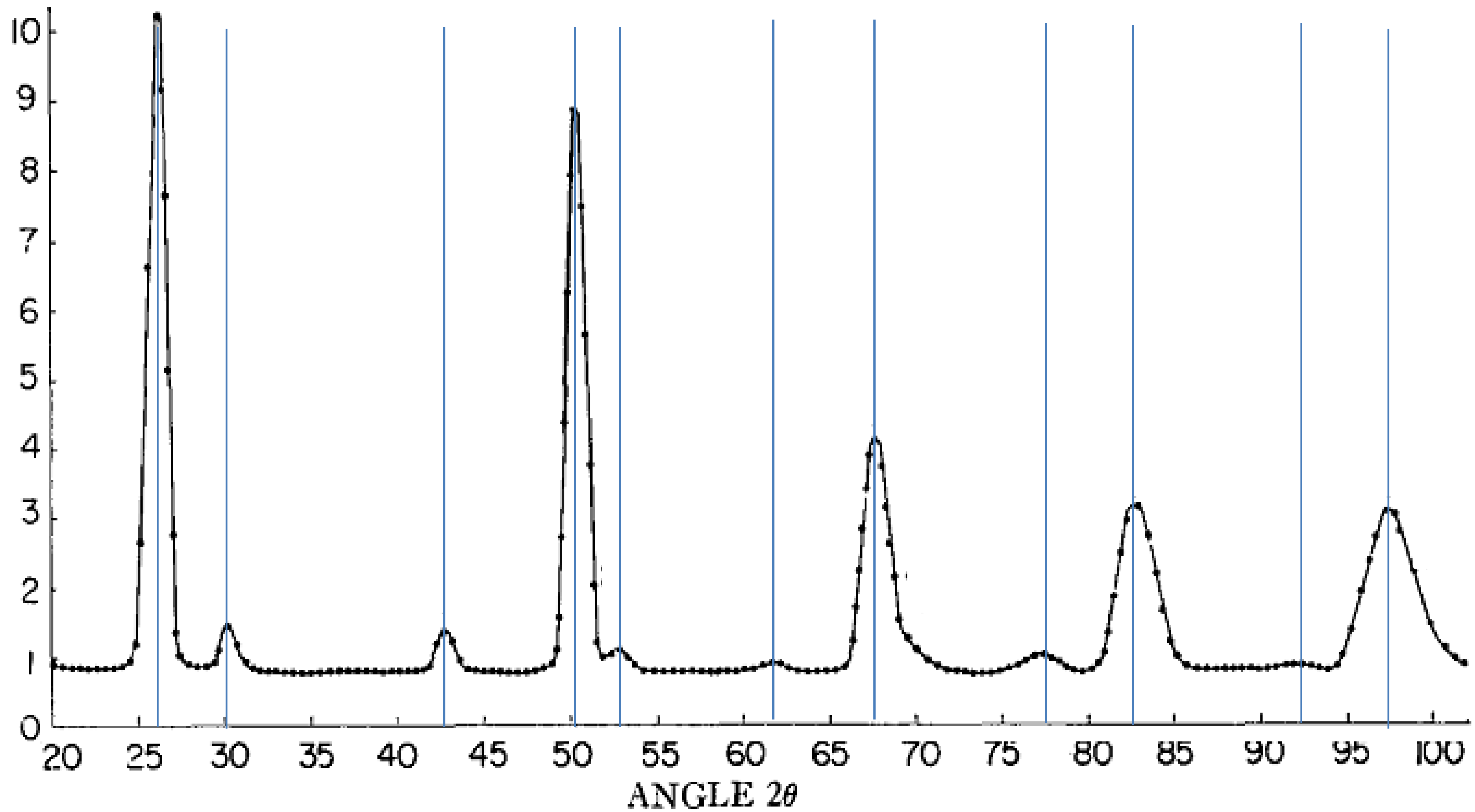
X-ray λ=1.54 Angstrom



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 don't matter much) , c having much more intensity than b is only consistent with BCC

λ = 1.09 Angstrom TiC neutron powder diffraction



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

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

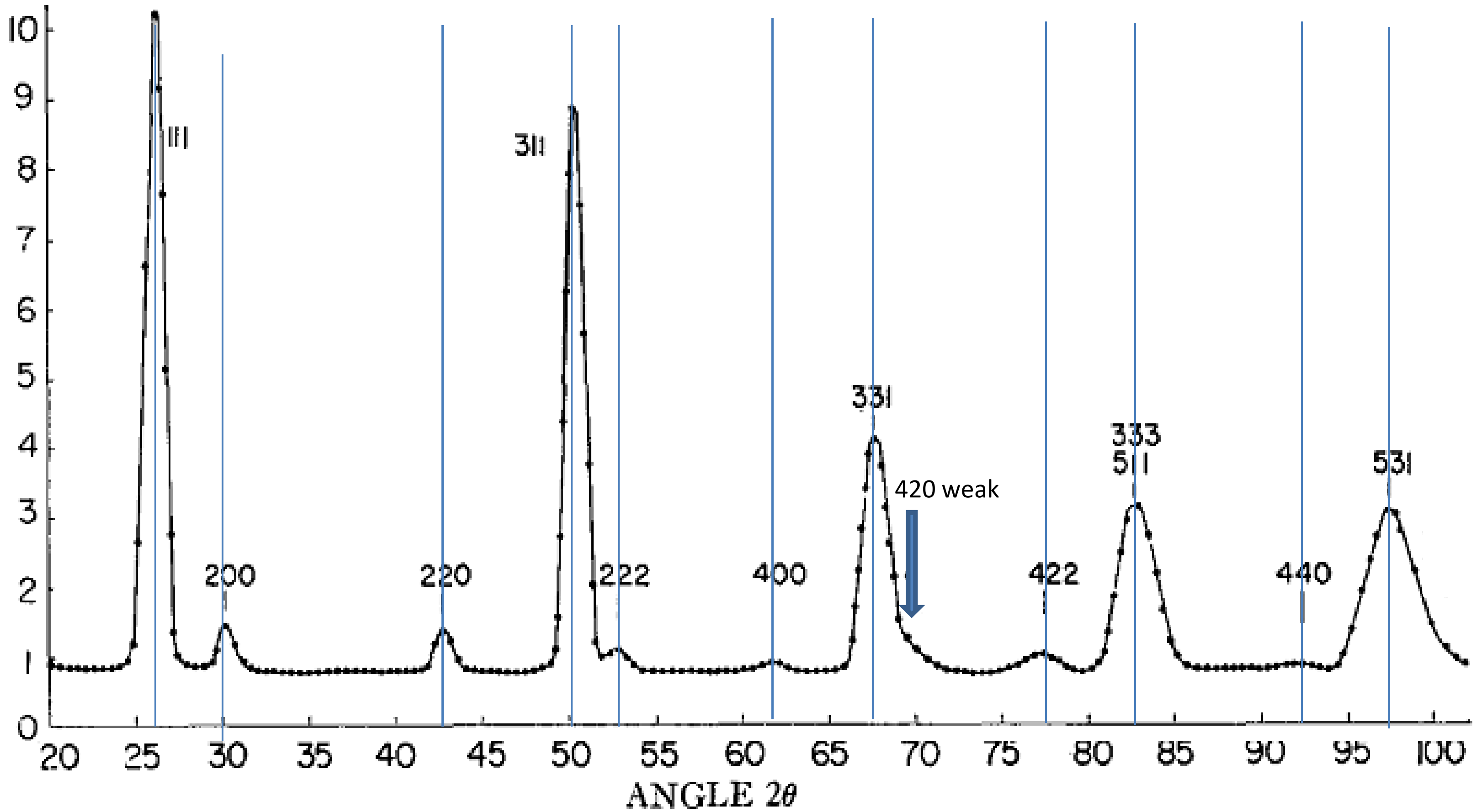
$$a^2/d^2 = h^2 + k^2 + l^2$$

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

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 ...

λ = 1.09 Angstrom   TiC



h+k+l:	3	2	4	5	6	4	7	6	8	7,9	8	9
Multiplicity:	8	6	12	24	8	6	24	24	24	24+6	24	24

can we figure out what the unit cell looks like?

NaCl structure

Ti @ [0,0,0]
C @ [1/2,1/2,1/2]

$$|S|^2 = \left| b_{Ti} + b_C (-1)^{h+k+l} \right|^2$$

= $|b_{Ti} - b_C|^2$ for h+k+l odd

= $|b_{Ti} + b_C|^2$ for h+k+l even

ZnS structure

Ti @ [0,0,0]
C @ [1/4,1/4,1/4]

$$|S|^2 = \left| b_{Ti} + b_C (i)^{h+k+l} \right|^2$$

= $b_{Ti}^2 + b_C^2$ for h+k+l odd

= $|b_{Ti} + b_C|^2$ for h+k+l = 4m

= $|b_{Ti} - b_C|^2$ for h+k+l = 4m+2

Conclude must be NaCl structure

X-ray scattering on liquids
– like powder but peaks not sharp.