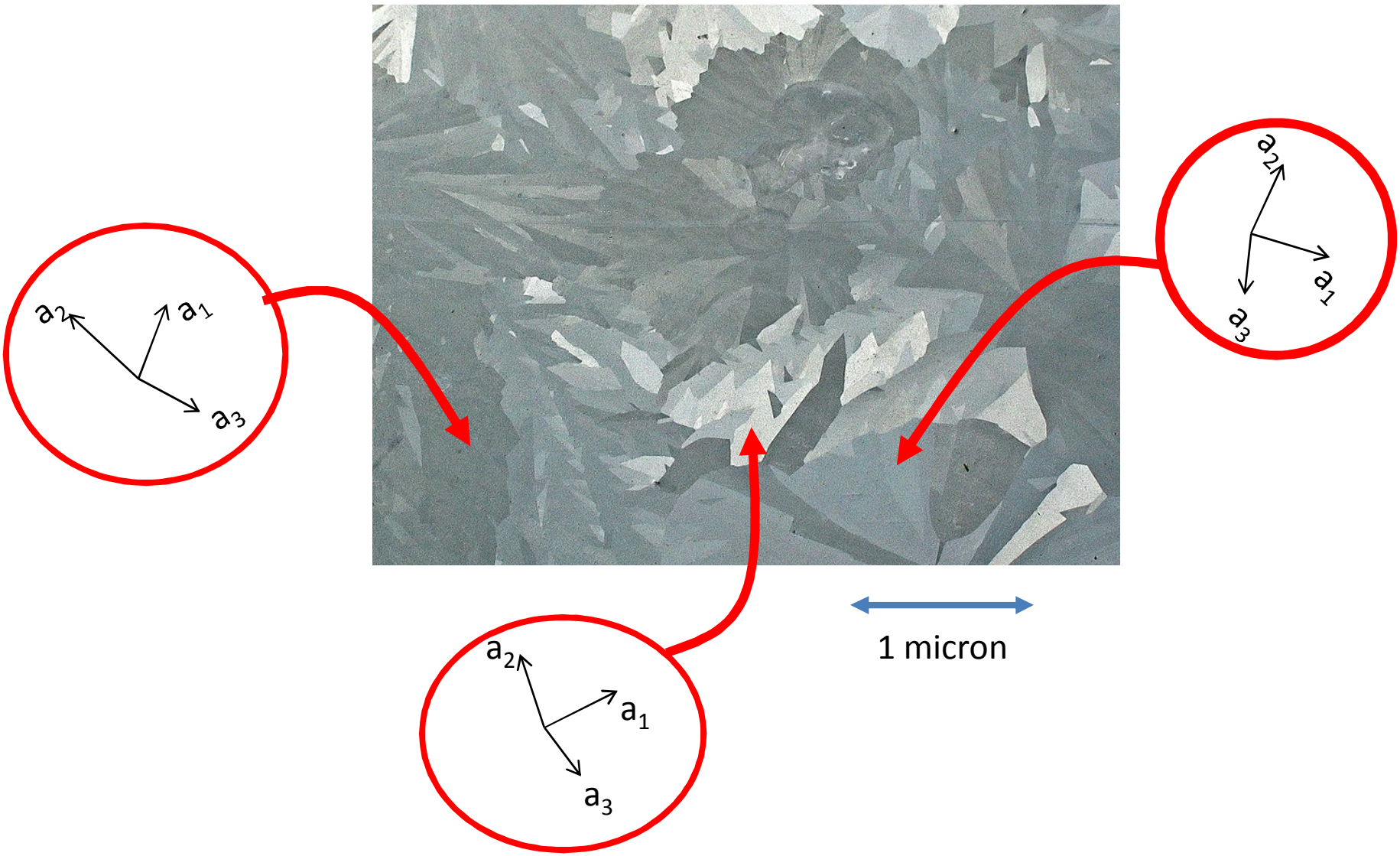
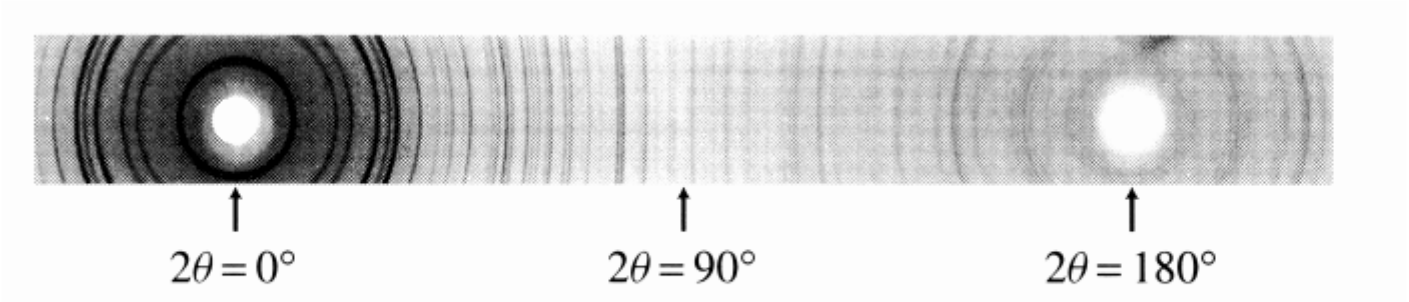
Slides
Condensed Matter Physics
Lecture 13

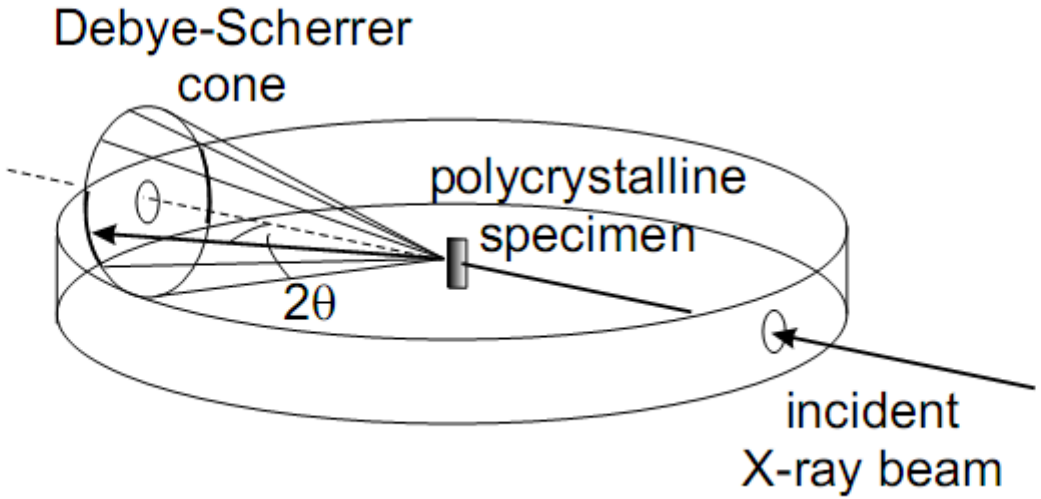
Nice single crystals (NaCl)

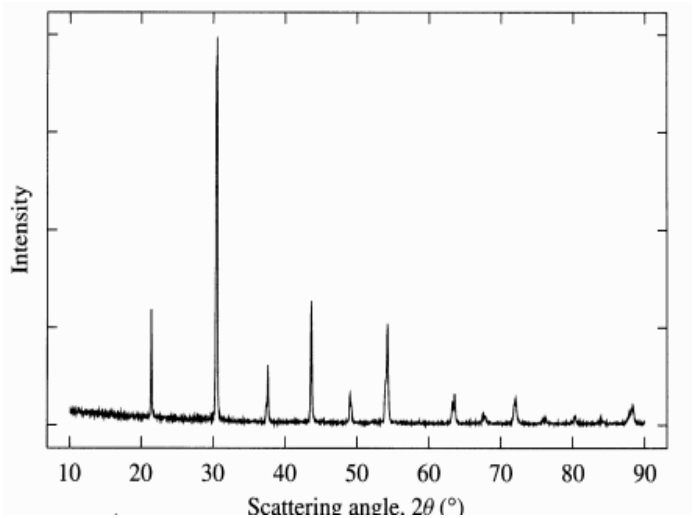


Polycrystalline Material

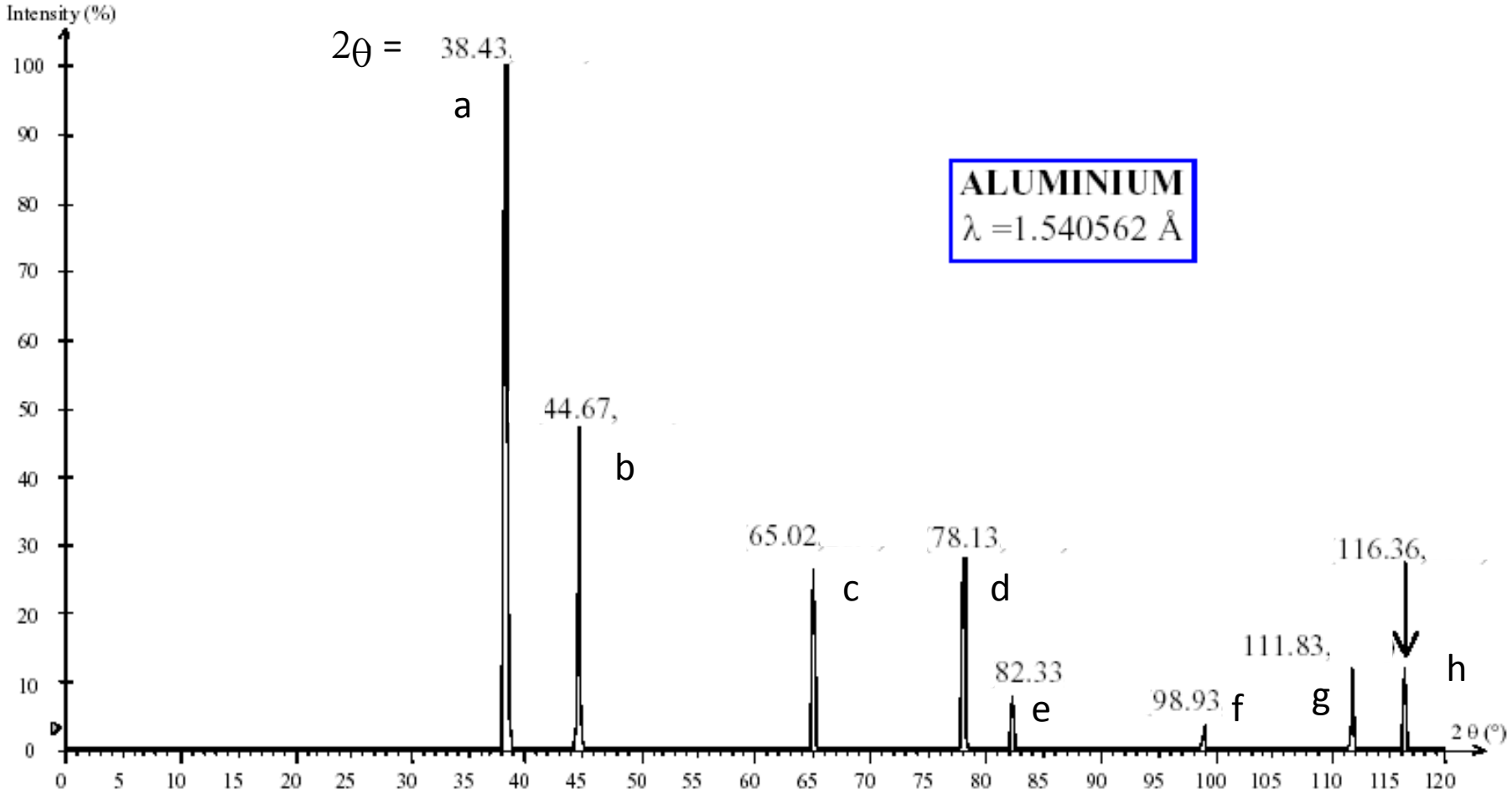


X-ray diffraction rings recorded on a photographic film





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



Scattering Selection Rules

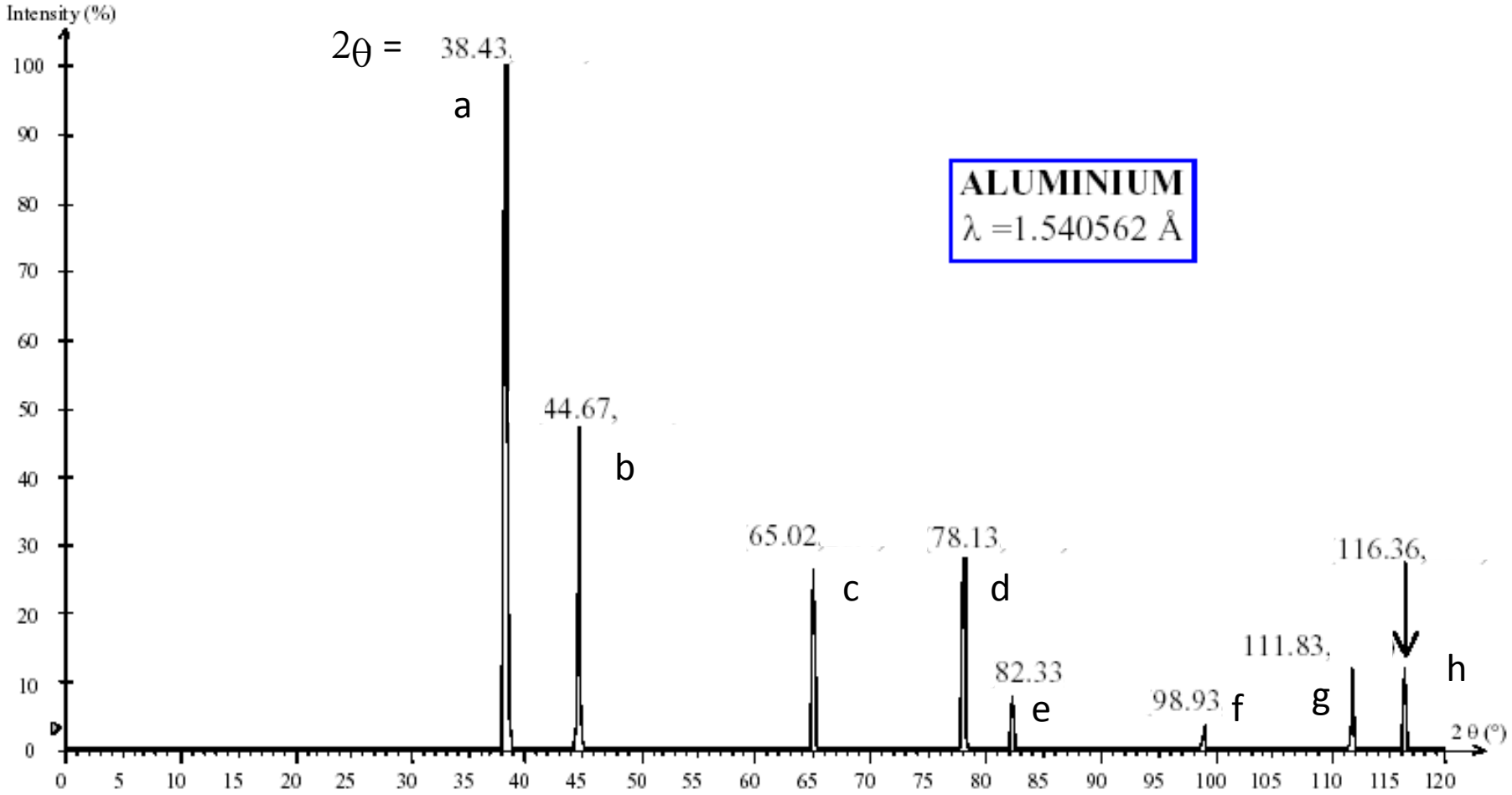
P = Primitive (simple) cubic — All hkl
I = BCC — $h+k+l$ = even
F = FCC — h,k,l all even or all odd

$\{hkl\}$	$N=h^2+k^2+l^2$	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.



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

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

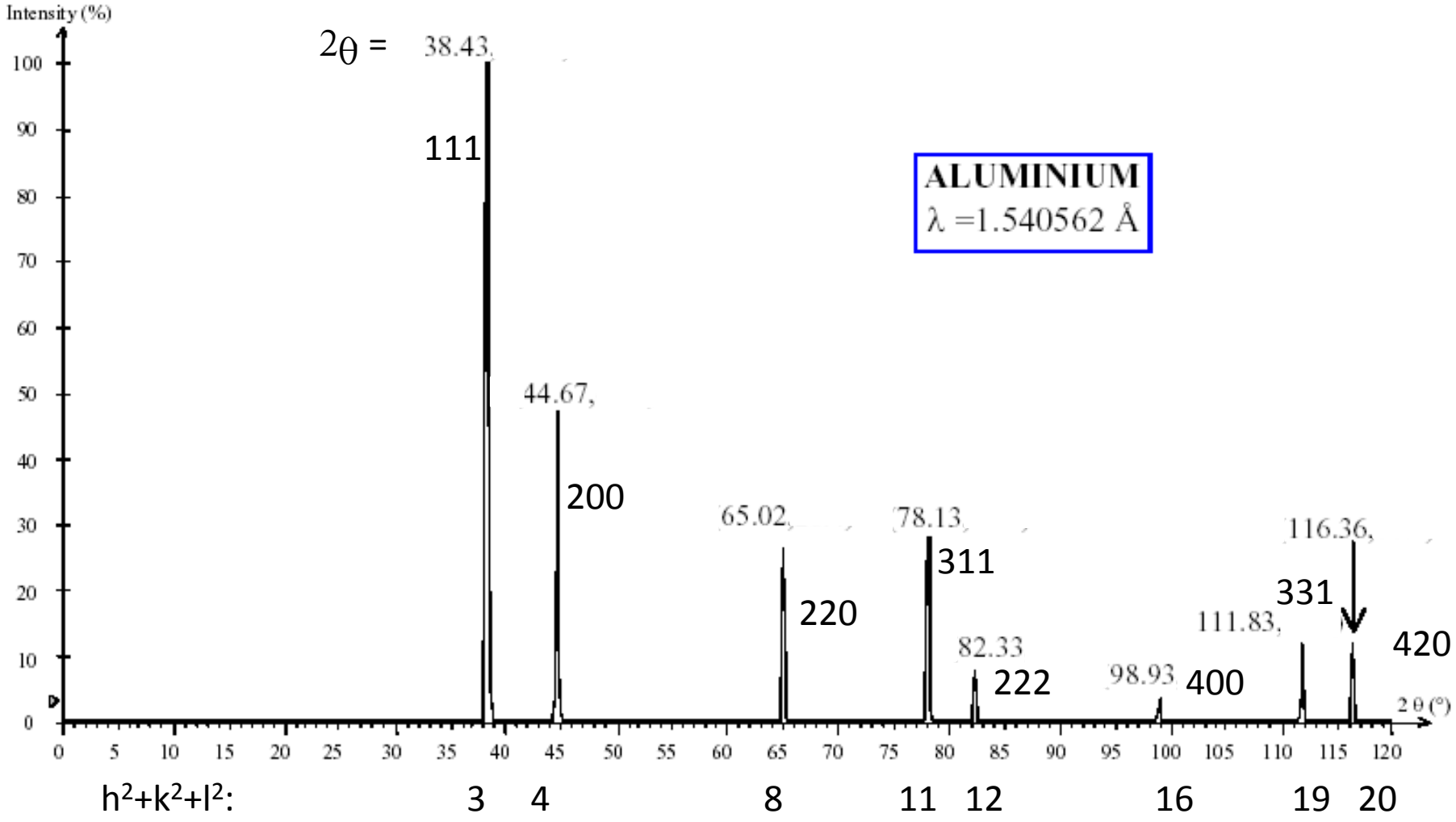
$$N = h^2 + k^2 + l^2$$

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

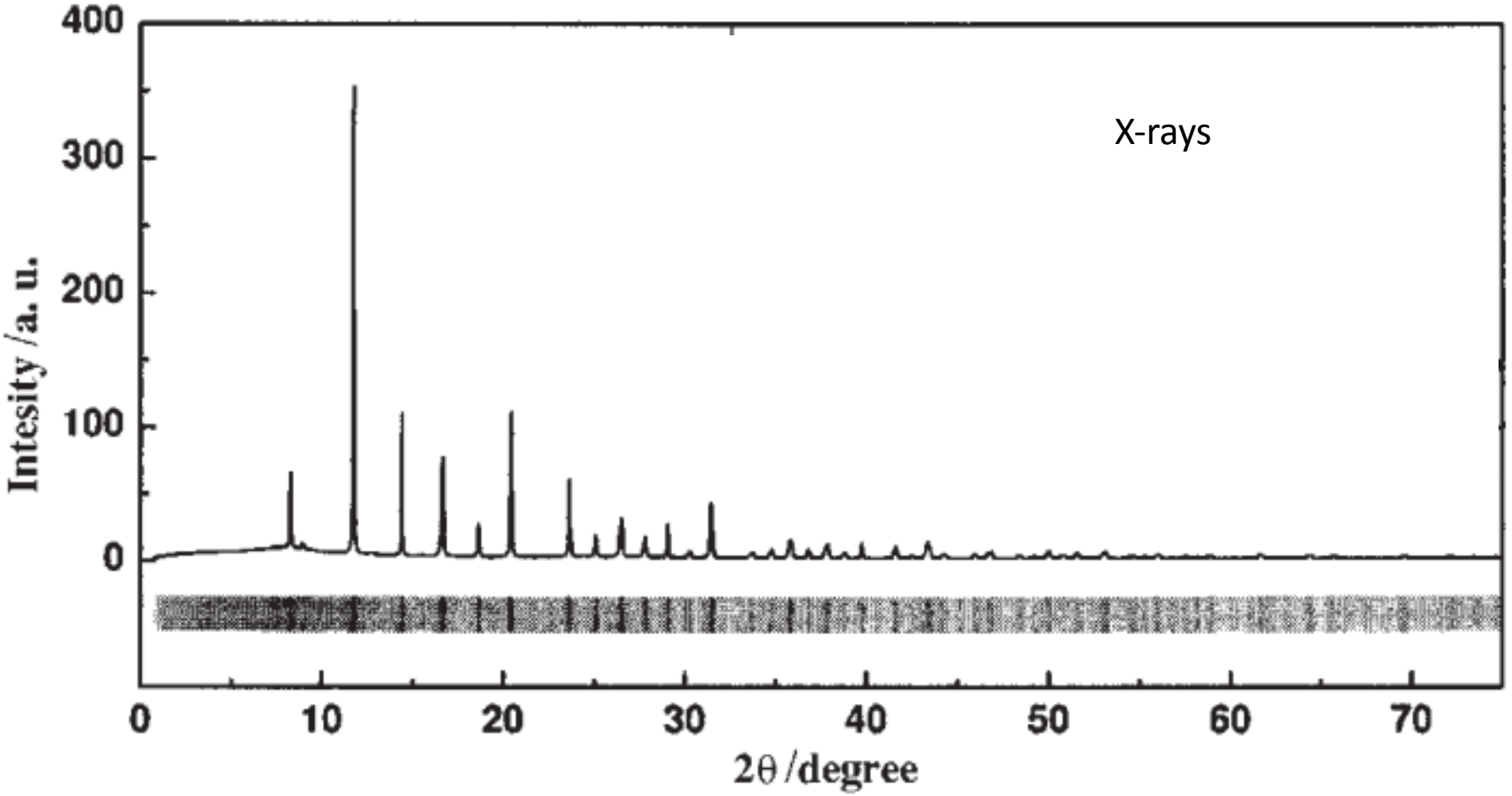
Peak	Angle 2θ		d_a^2/d^2	$3d^2/d_a^2$	N	$\{hkl\}$	a
a	38.43	2.3405Å	1.0000	3.0000	3	111	4.0538Å
b	44.67	2.0269Å	1.3333	3.9999	4	200	4.0539Å
c	65.02	1.4332Å	2.6667	8.0002	8	220	4.0538Å
d	78.13	1.2223Å	3.6666	10.9999	11	311	4.0538Å
e	82.33	1.1702Å	4.0000	12.0001	12	222	4.0538Å
f	98.93	1.0135Å	5.3327	15.9980	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.

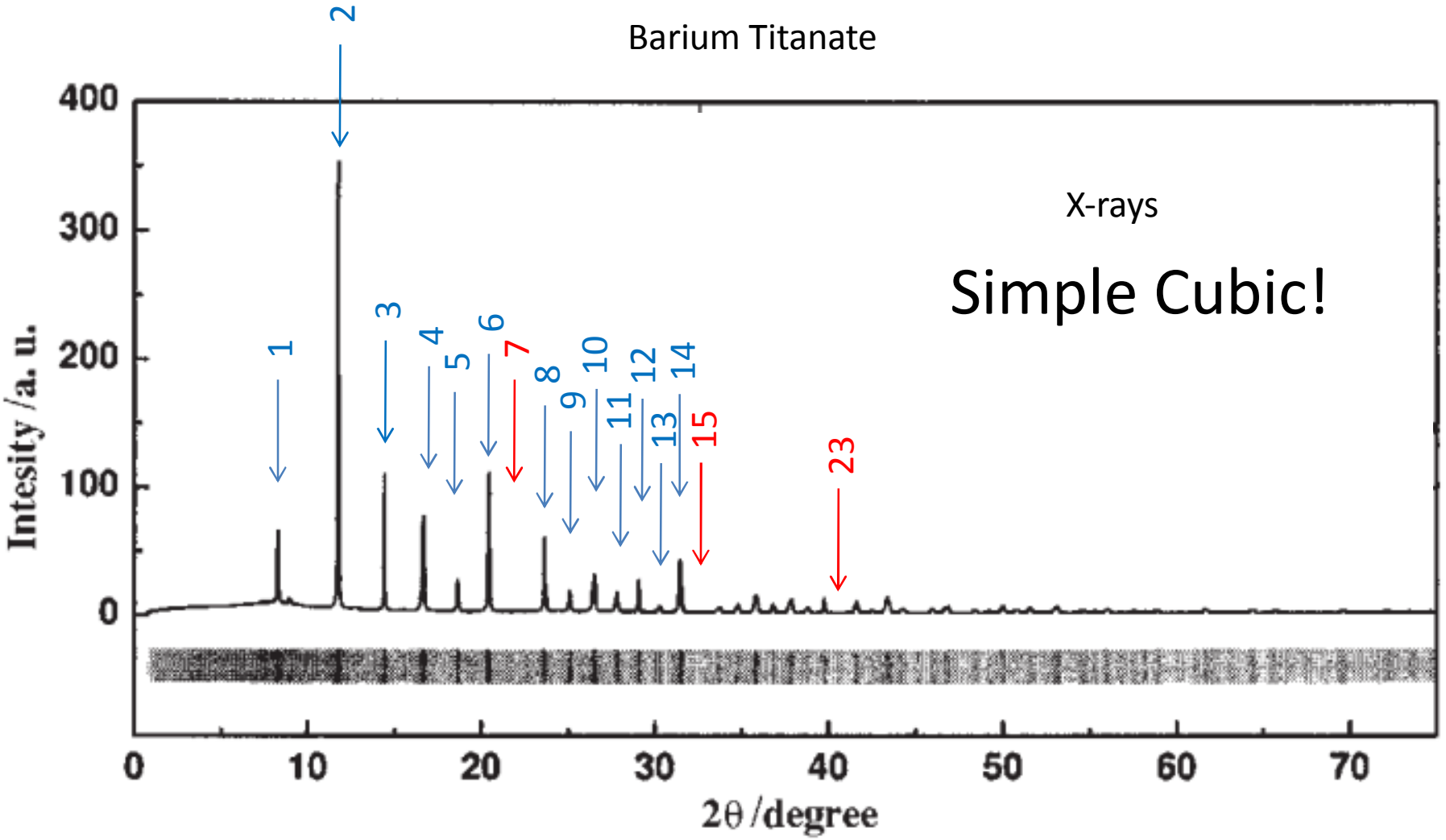


Barium Titanate



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

Barium Titanate



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

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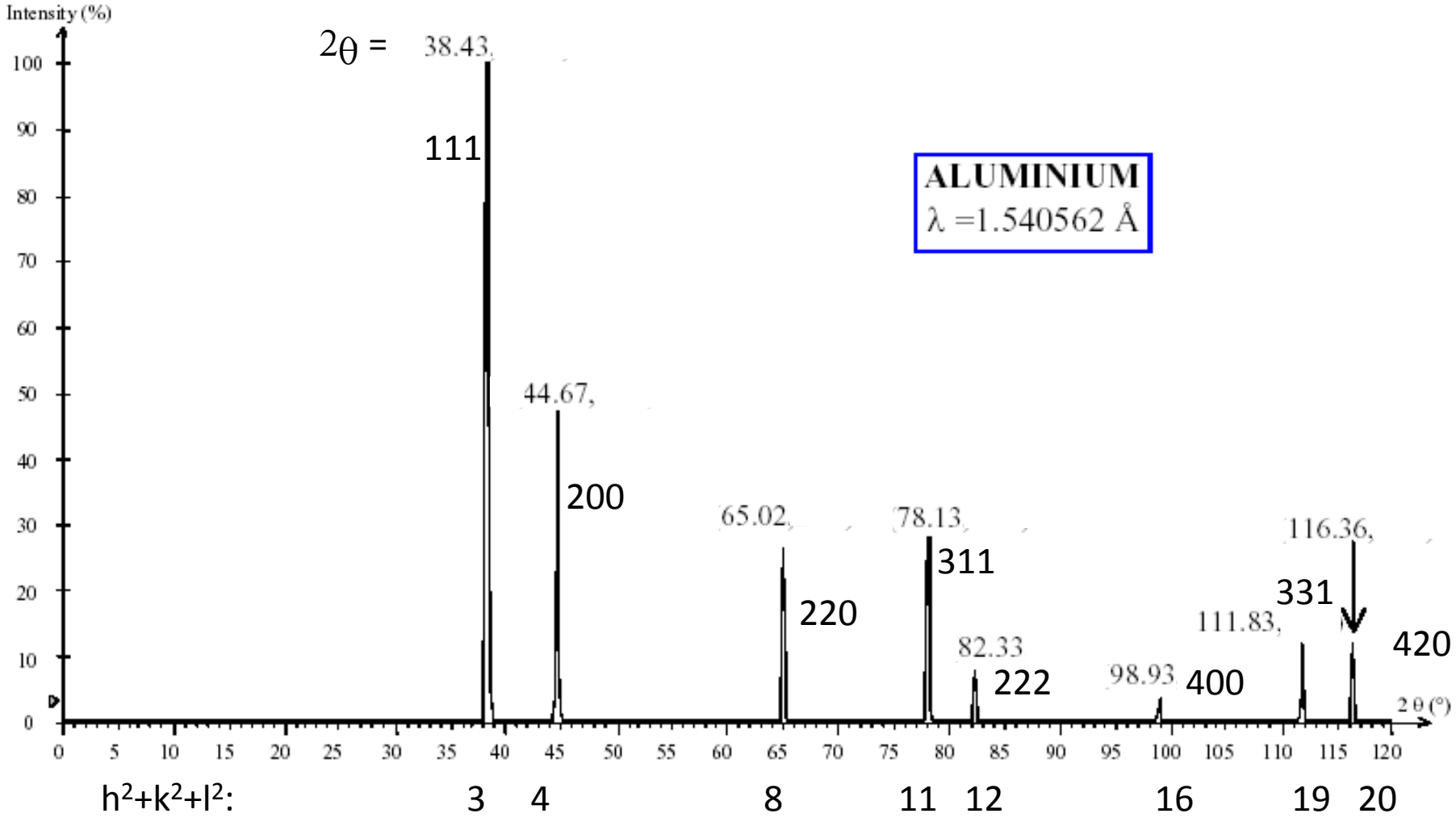
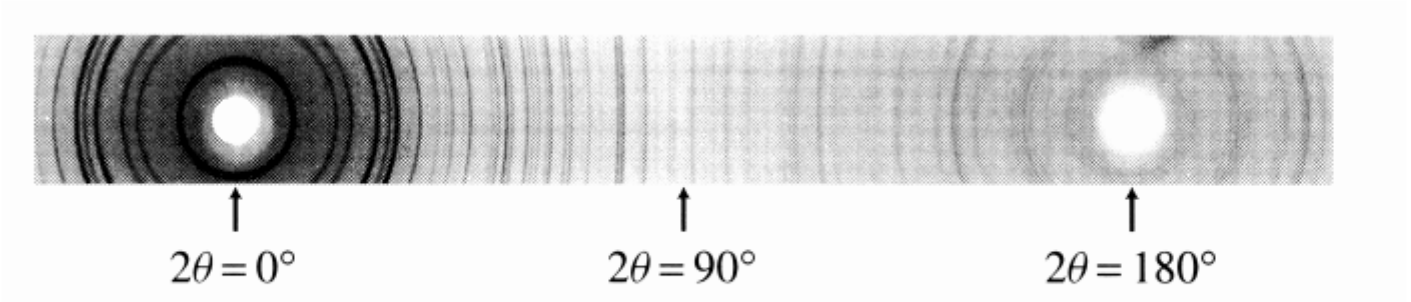
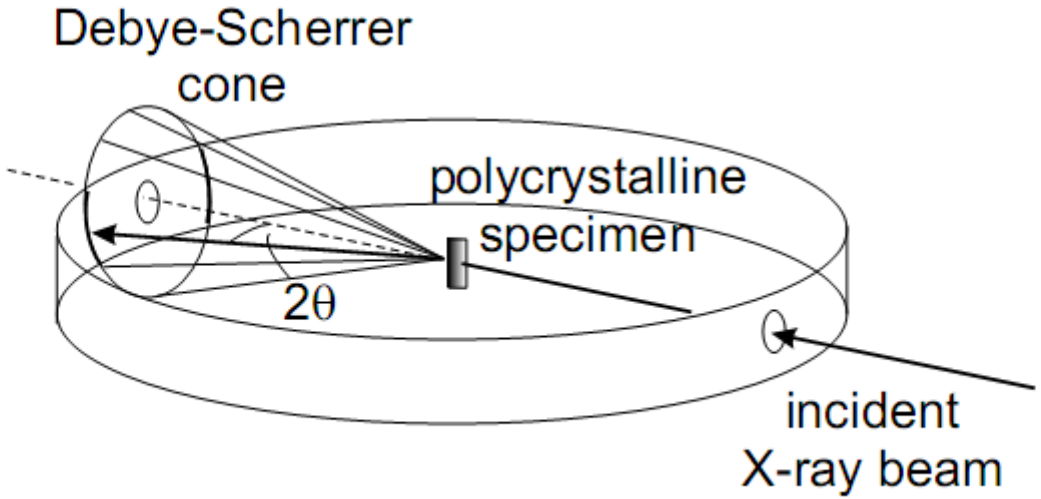
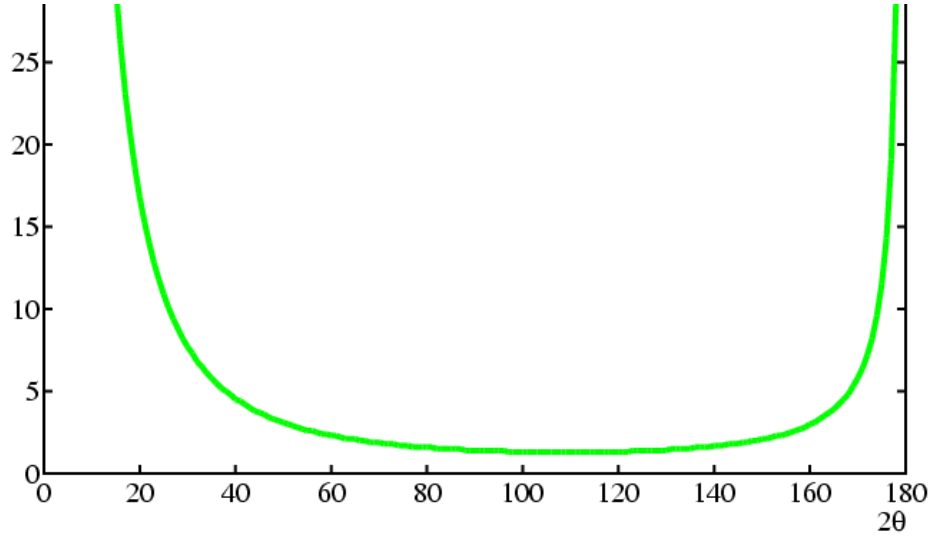




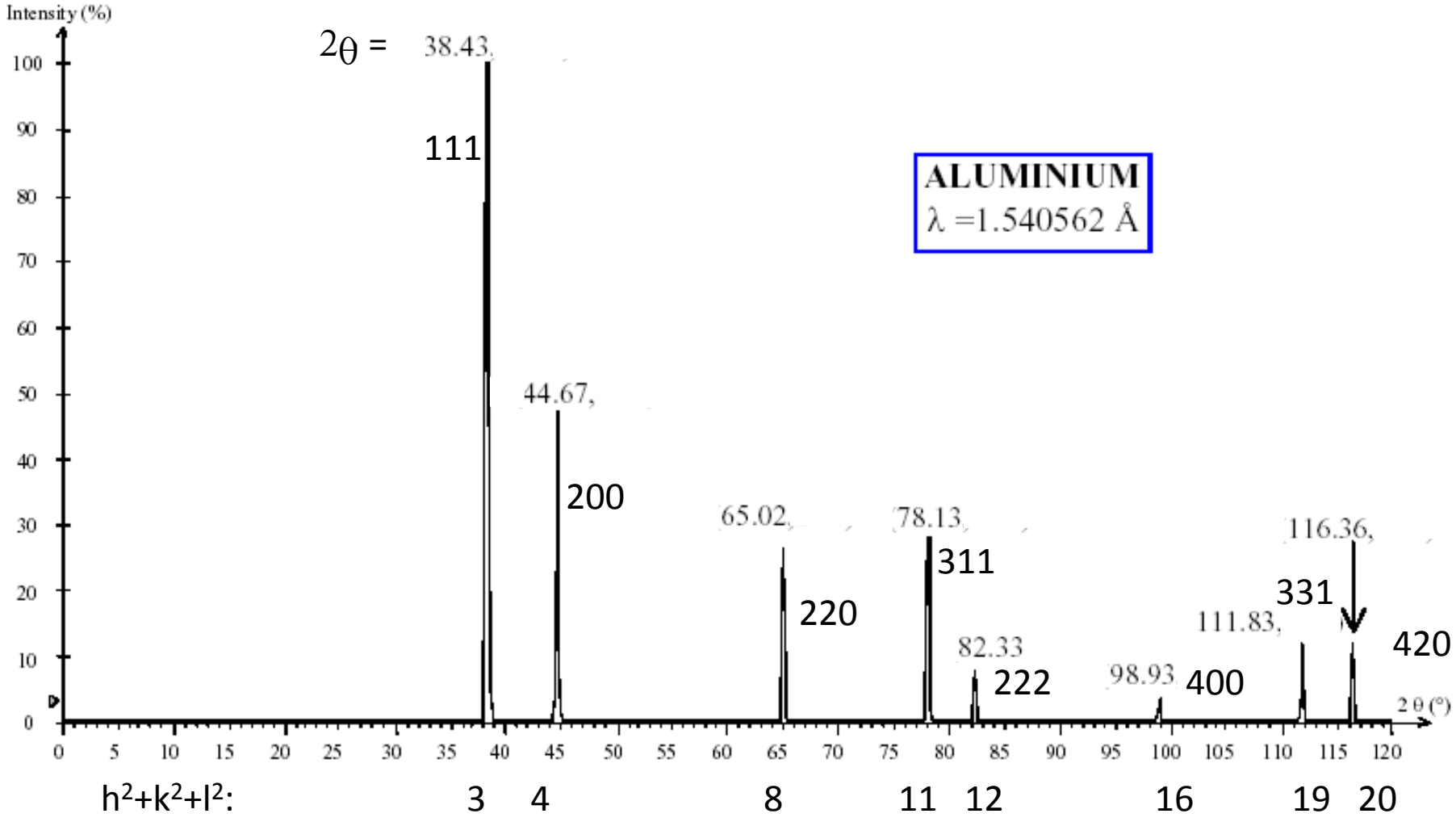
X-ray diffraction rings recorded on a photographic film

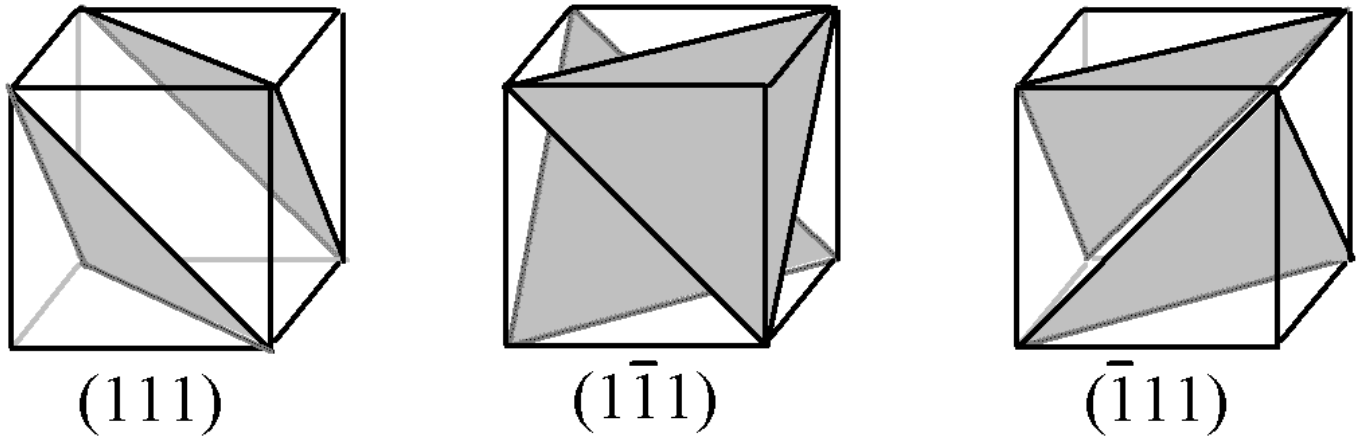




Geometric Lorentz Factor

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





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

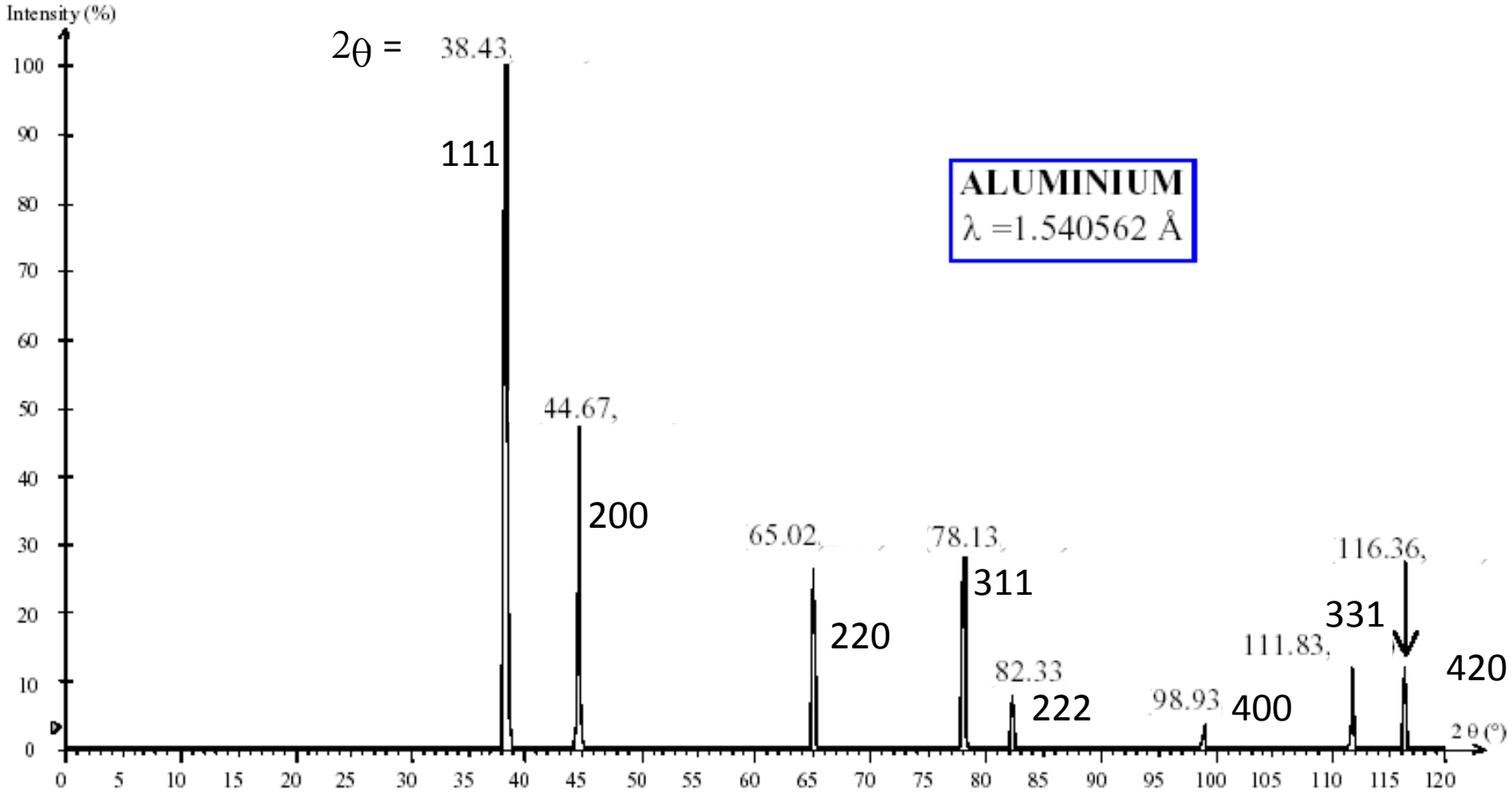
P = Primitive (simple) cubic — All hkl
I = BCC — $h+k+l$ = even
F = FCC — h,k,l all even or all odd

$\{hkl\}$	$N=h^2+k^2+l^2$	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

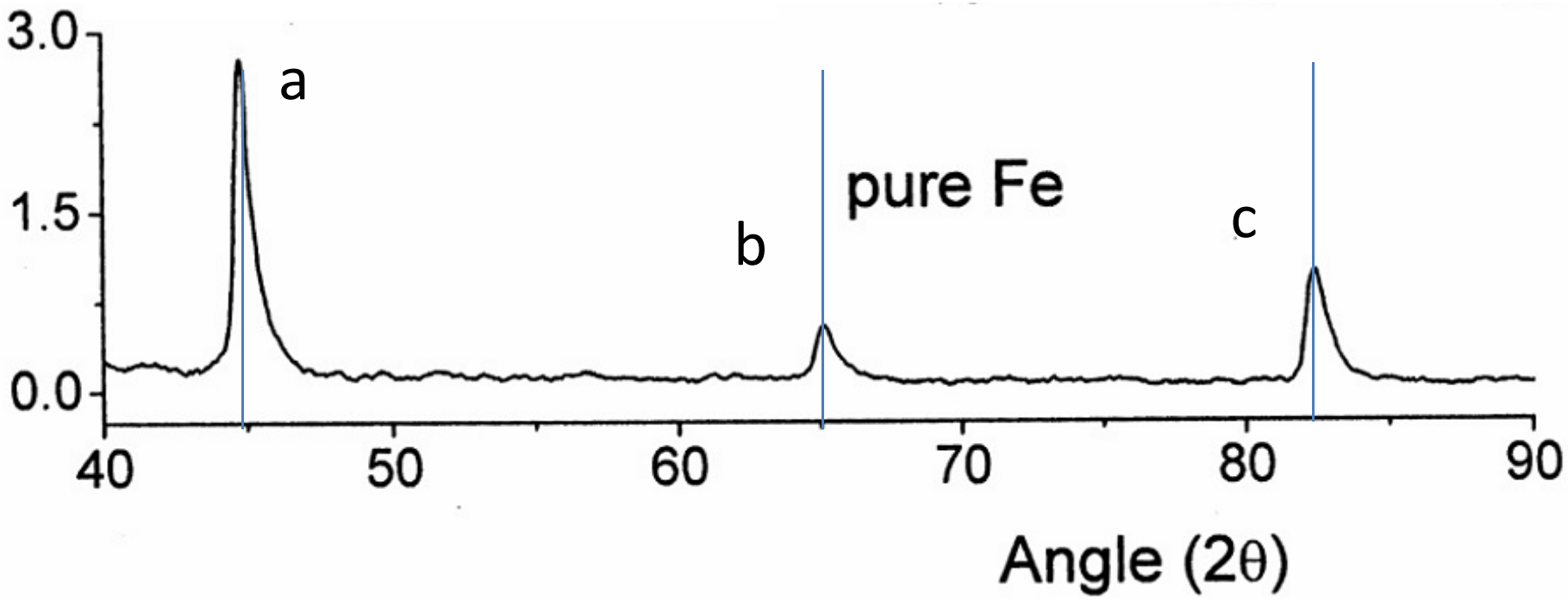
P: 1,2,3,4,5,6,8,9, ….. (= all integers excluding 7, 15, 23,…)
I : 2,4,6,8,10,12,14 … (= even integers excluding 28, 60…)
F: 3,4,8,11,12,16,19,20 ….

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

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

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

Peak	Angle 2θ		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}

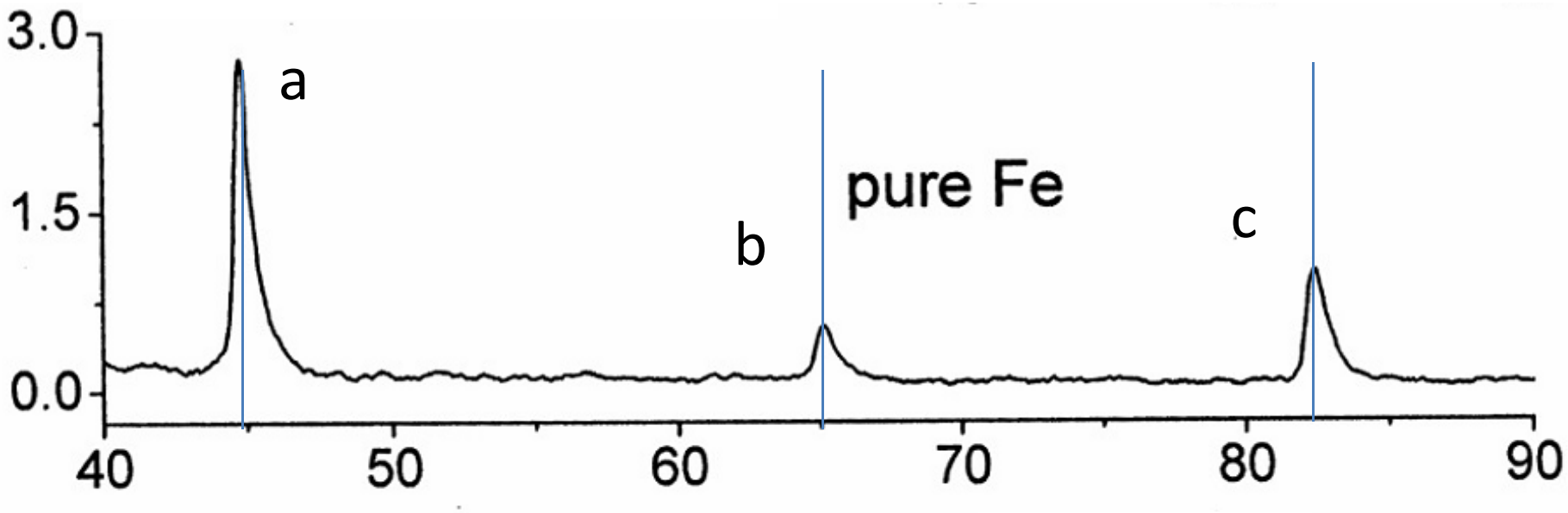
$$a = d\sqrt{h^2 + k^2 + l^2}$$

= 2.03 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

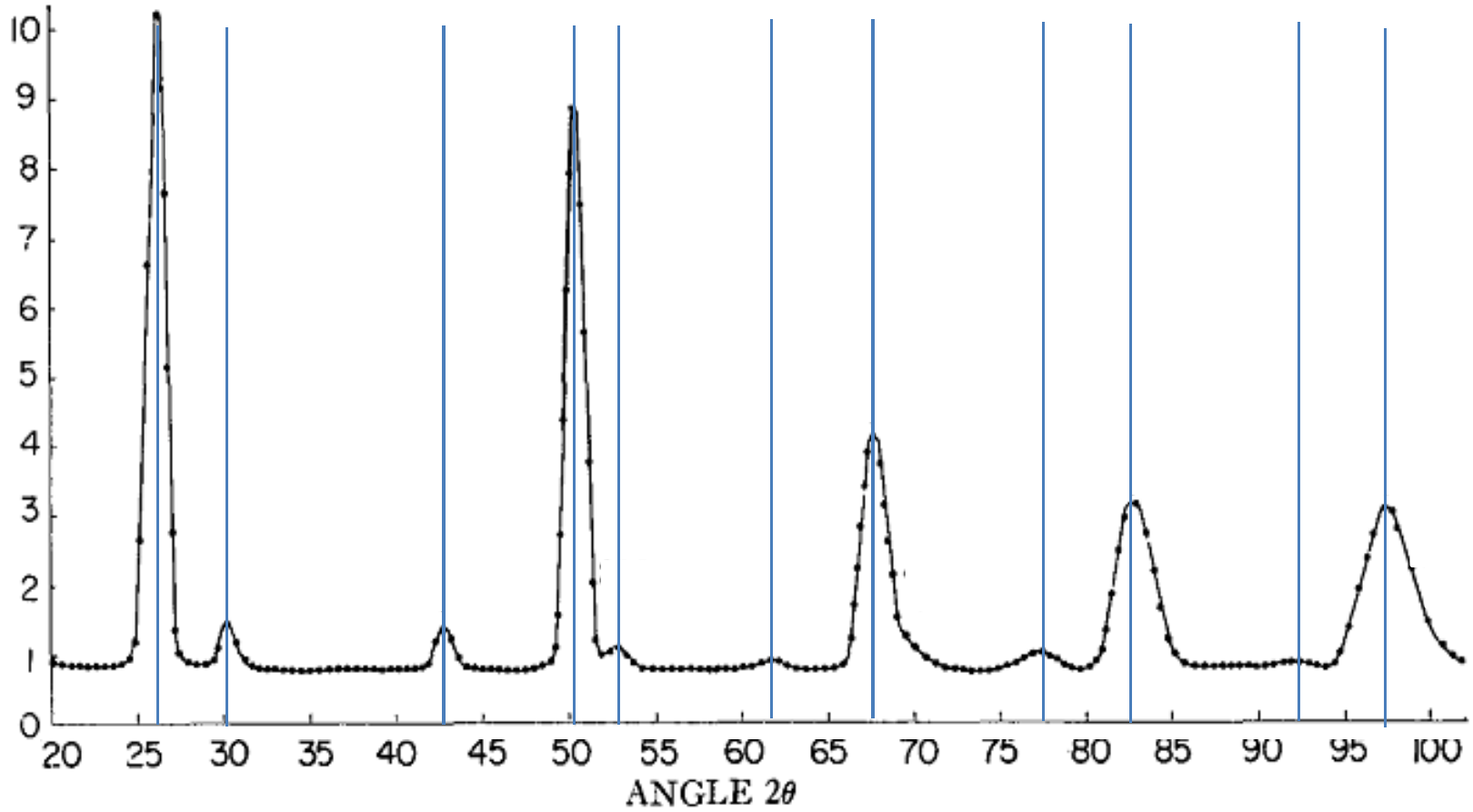
X-ray λ=1.54 Angstrom



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 also decaying) , 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).

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

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

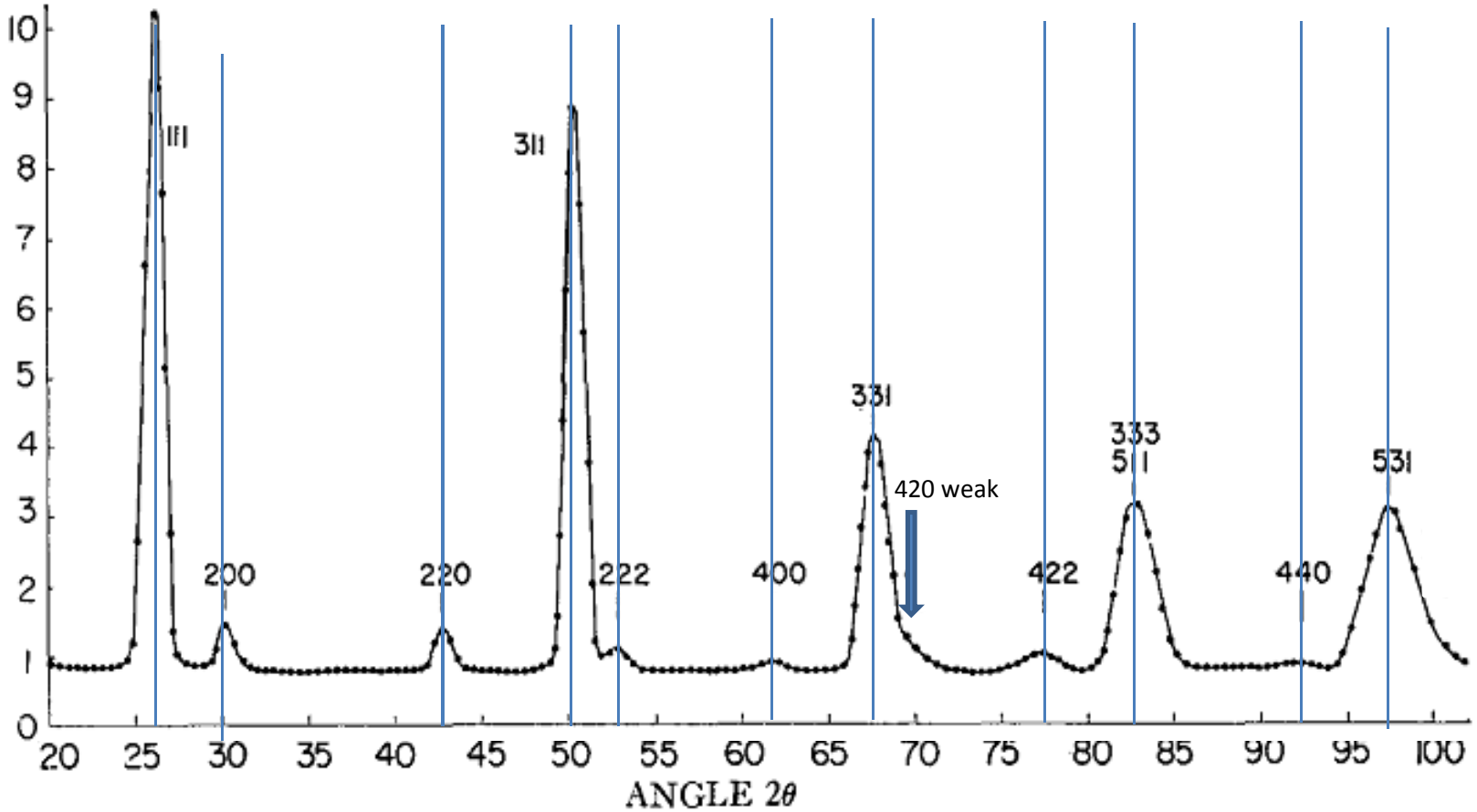
$$N = h^2 + k^2 + l^2$$

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

Peak	Angle 2θ		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

The Rutherford-Appleton Lab in Oxfordshire

Synchrotron X-ray Source

Spallation Neutron Source