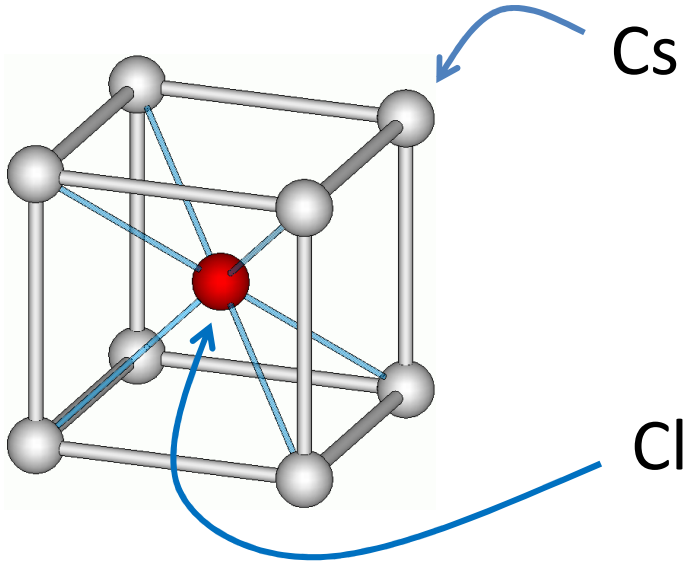
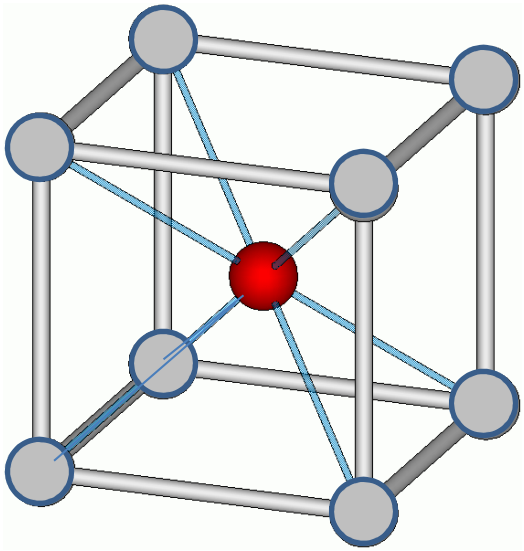
Slides
Condensed Matter Physics
Lecture 13



Cesium Chloride (CsCl): A simple cubic Lattice with a Basis

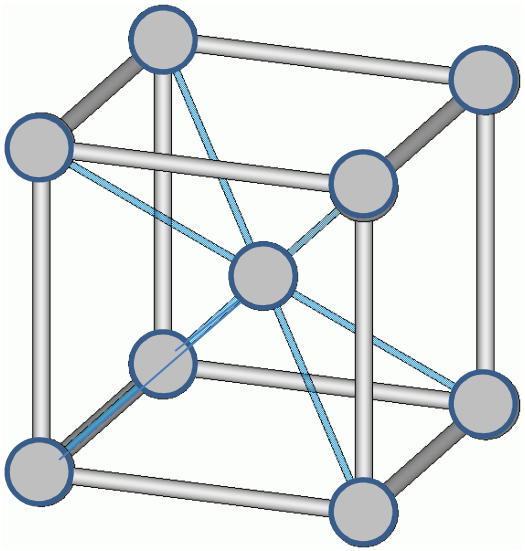
Basis:

Cs at[0, 0, 0] (i.e., on the simple cubic)
Cl at [½, ½, ½] (i.e., in the middle of each cube)



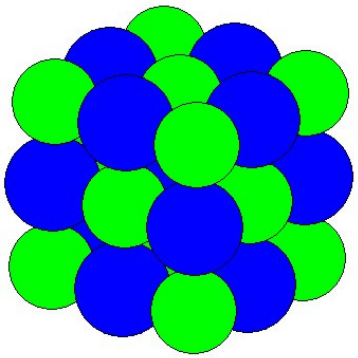
CsCl =Simple Cubic
with Basis

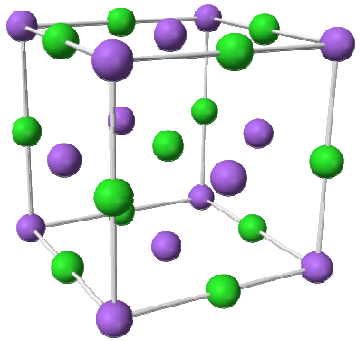
Cs at [0, 0, 0]
Cl at [½, ½, ½]

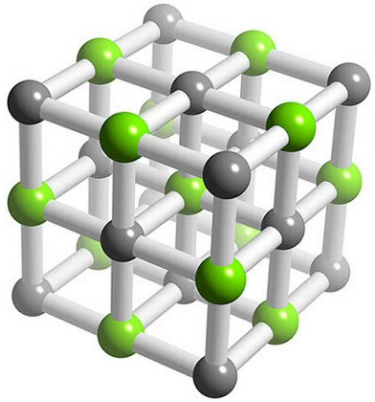


Cs = Simple Cubic
with Basis
= BCC

Cs at [0, 0, 0]
Cs at [½, ½, ½]







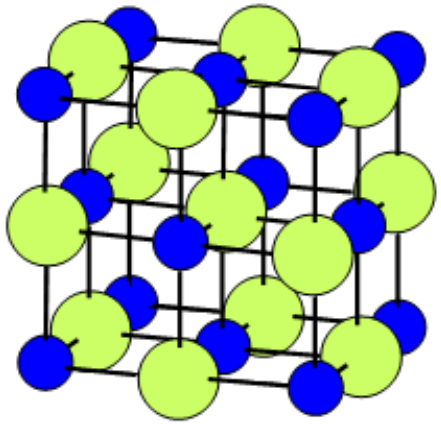
sodium chloride (NaCl)

lattice: cubic F

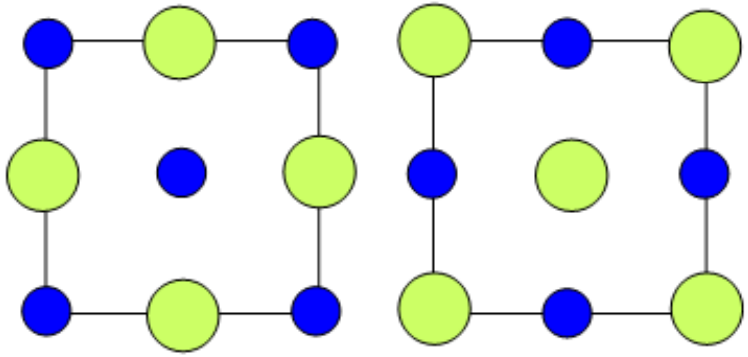
basis :

Na 000

Cl ½½½



Plan view

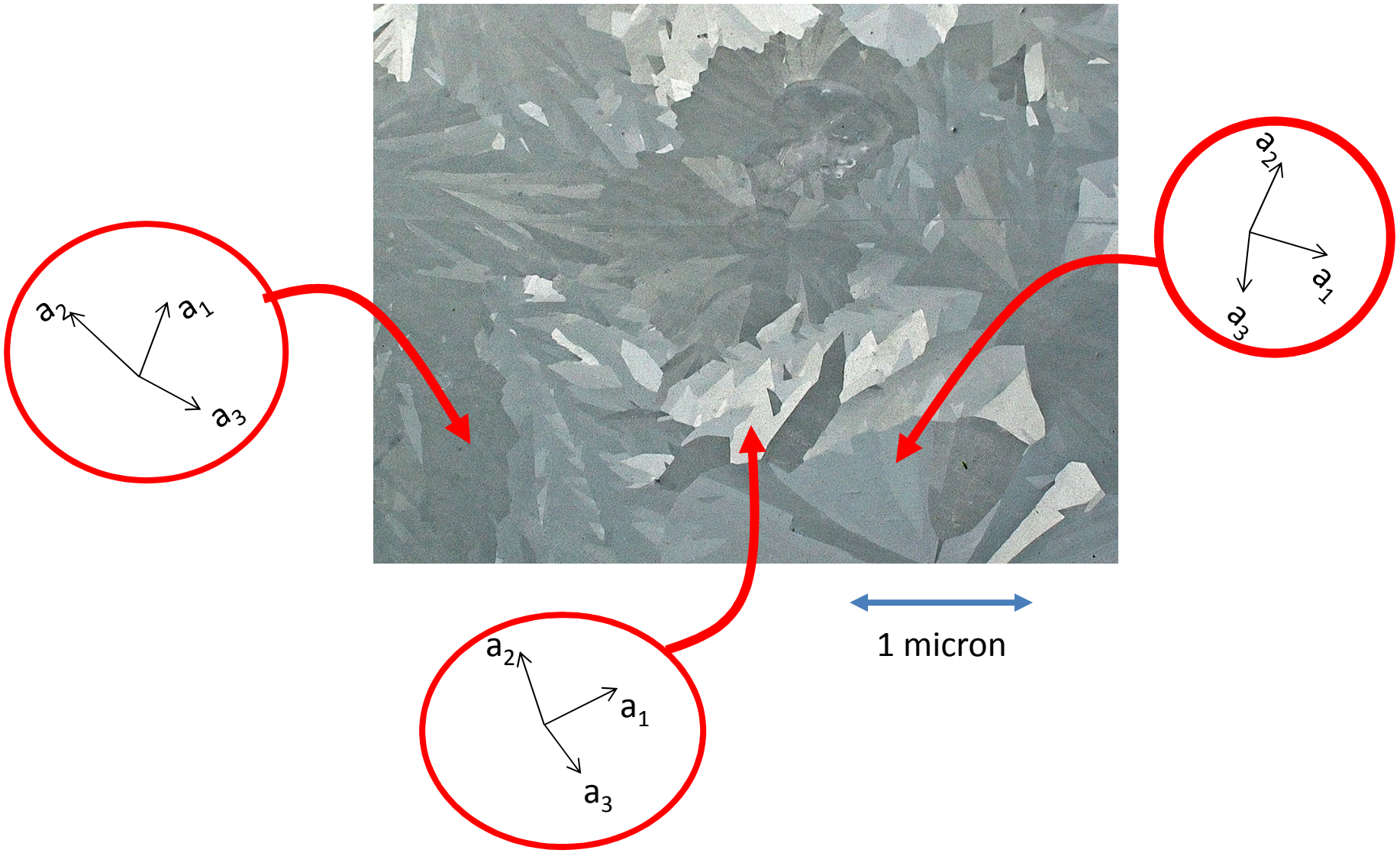


$z = 0$ layer

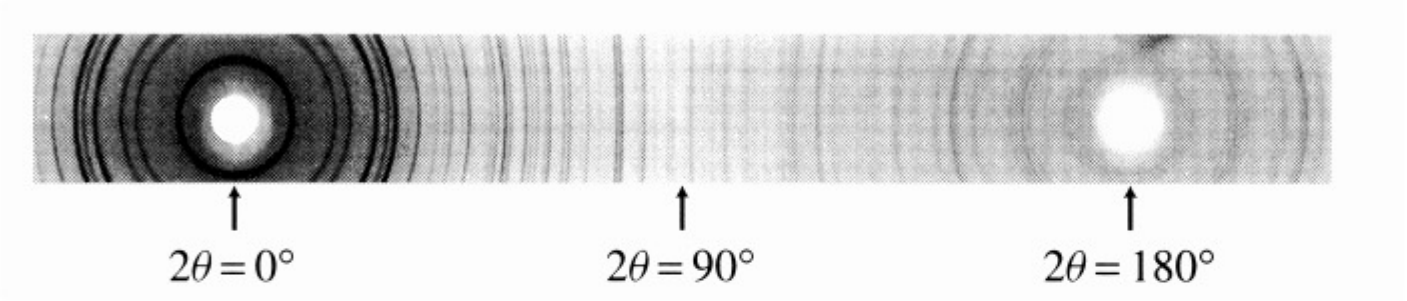
$z = ½$ layer

Na forms FCC lattice.

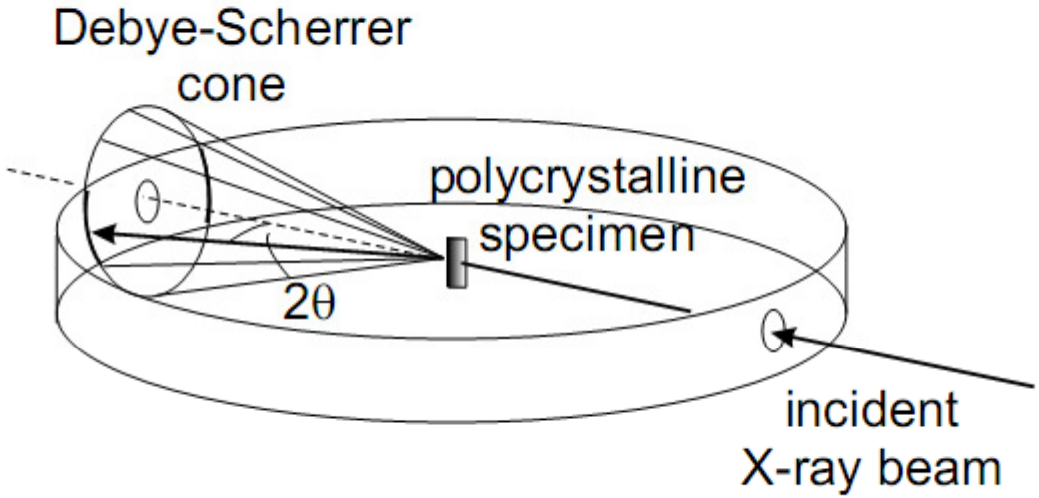
Cl is displaced (1/2,1/2,1/2) from each Na

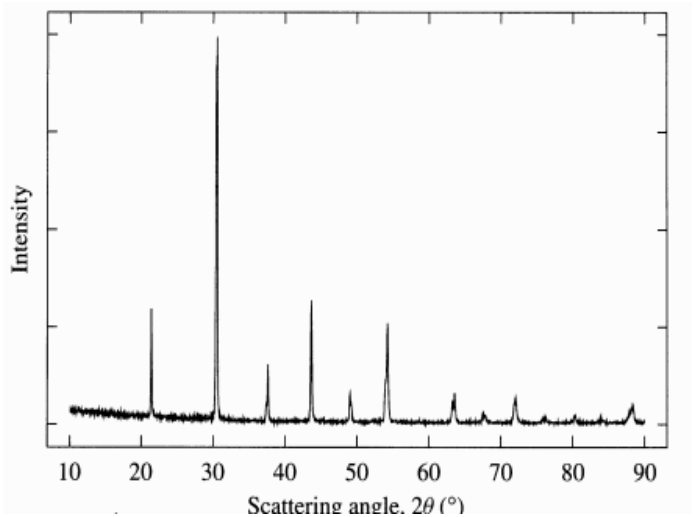


Polycrystalline Material

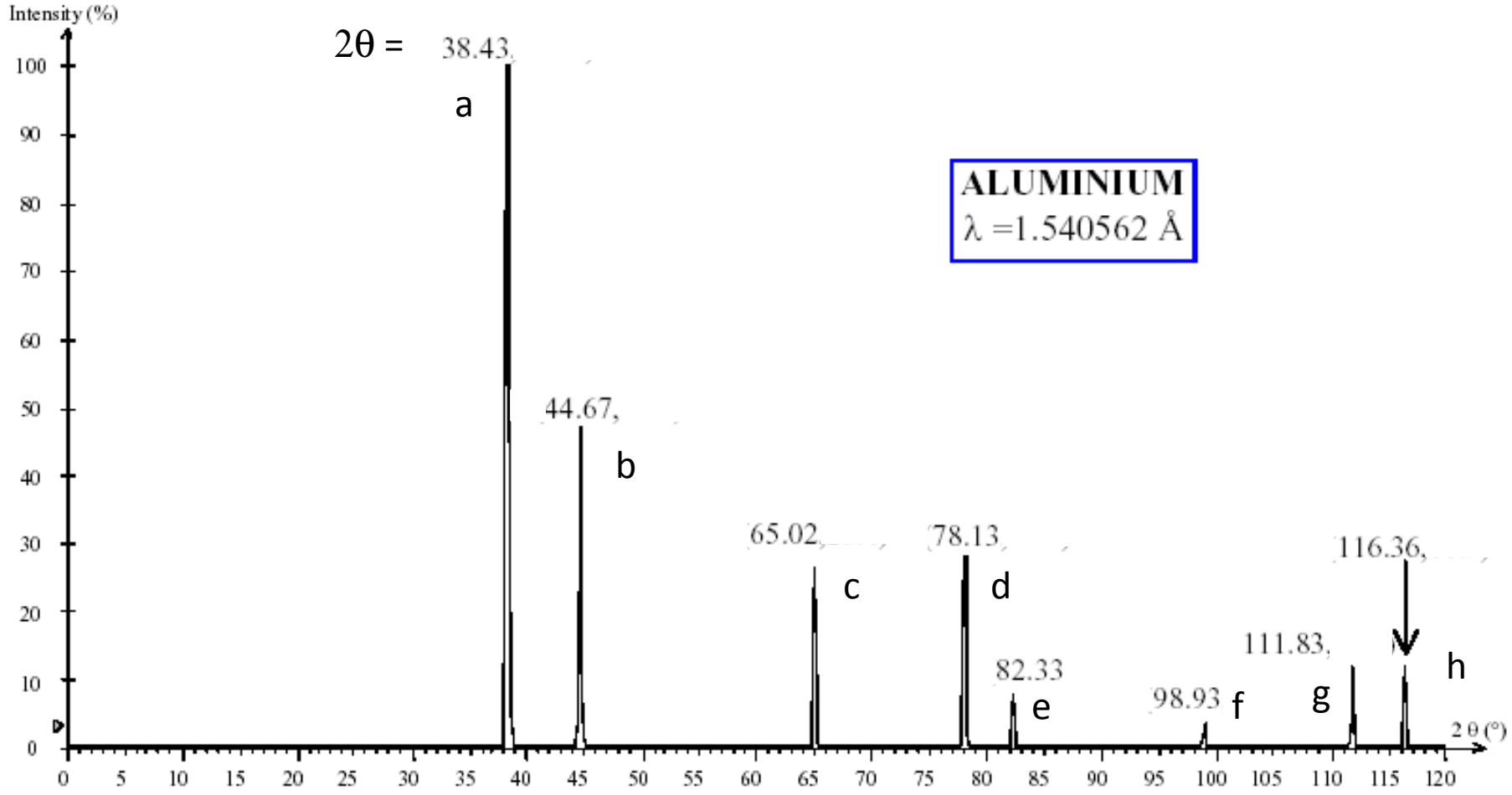


X-ray diffraction rings recorded on a photographic film





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



Scattering Selection Rules

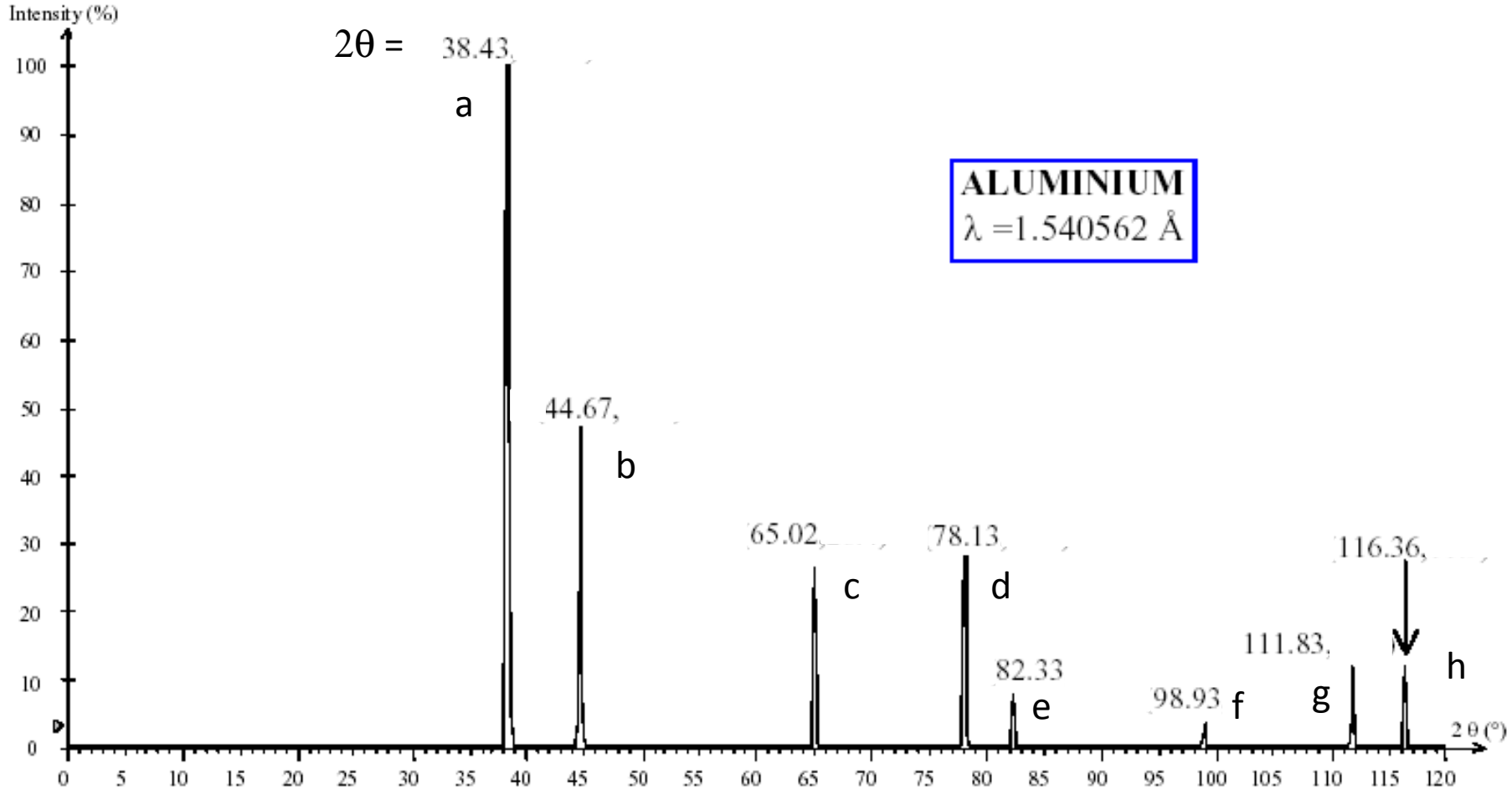
P = Primitive (simple) cubic — All hkl
I = BCC — $h+k+l$ = even
F = FCC — h,k,l all even or all odd

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



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

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

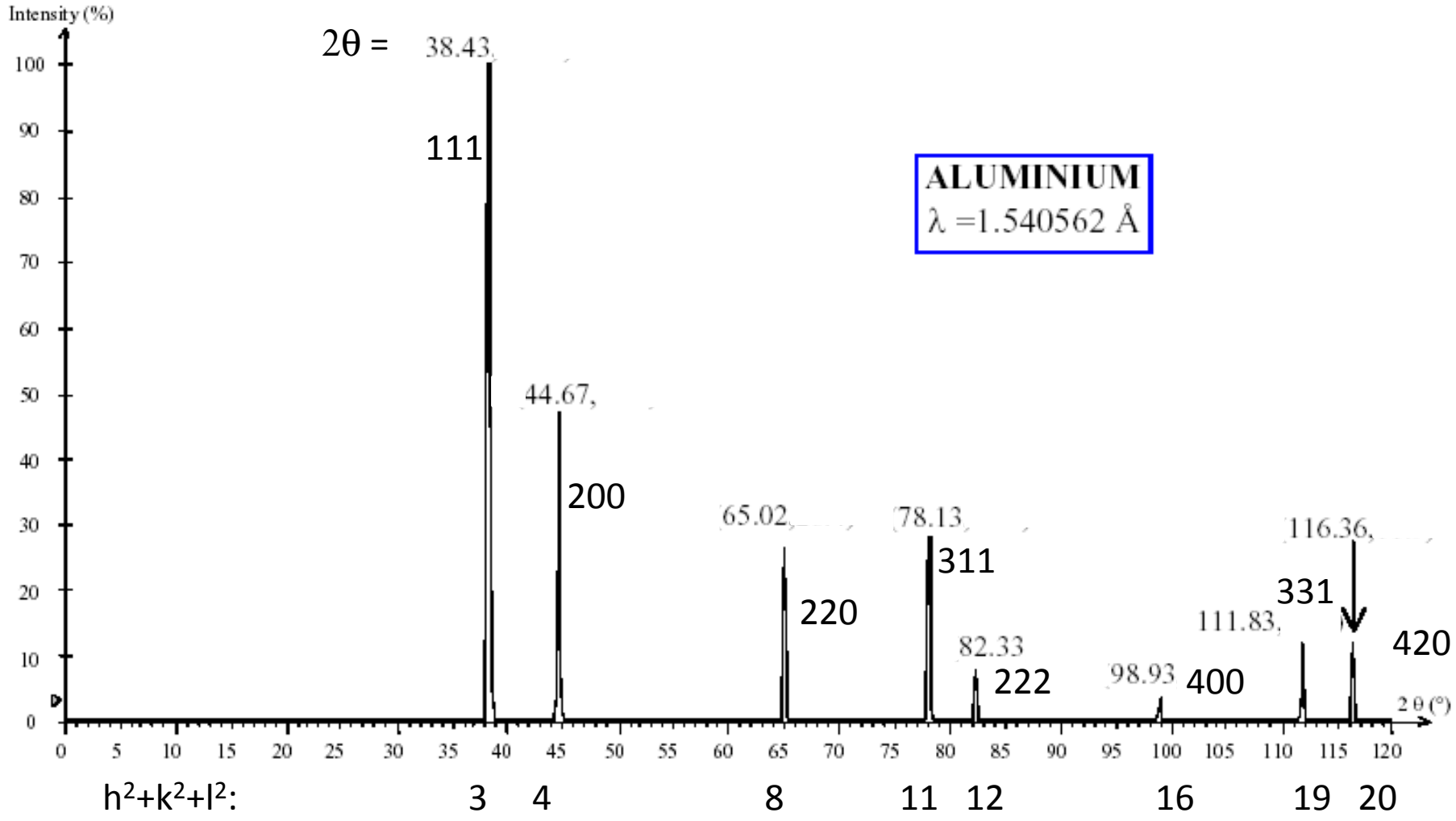
$$N = h^2 + k^2 + l^2$$

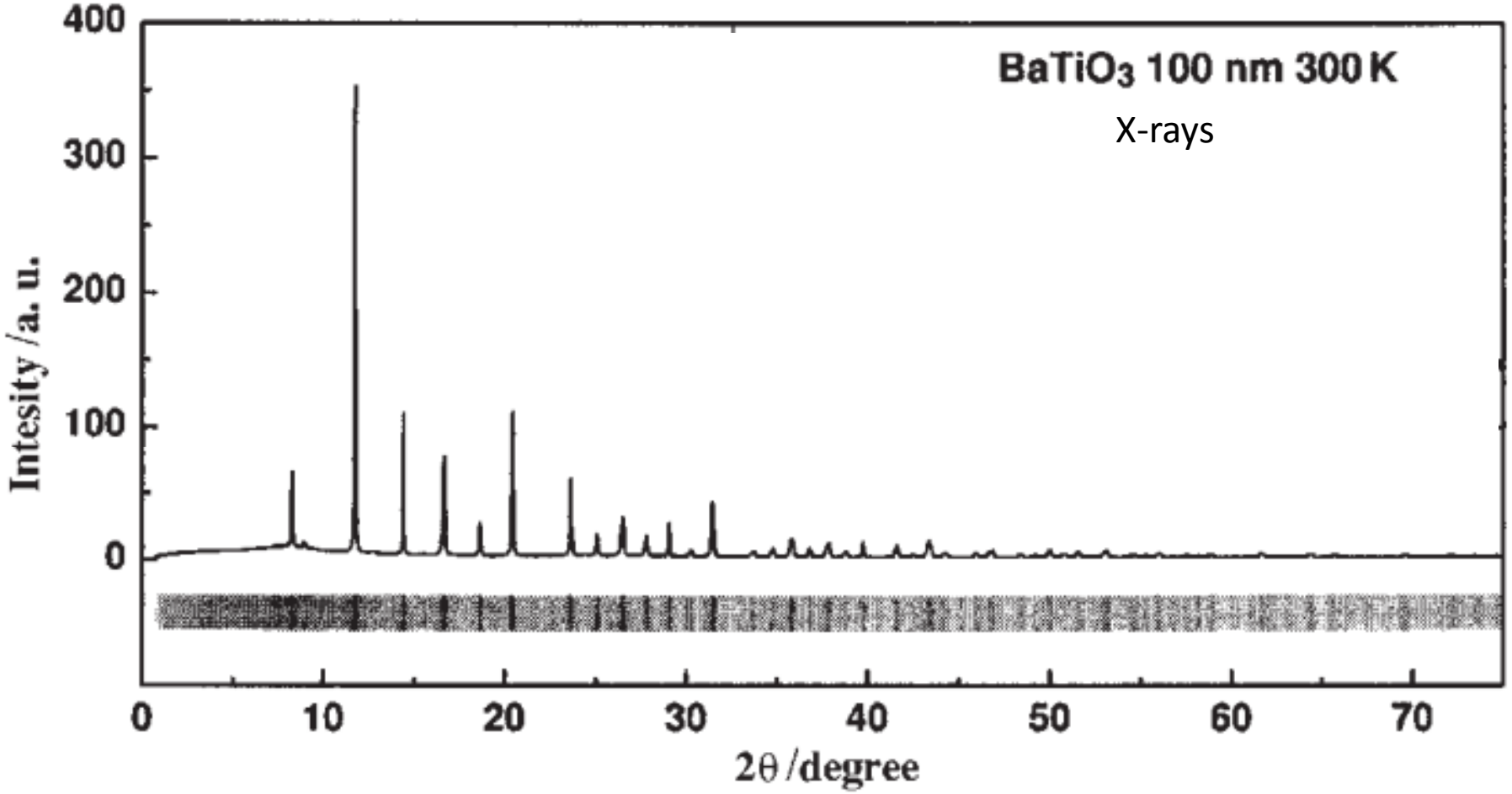
$$d = \frac{\lambda}{2\sin\theta}$$

Peak	Angle 2θ	d	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

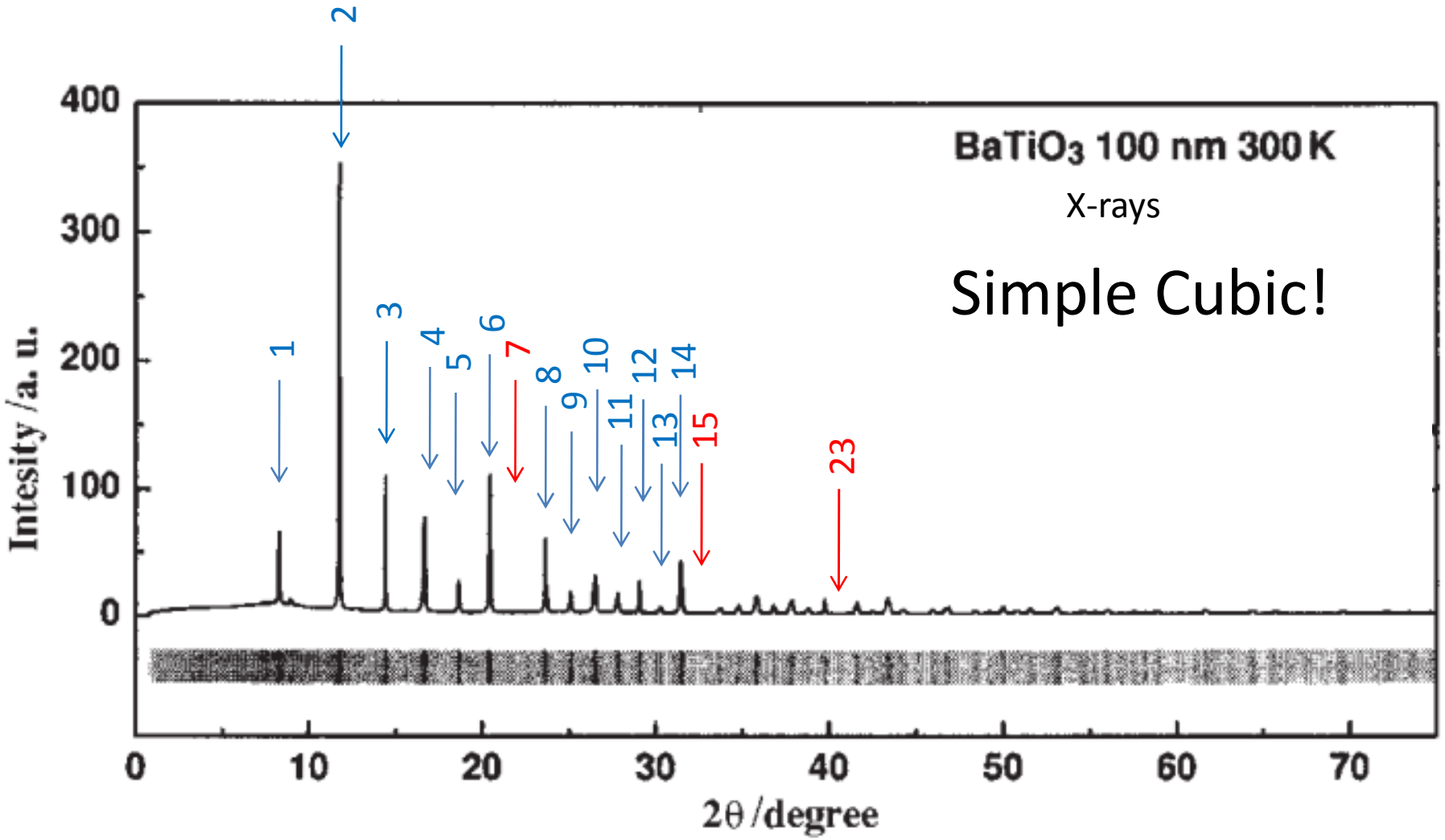
FCC! : h,k,l all even or all odd : N = 3,4,8,11,12 …

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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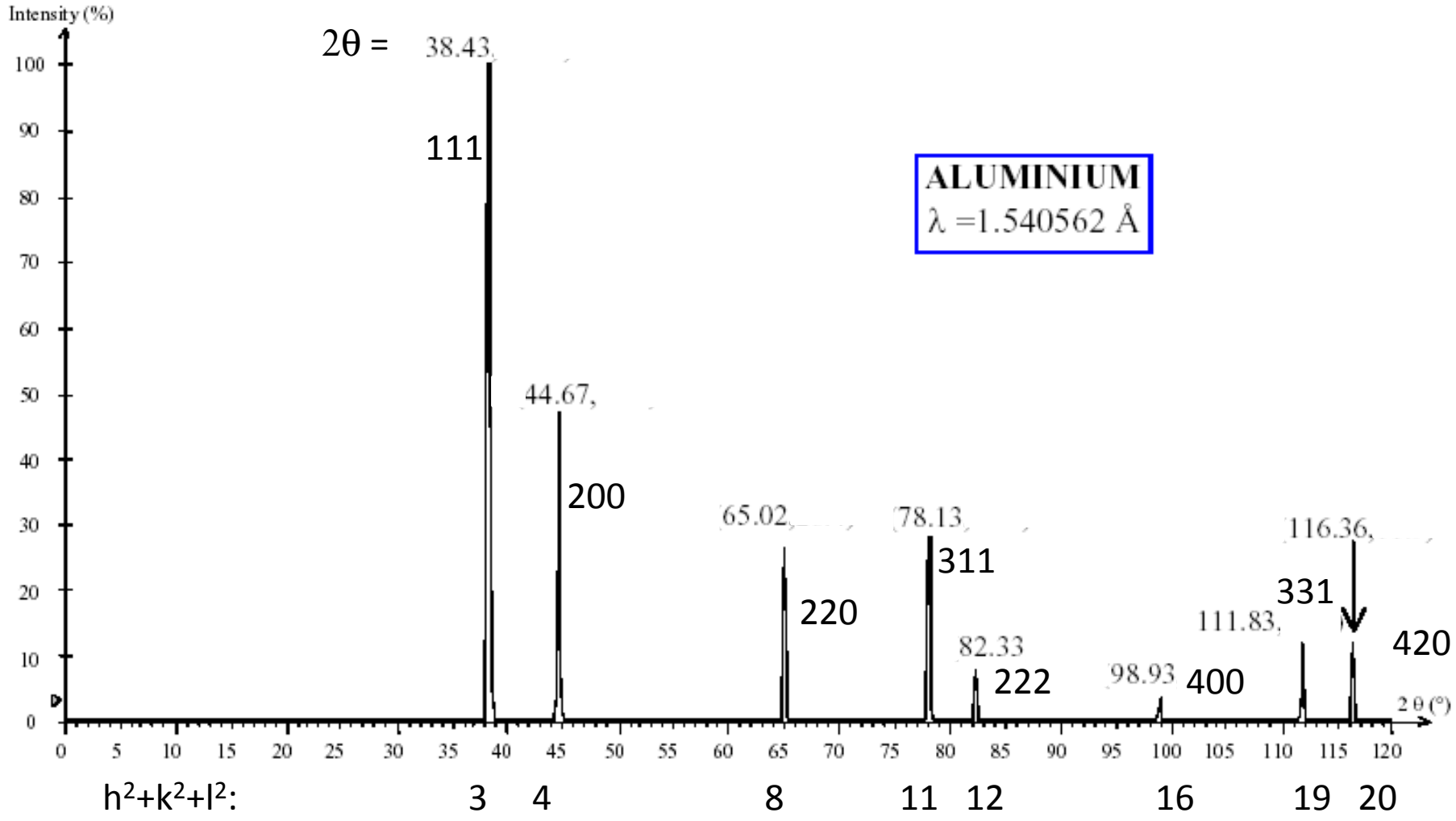

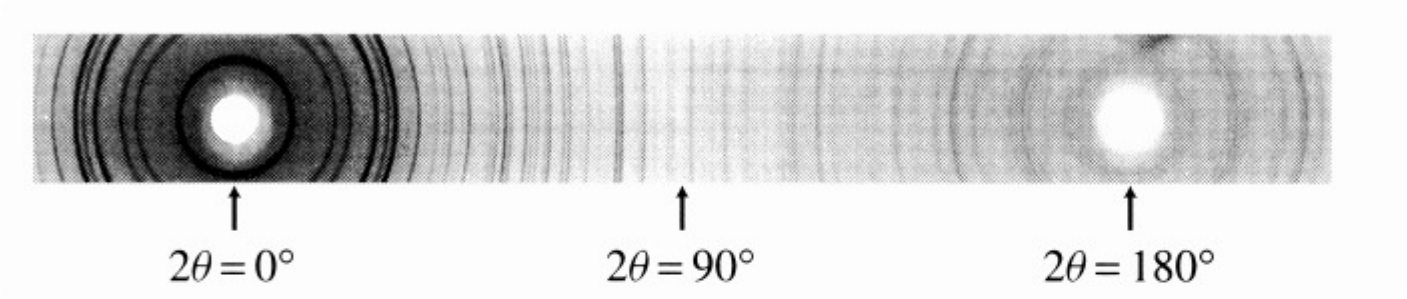

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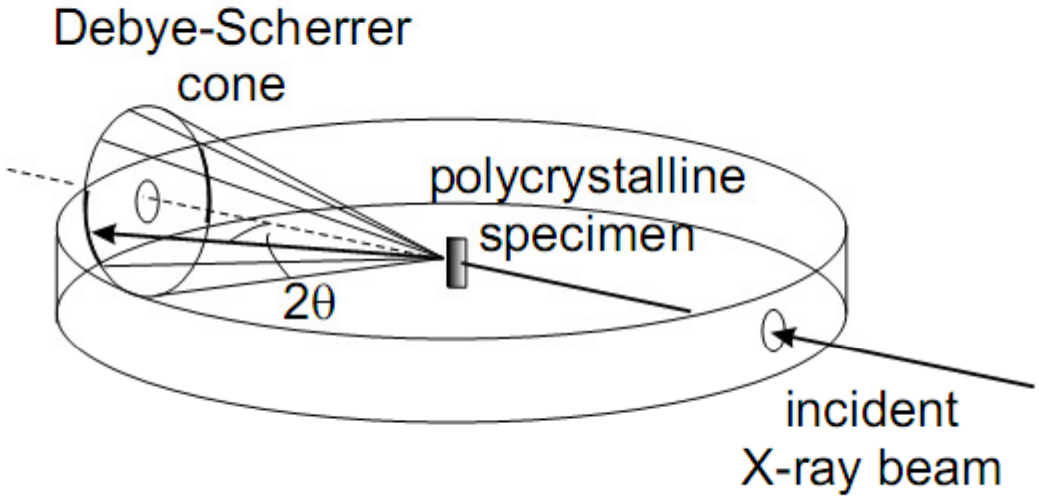
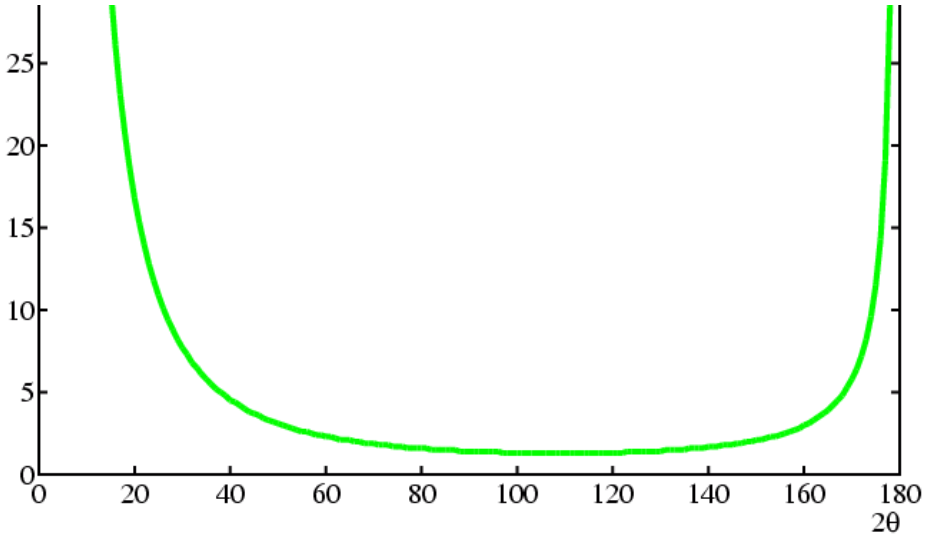
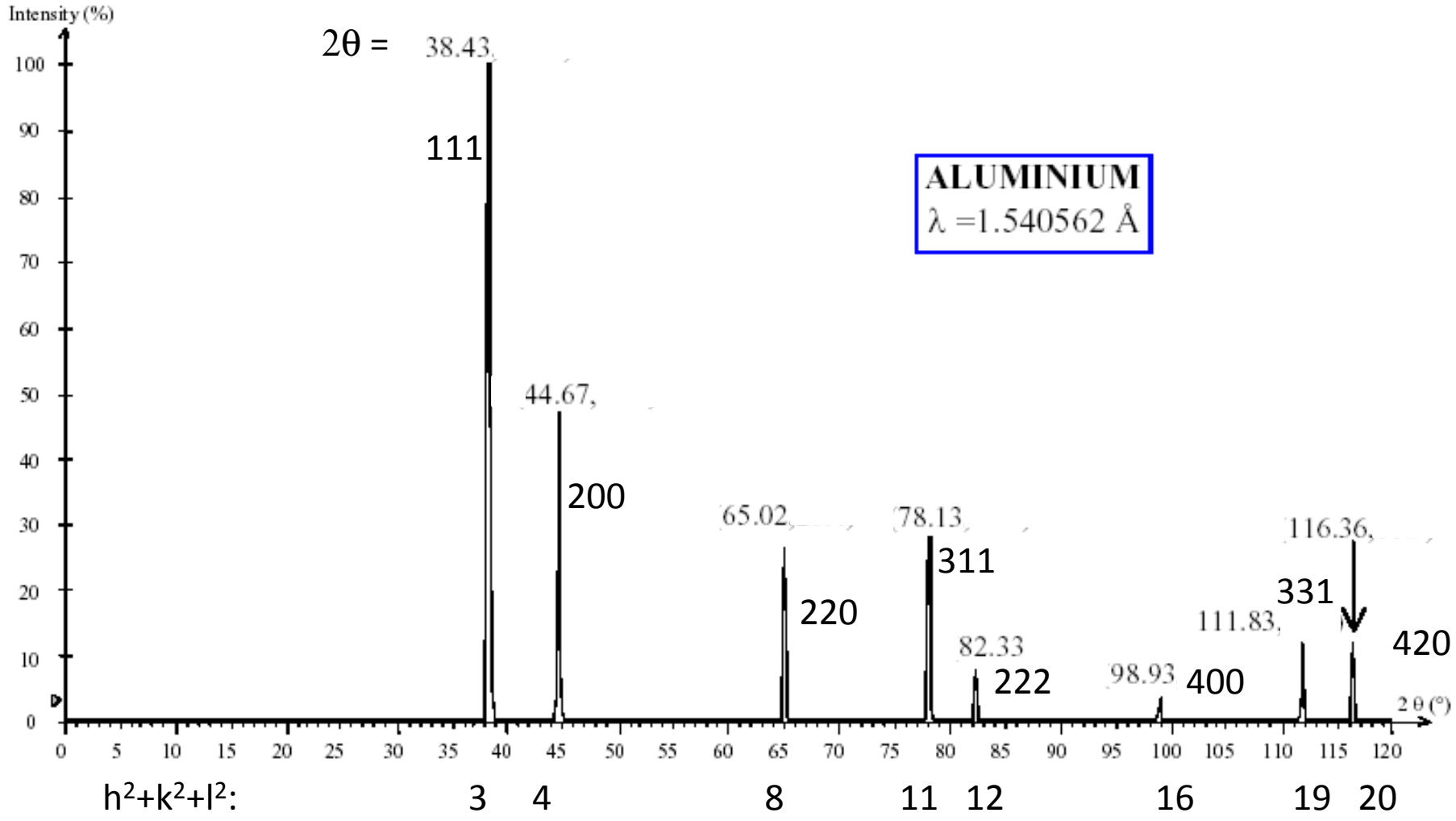
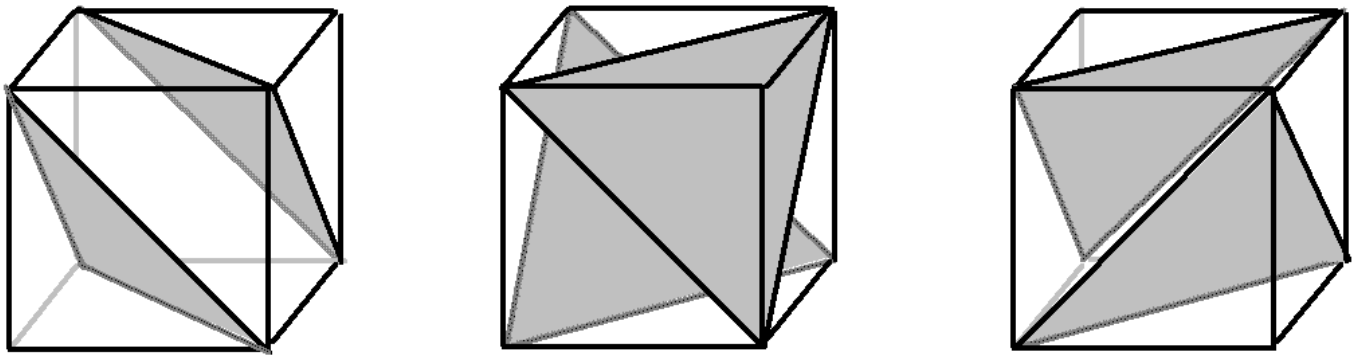




Geometric Lorentz Factor

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,…)
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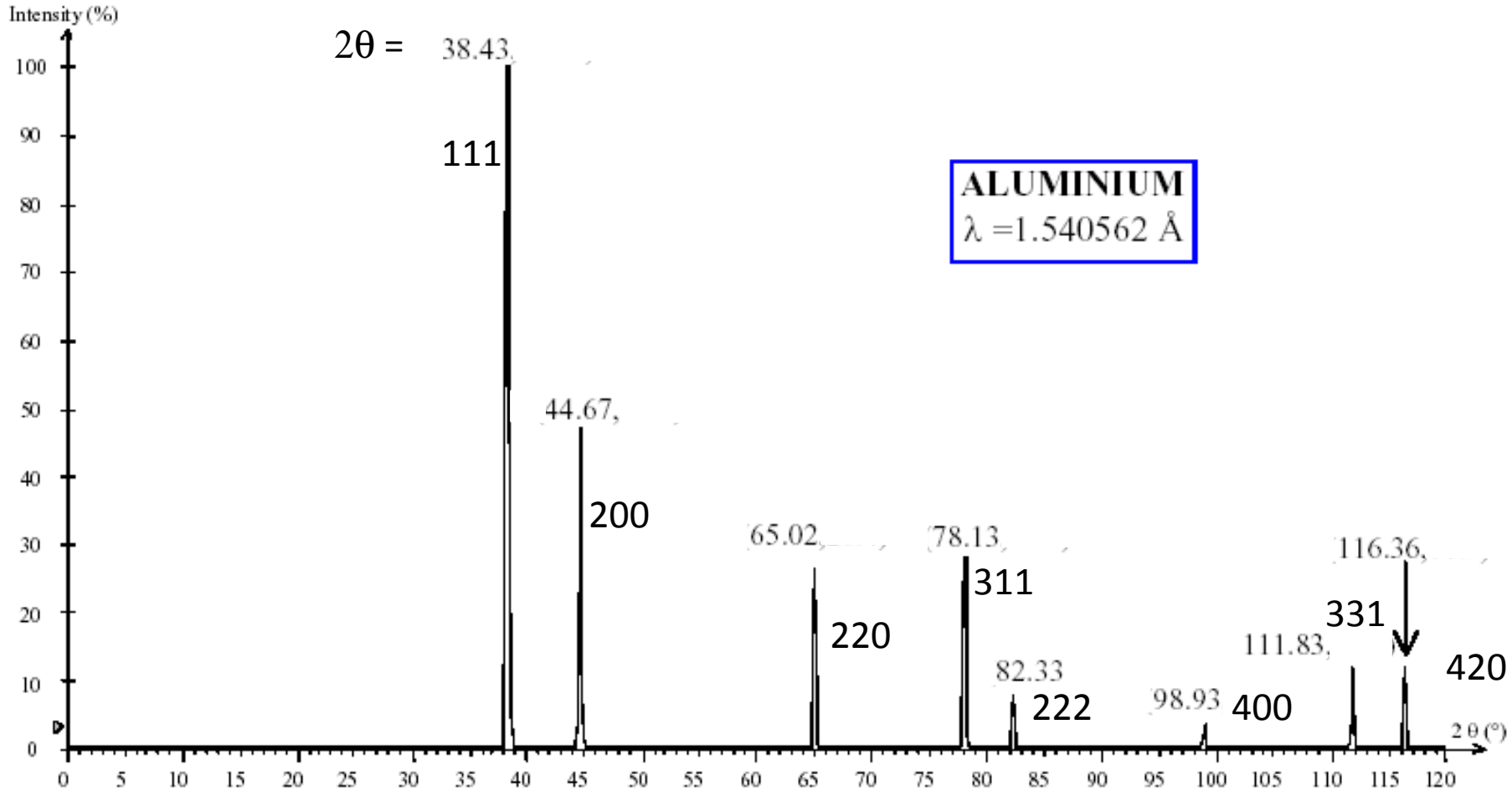

$h^2+k^2+l^2$:	3	4	8	11	12	16	19	20
Multiplicity:	8	6	12	24	8	6	24	24