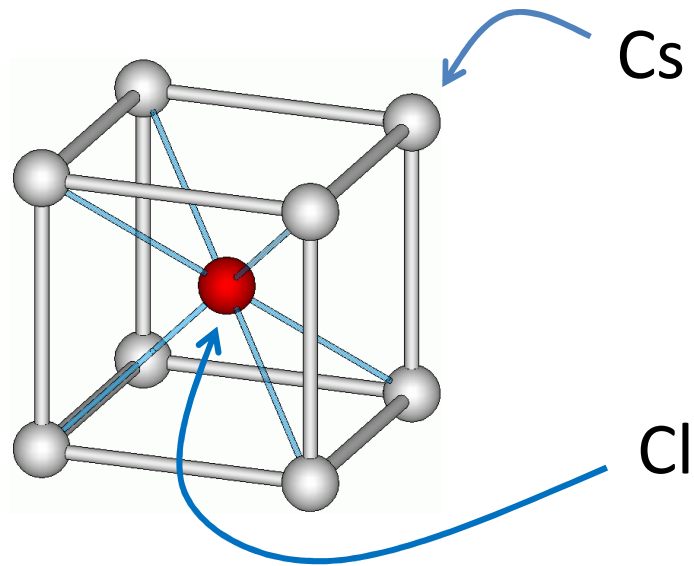


Slides
Condensed Matter Physics
Lecture 13

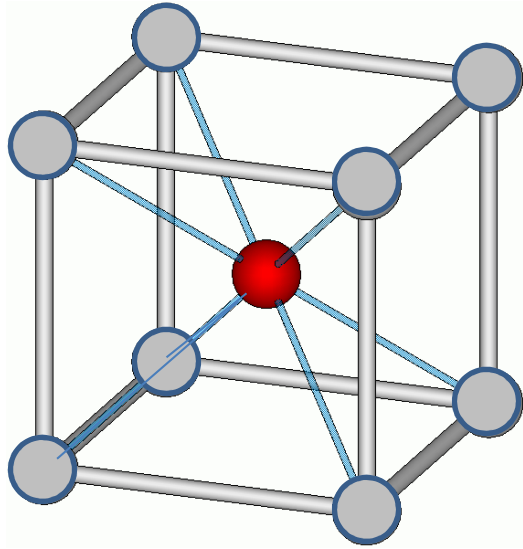


Cesium Chloride (CsCl): A simple cubic Lattice with a Basis

Basis:

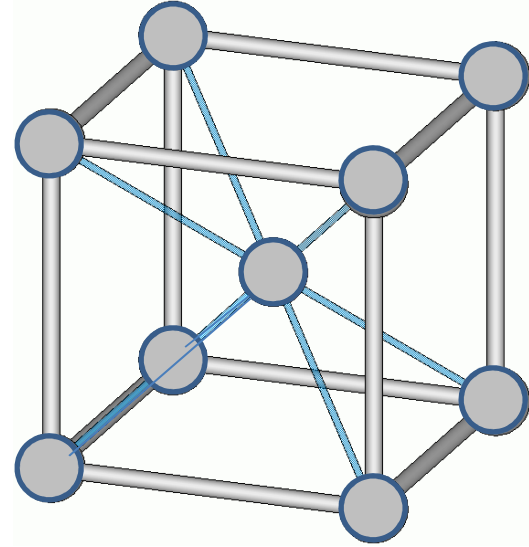
Cs at $[0, 0, 0]$ (i.e., on the simple cubic)

Cl at $[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$ (i.e., in the middle of each cube)



CsCl = Simple Cubic
with Basis

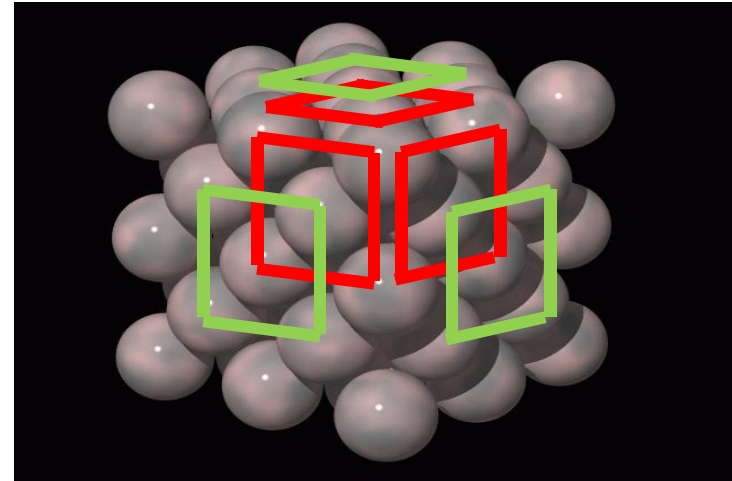
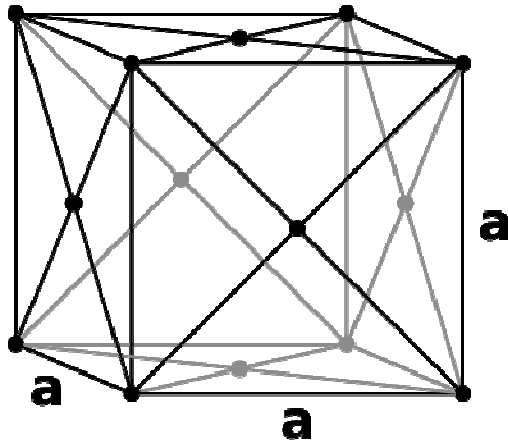
Cs at $[0, 0, 0]$
Cl at $[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$



Cs = Simple Cubic
with Basis
= BCC

Cs at $[0, 0, 0]$
Cs at $[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$

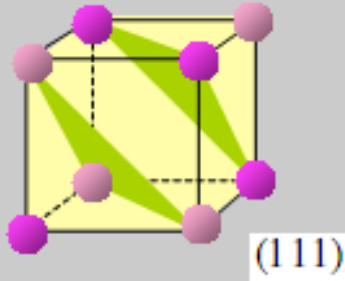
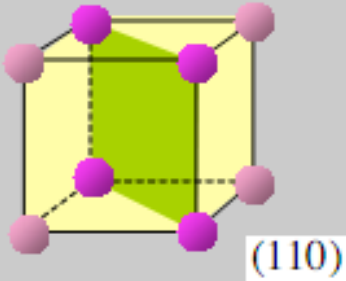
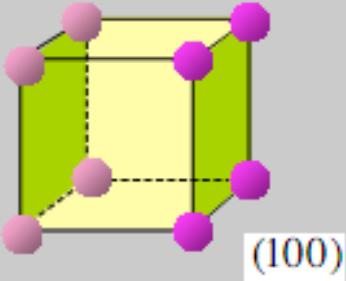
Unit cell of Face Centered Cubic Lattice (FCC) (Notated cubic-F)



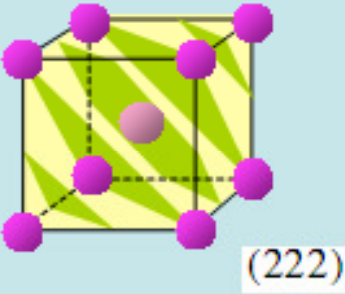
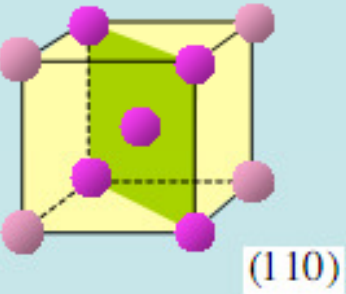
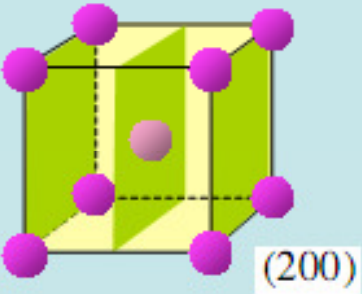
FCC = Simple Cubic with Basis

Basis = $[0,0,0]$, $[\frac{1}{2}, \frac{1}{2}, 0]$, $[\frac{1}{2}, 0, \frac{1}{2}]$, $[0, \frac{1}{2}, \frac{1}{2}]$

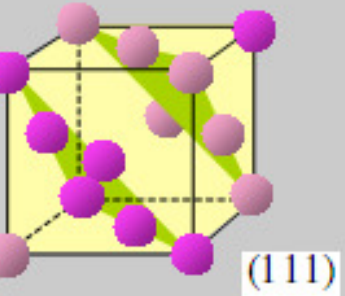
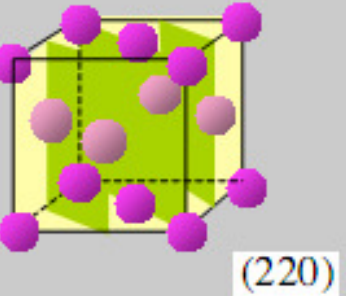
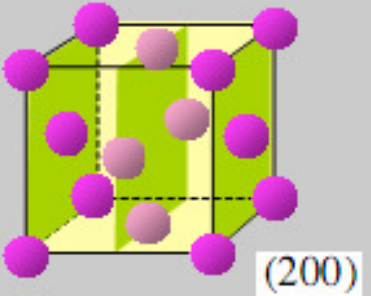
SC

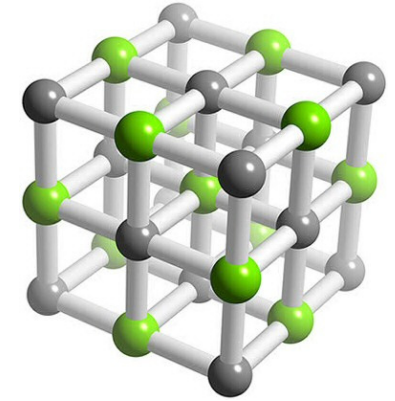
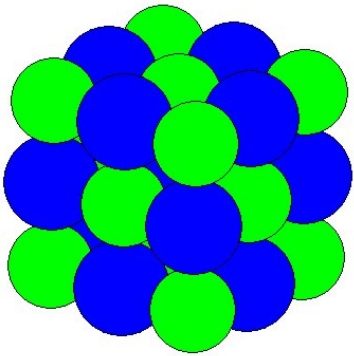


bcc



fcc





sodium chloride (NaCl)

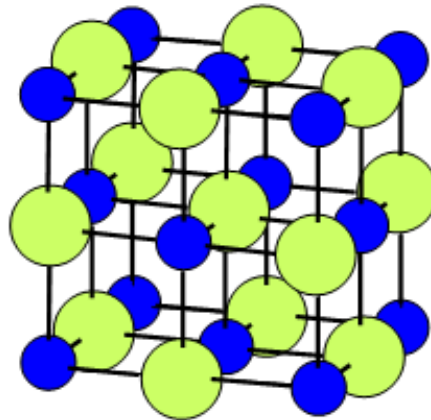
lattice: cubic F

basis :

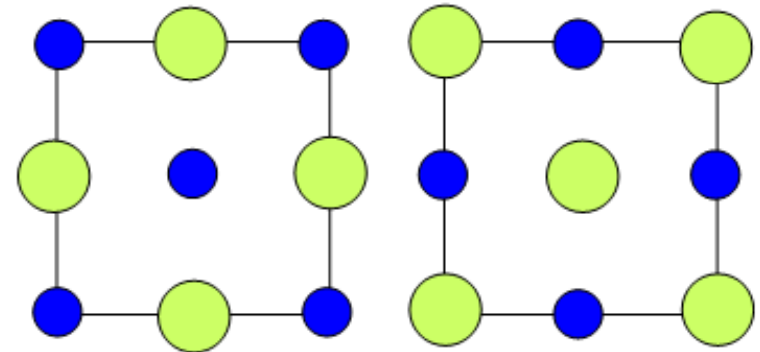
Na 000



Cl $\frac{1}{2}\frac{1}{2}\frac{1}{2}$



Plan view

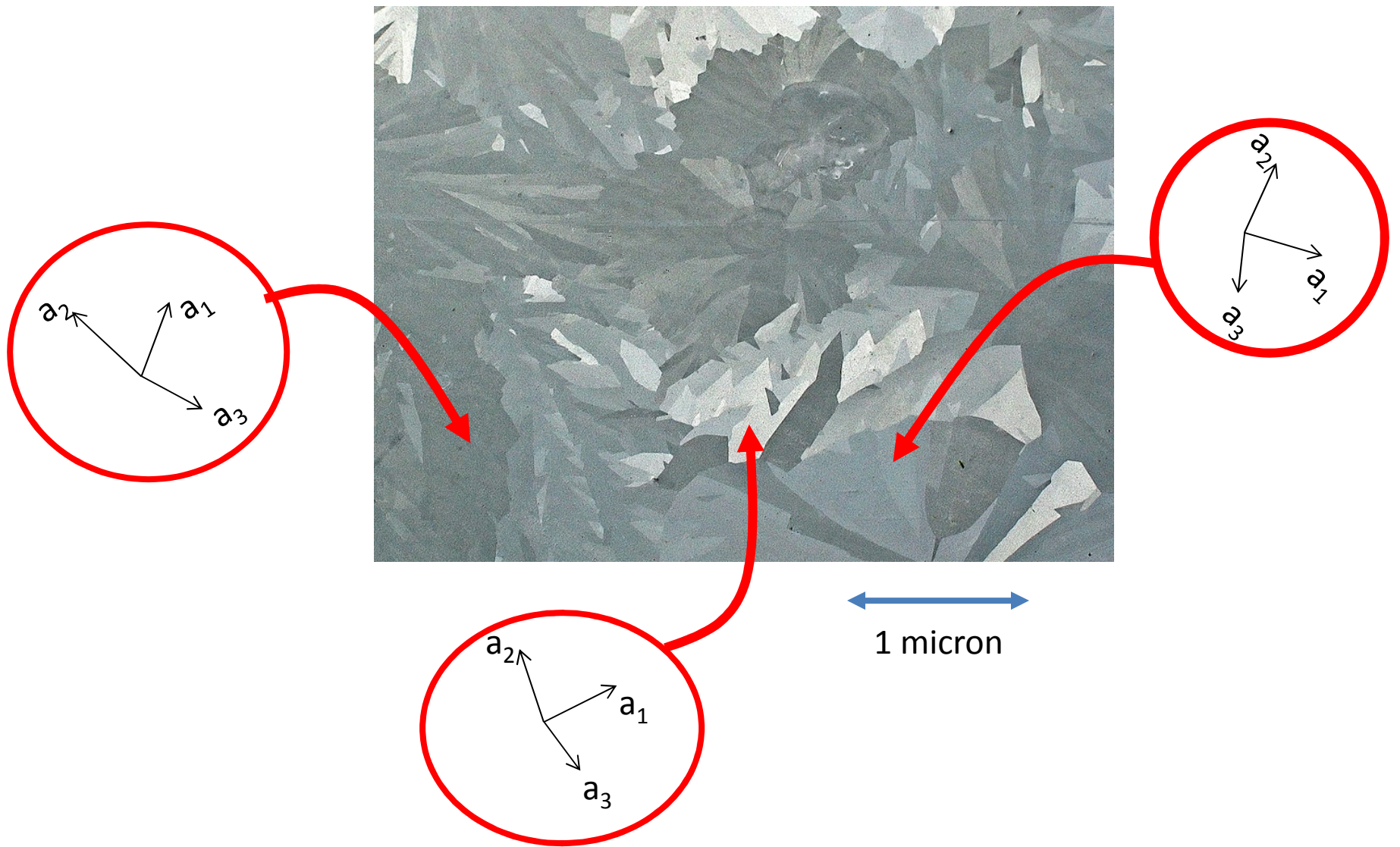


$z = 0$ layer

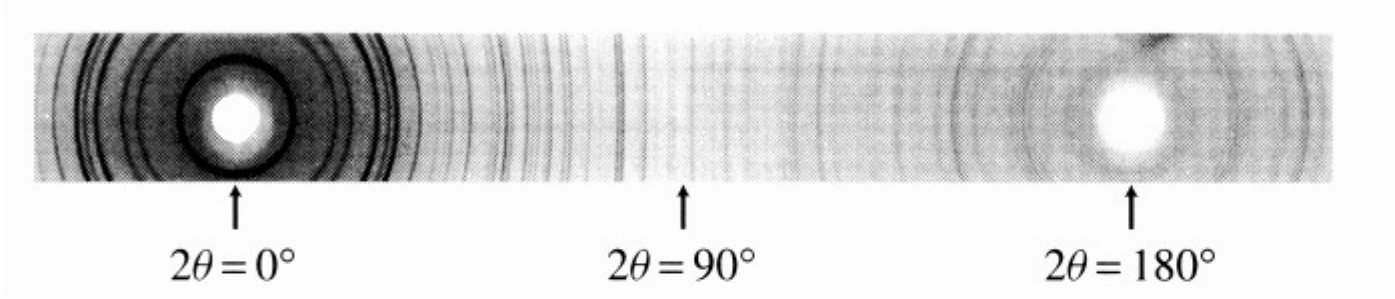
$z = \frac{1}{2}$ layer

Na forms FCC lattice.

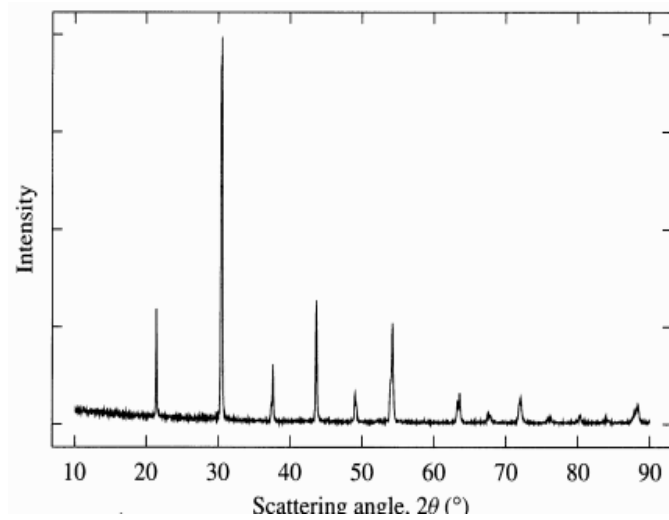
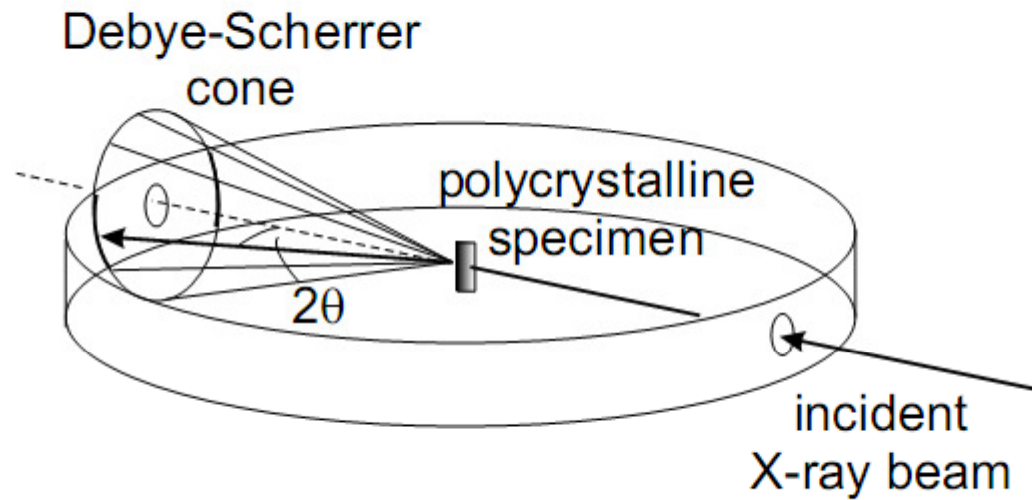
Cl is displaced $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ from each Na



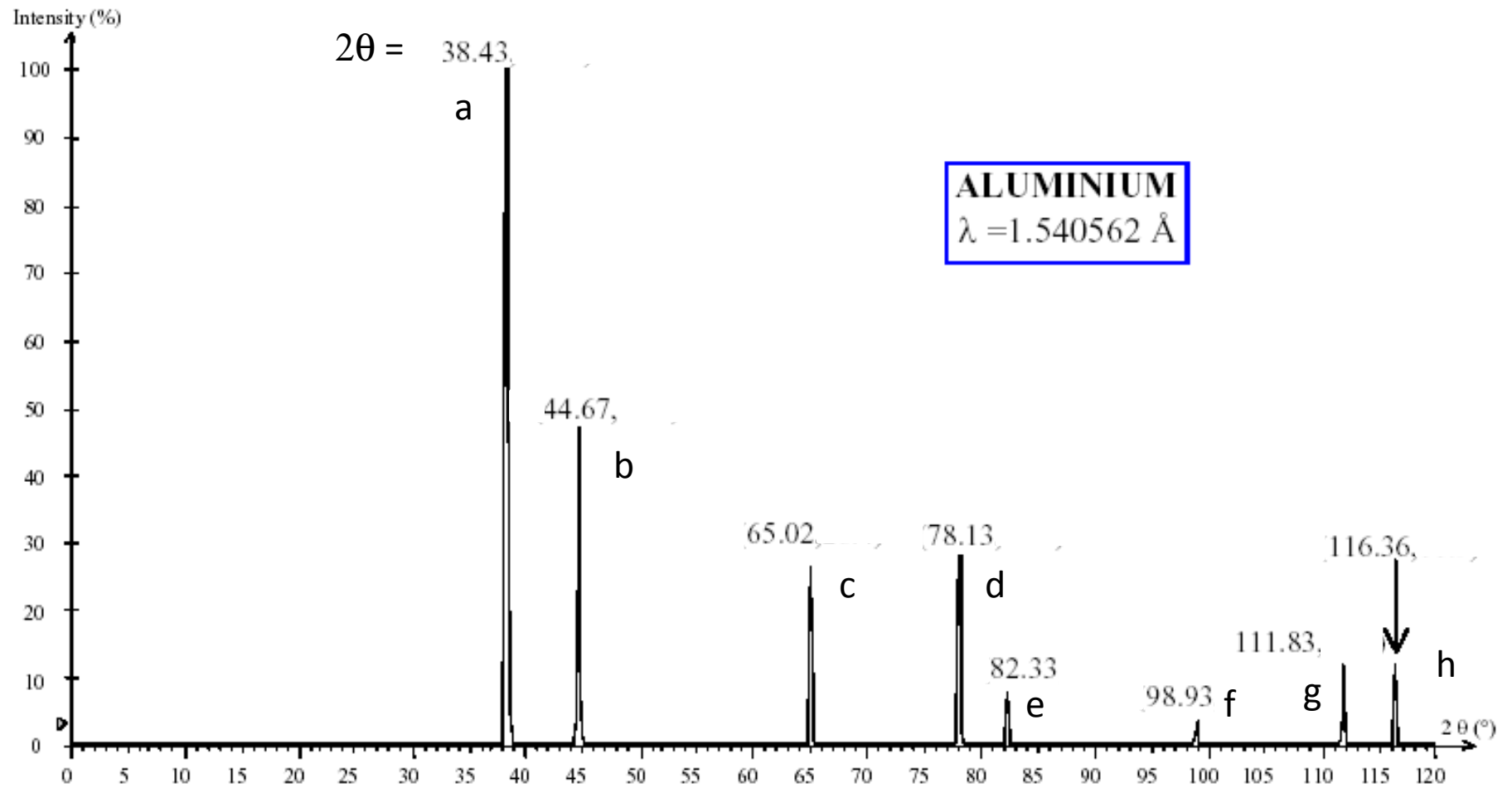
Polycrystalline Material



X-ray diffraction rings recorded on a photographic film



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



Scattering
Selection Rules

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

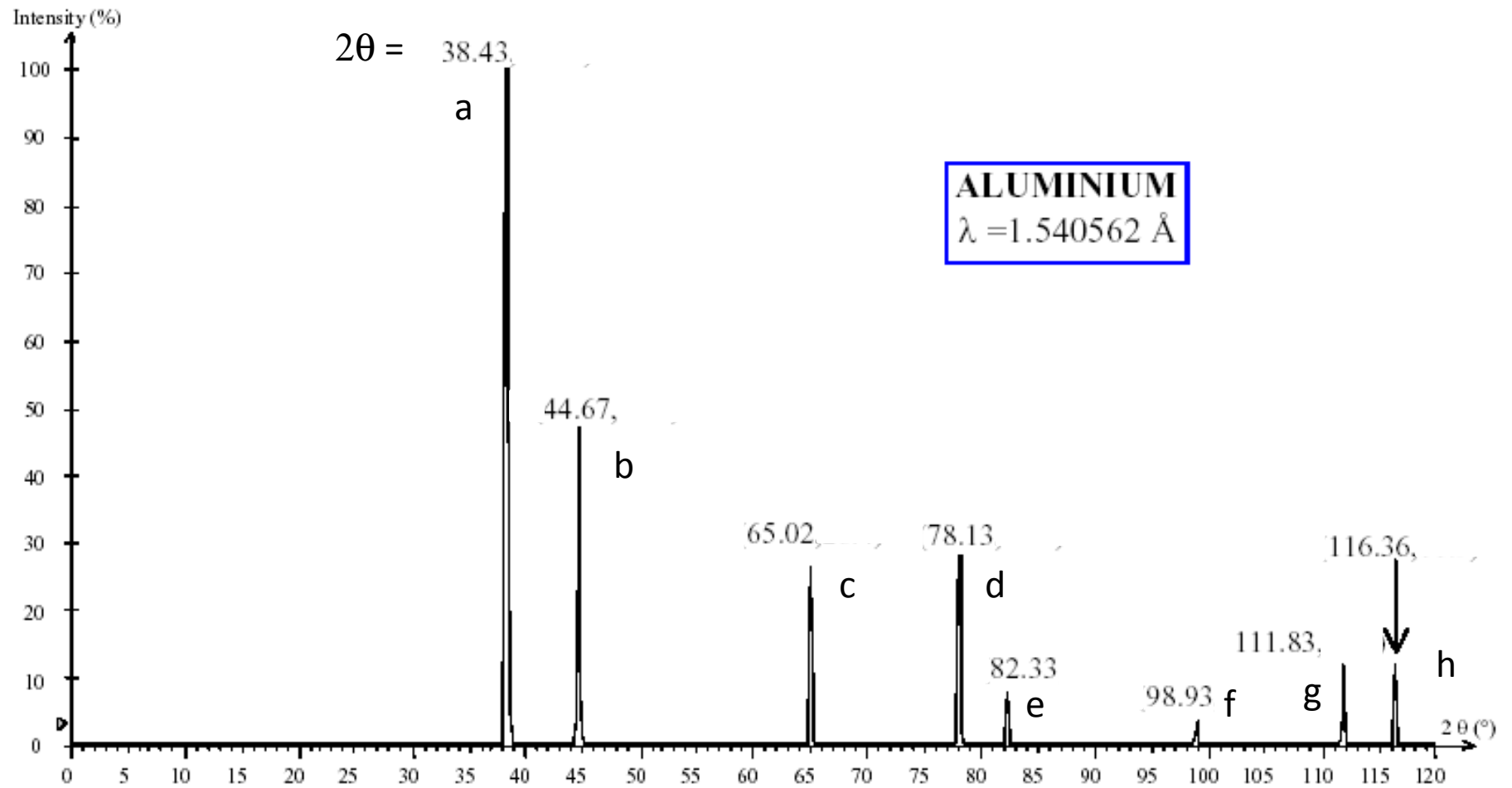
All hkl
 $h+k+l = \text{even}$
 h,k,l all even or all odd

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



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

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

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



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

$$d_a^2/d^2$$

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

$$N$$

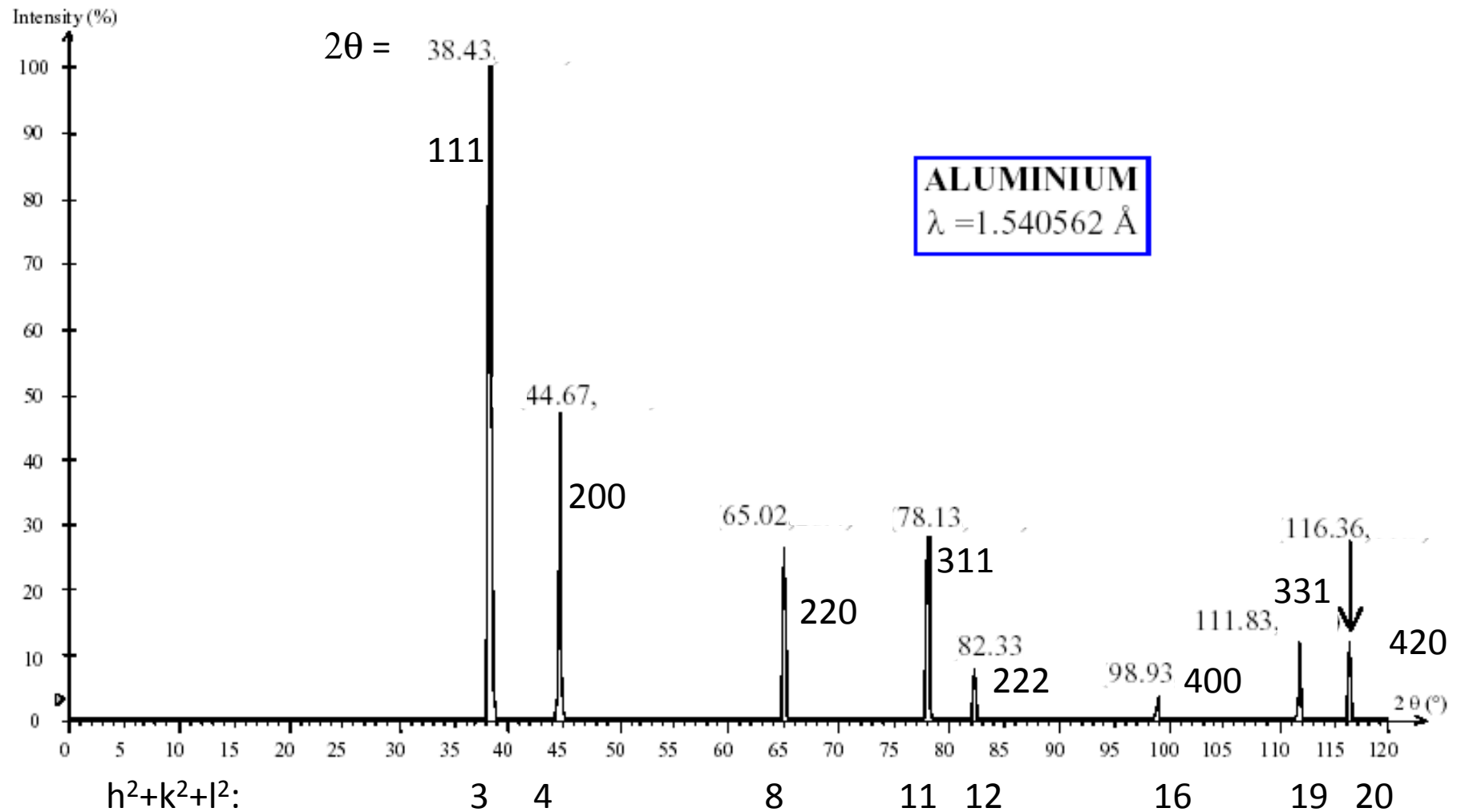
$$\{hkl\}$$

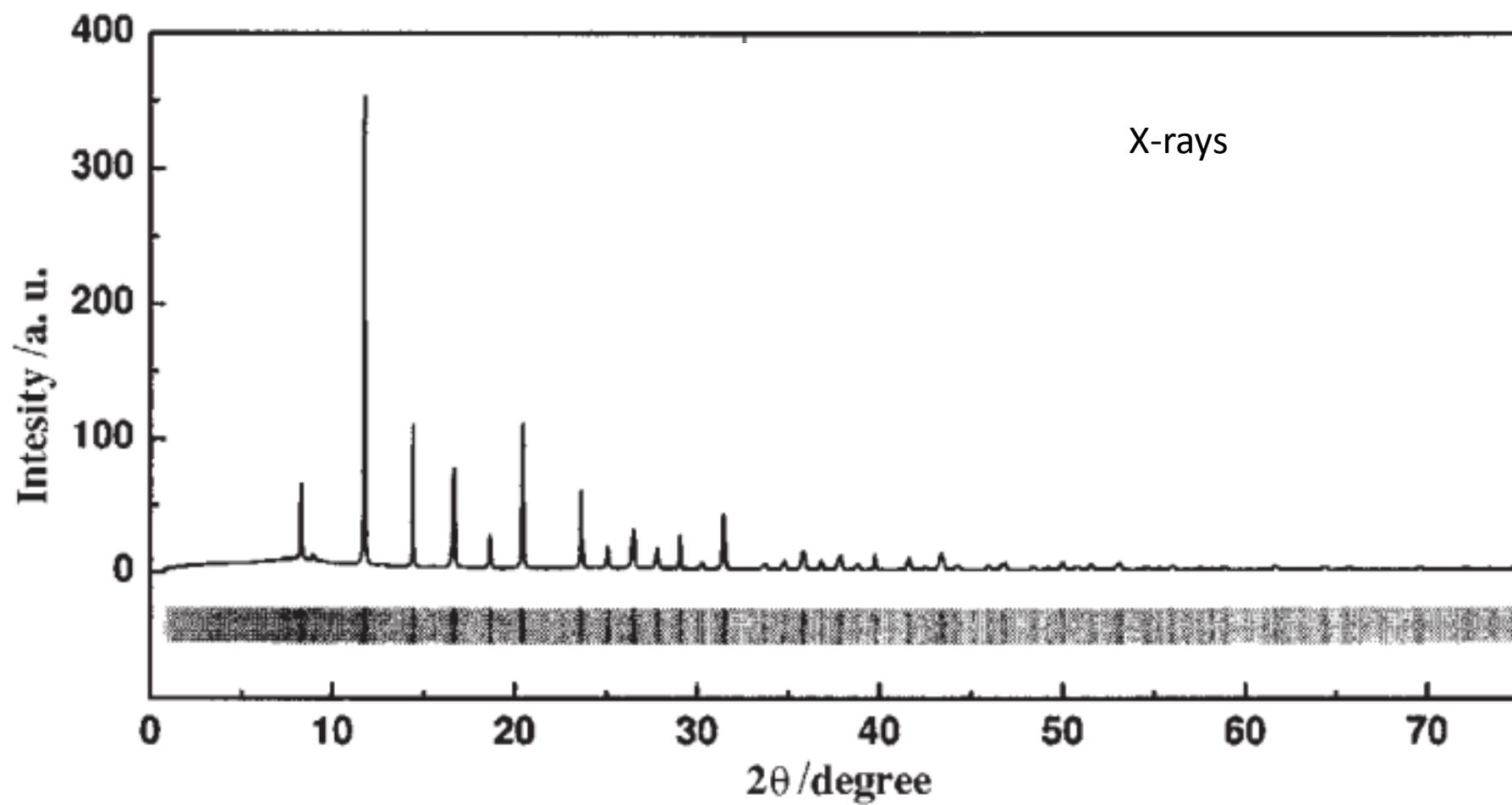
$$a$$

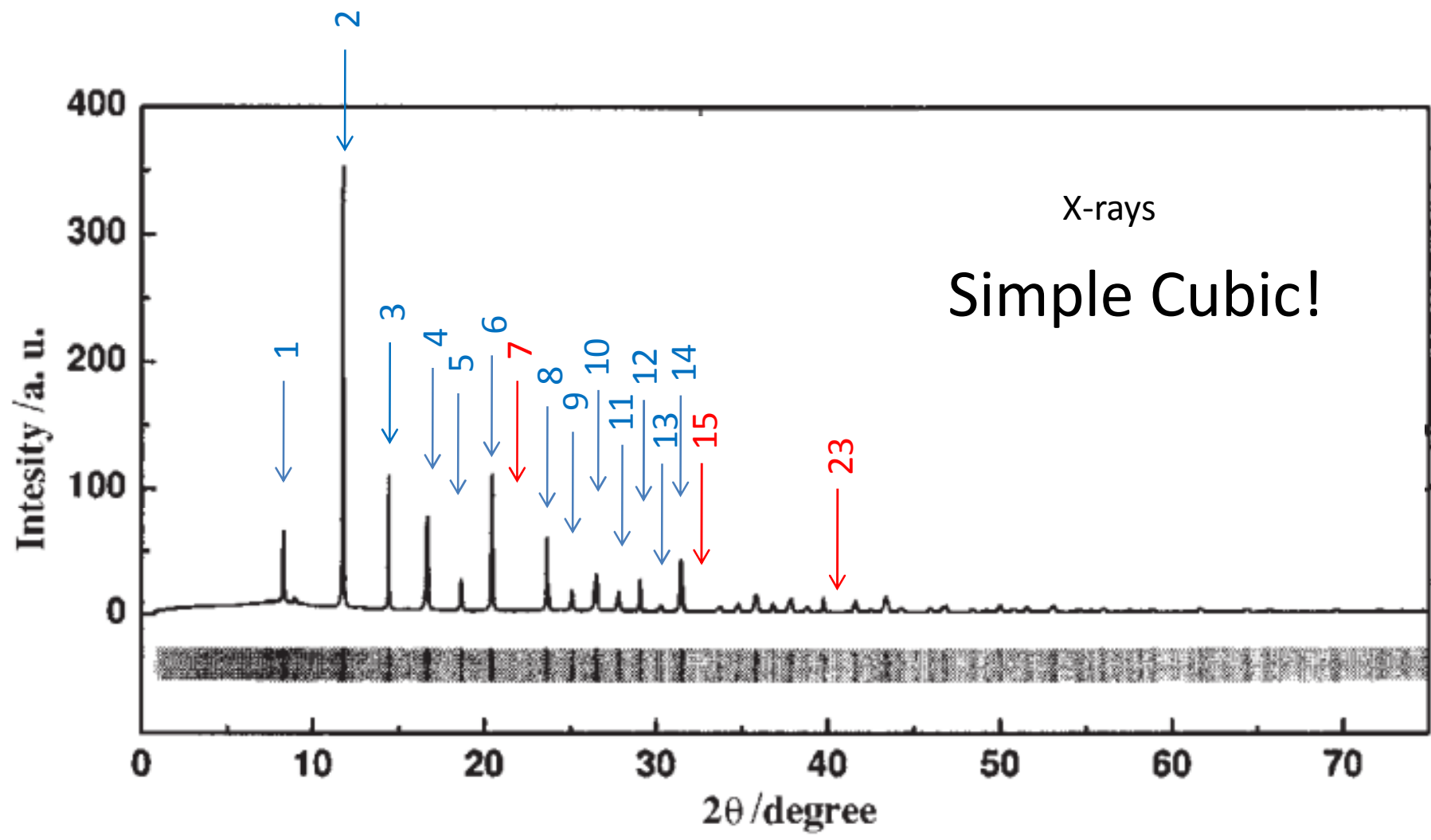
Peak	Angle 2θ	$d = \frac{\lambda}{2 \sin \theta}$	d_a^2/d^2	$3d^2/d_a^2$	N	$\{hkl\}$	a
a	38.43	2.3405Å	1.0000	3.0000	3	111	4.0538Å
b	44.67	2.0269Å	1.3333	3.9999	4	200	4.0539Å
c	65.02	1.4332Å	2.6667	8.0002	8	220	4.0538Å
d	78.13	1.2223Å	3.6666	10.9999	11	311	4.0538Å
e	82.33	1.1702Å	4.0000	12.0001	12	222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

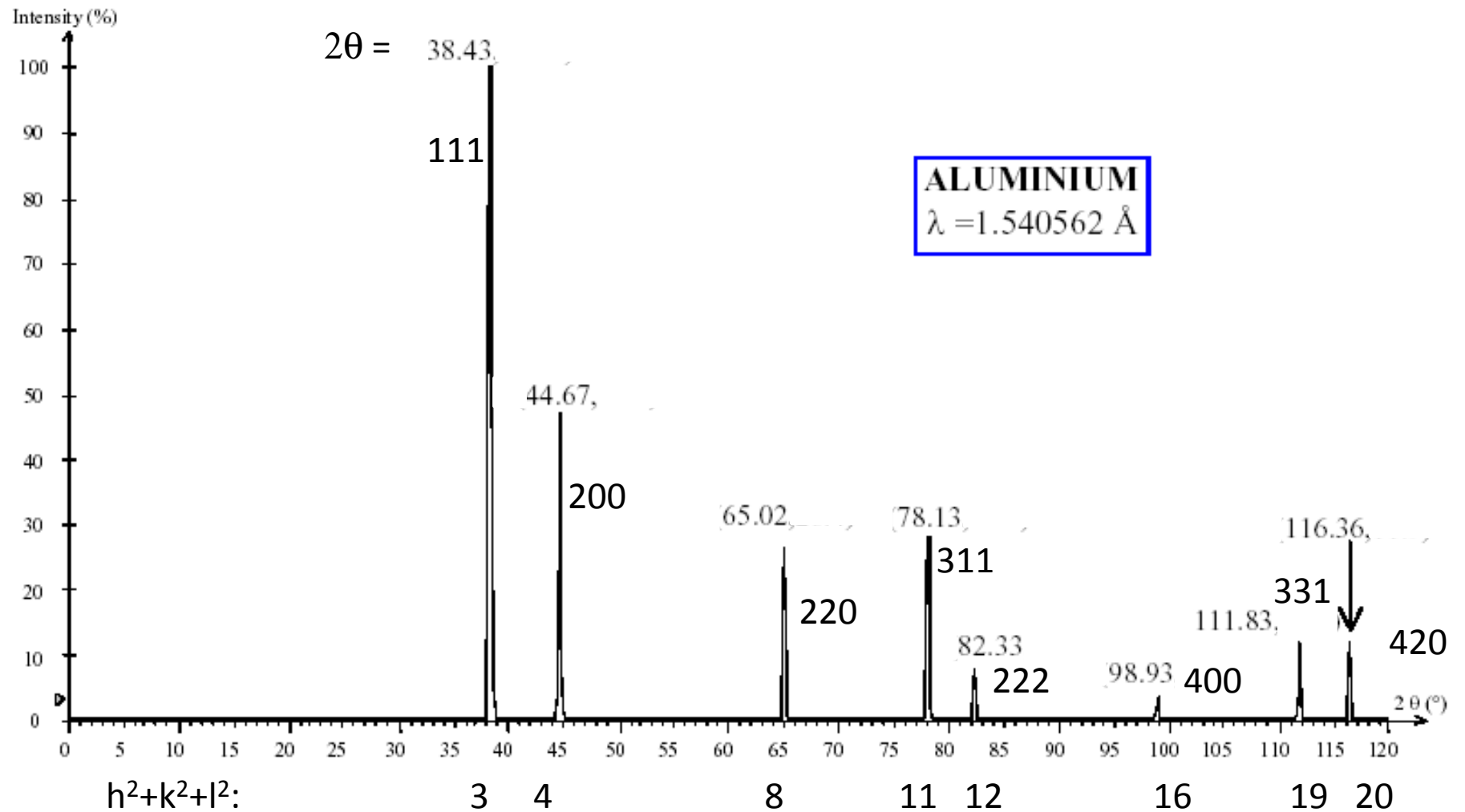
Consider the following XRD pattern for Aluminum, which was collected using $\text{CuK}\alpha$ radiation.

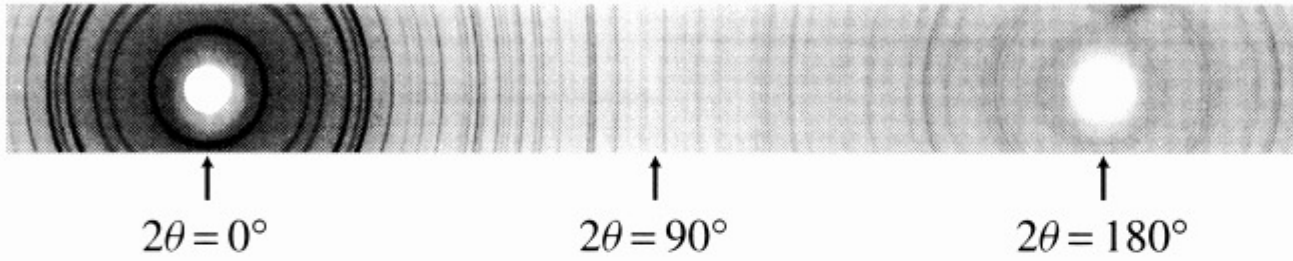






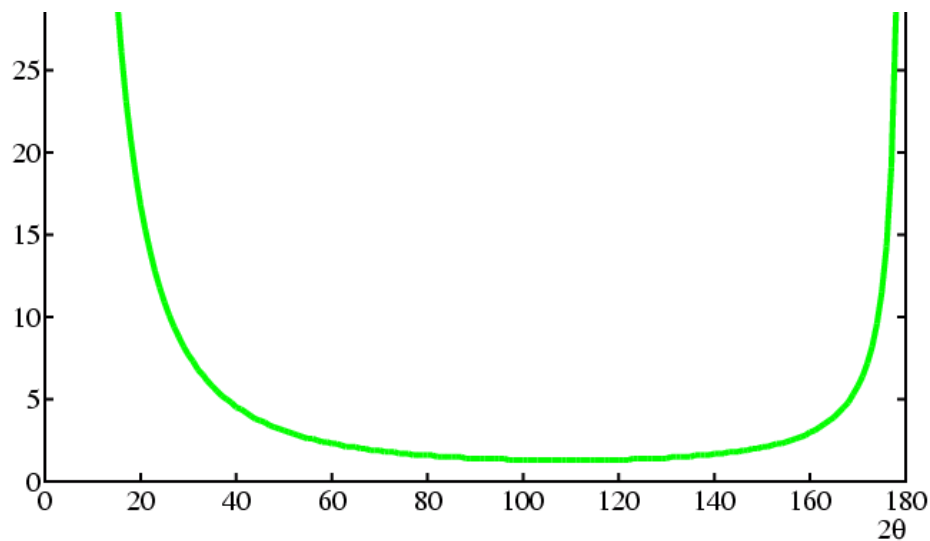
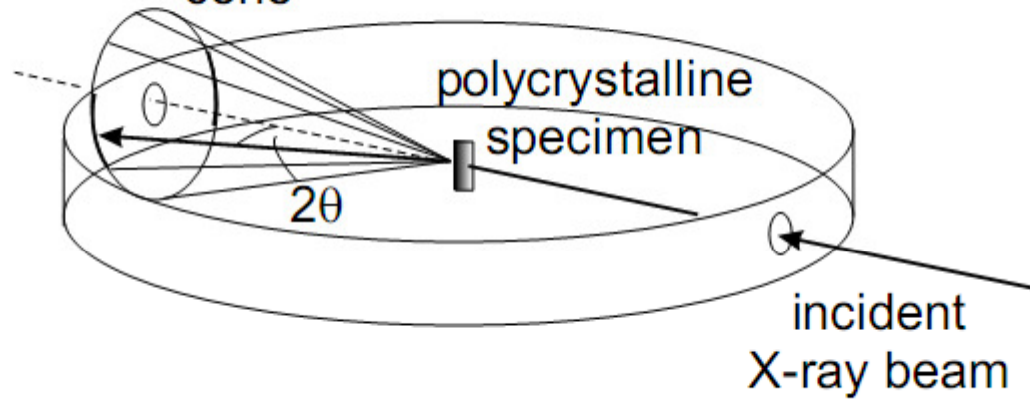
Consider the following XRD pattern for Aluminum, which was collected using $\text{CuK}\alpha$ radiation.





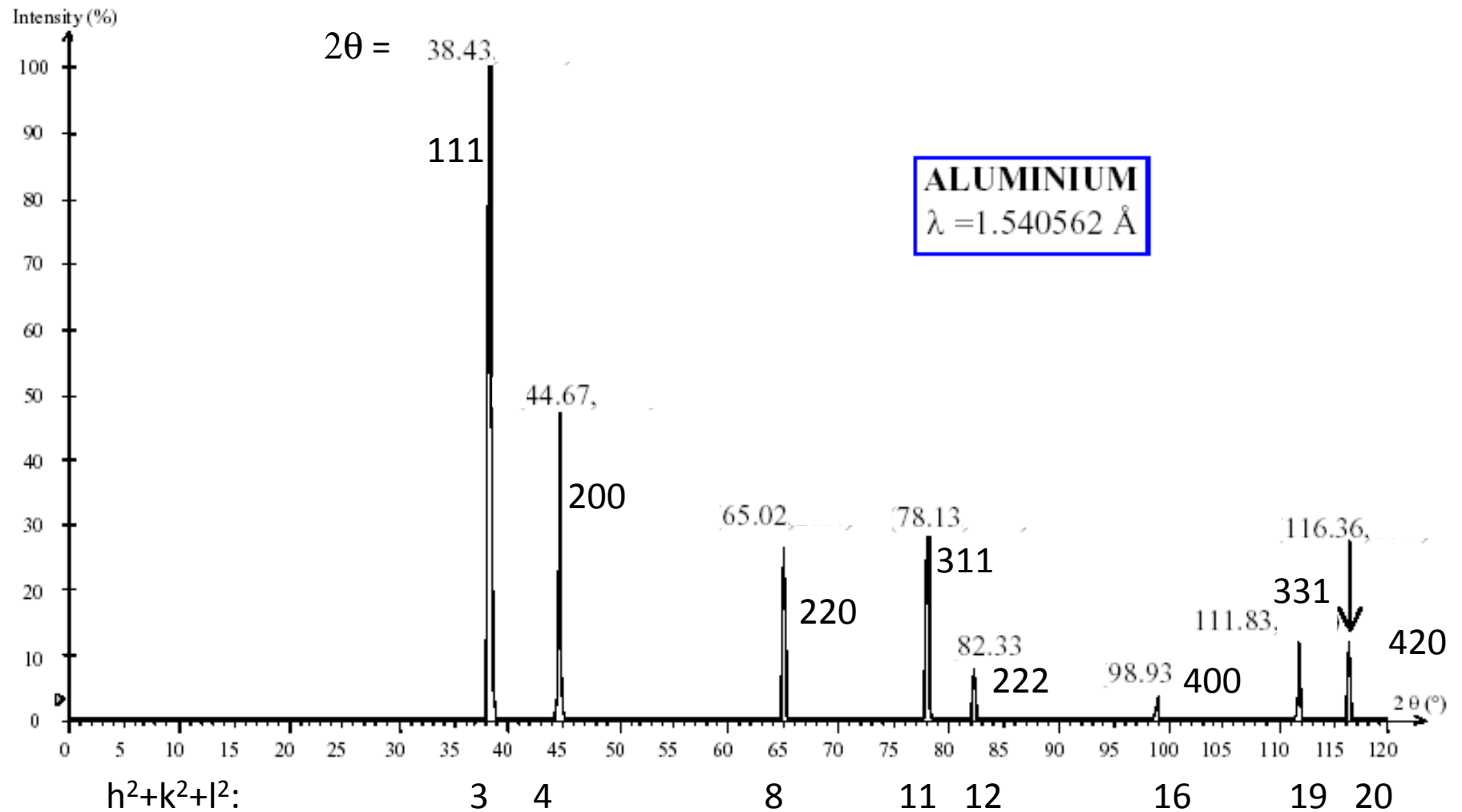
X-ray diffraction rings recorded on a photographic film

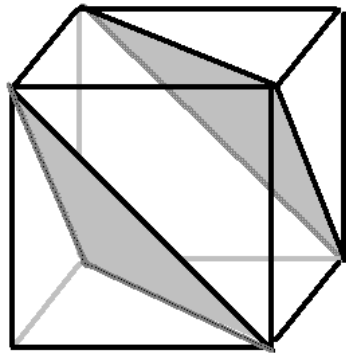
Debye-Scherrer cone



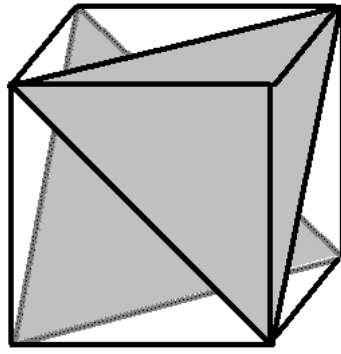
Geometric Lorentz Factor

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

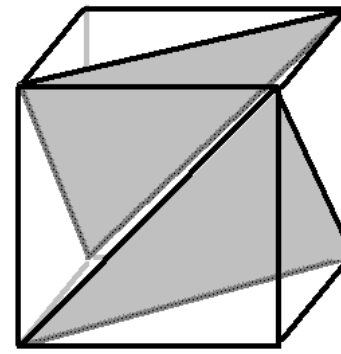




(111)



(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

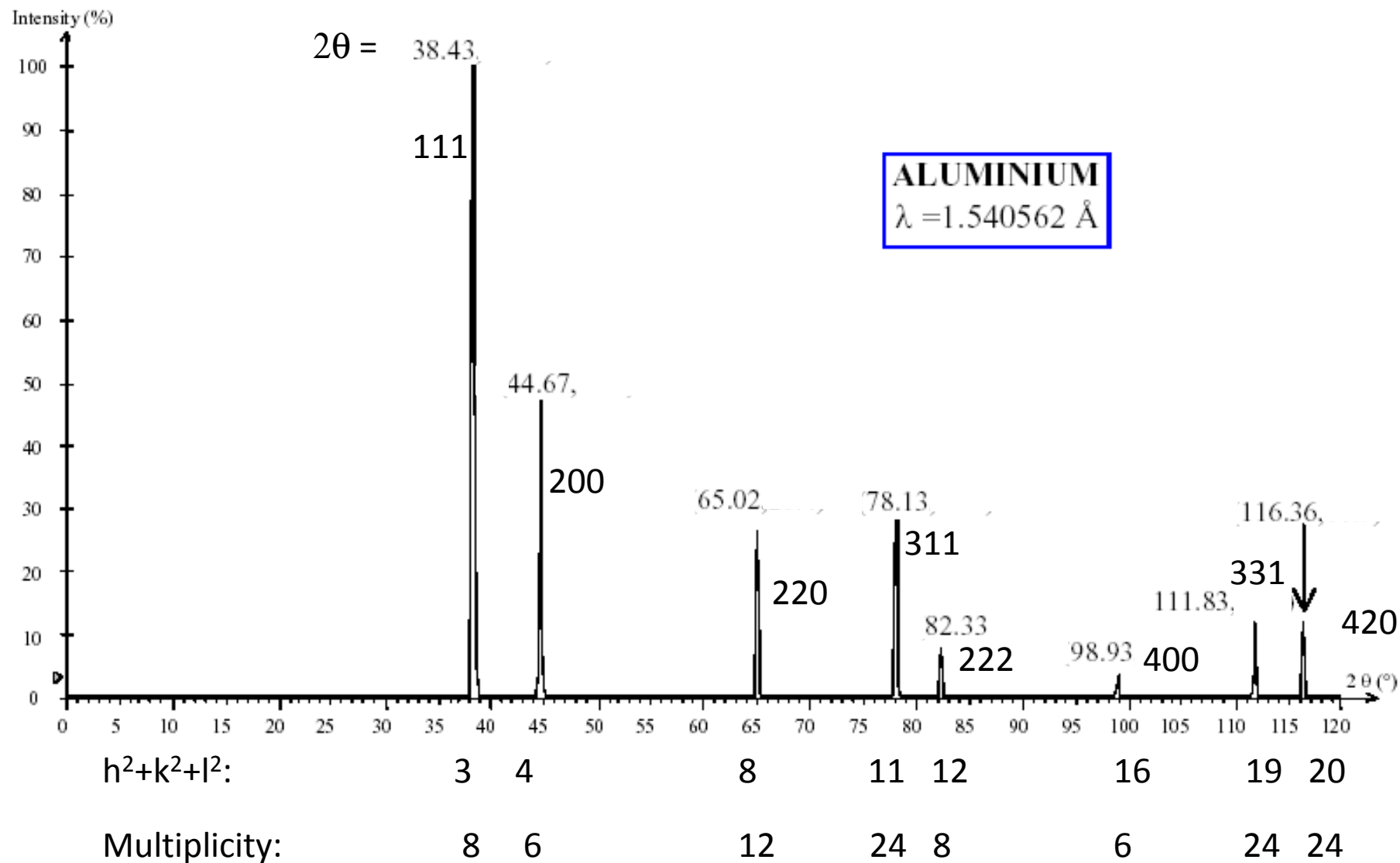
All hkl
 $h+k+l = \text{even}$
 h,k,l all even or all odd

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



The Rutherford-Appleton Lab in Oxfordshire



Spallation Neutron Source

Synchrotron X-ray Source