Slides
Condensed Matter Physics
Lecture 14

Scattering Selection Rules

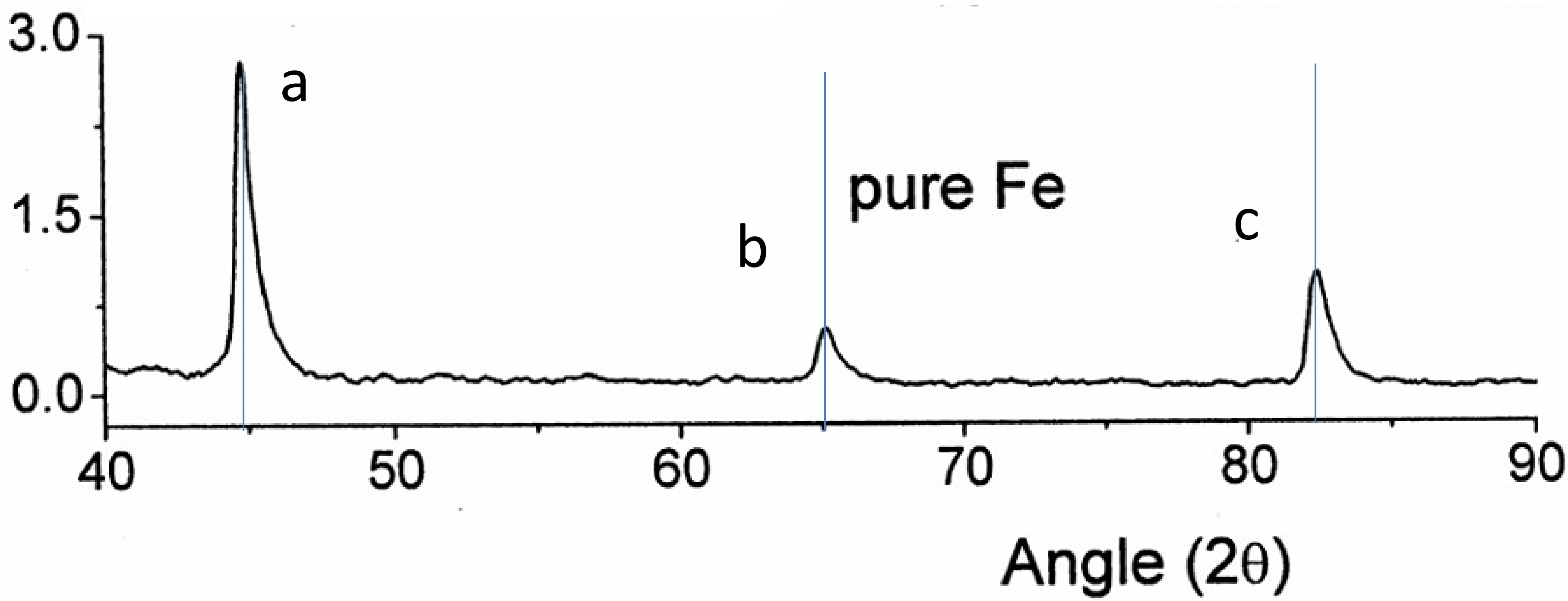
P = Primitive (simple) cubic — All *hkl*
I = BCC — $h+k+l$ = even
F= FCC — h,k,l all even or all odd

{*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 ….

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	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}

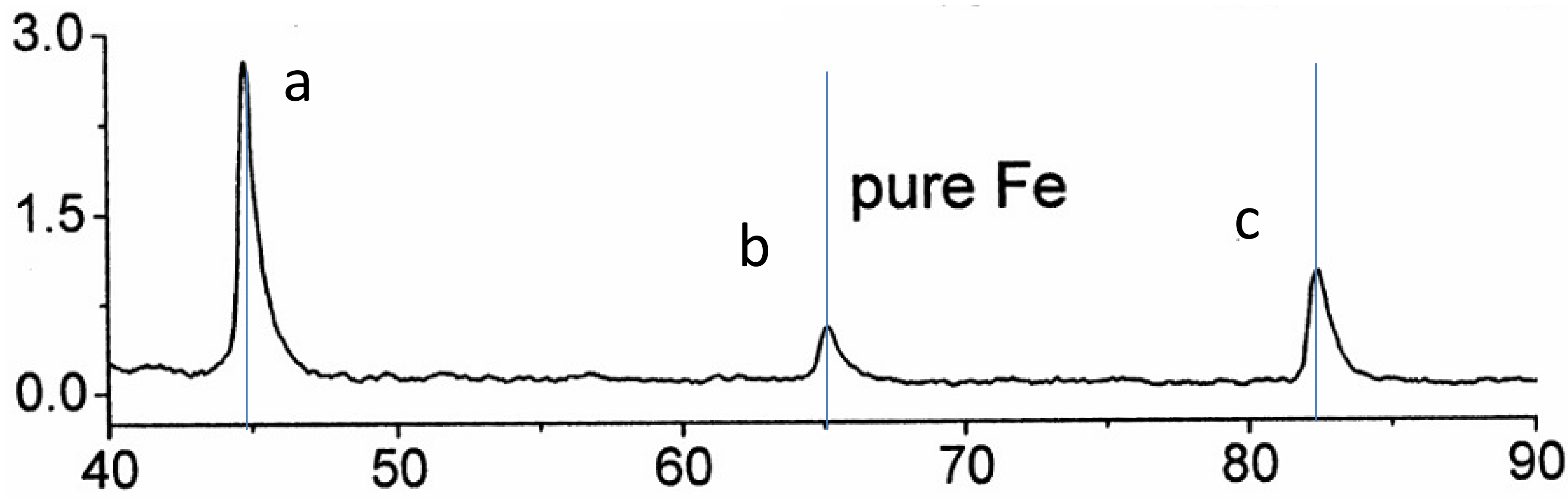
$$a = d\sqrt{h^2 + k^2 + l^2}$$

= 2.03 Å if we choose simple cubic

= 2.86 Å if we choose BCC

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

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200	4	6	*	*	*
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400	16	6	*	*	*

Sequence of N values

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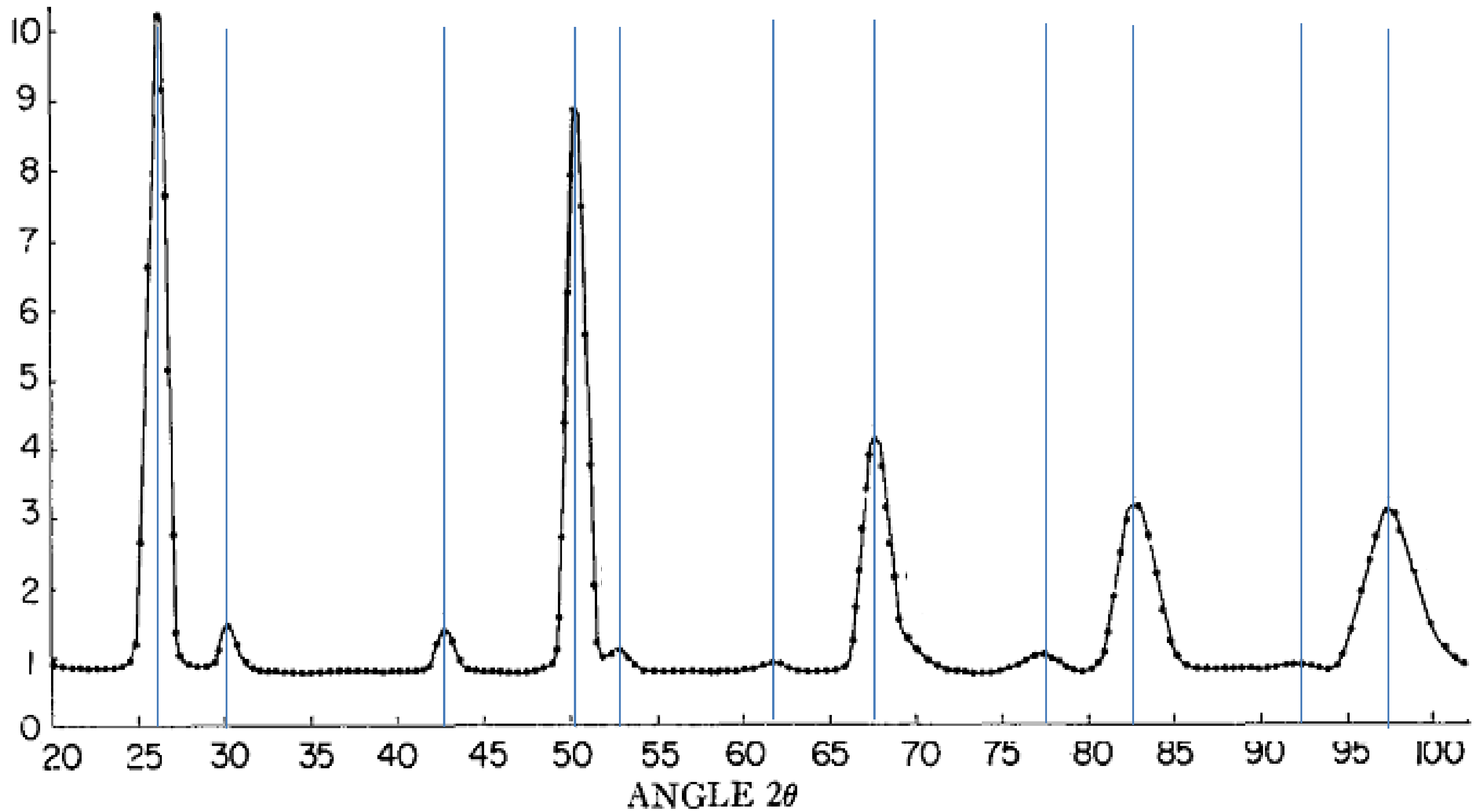
F: 3,4,8,11,12,16,19,20 ….

λ = 1.09 Angstrom TiC neutron powder diffraction



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

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

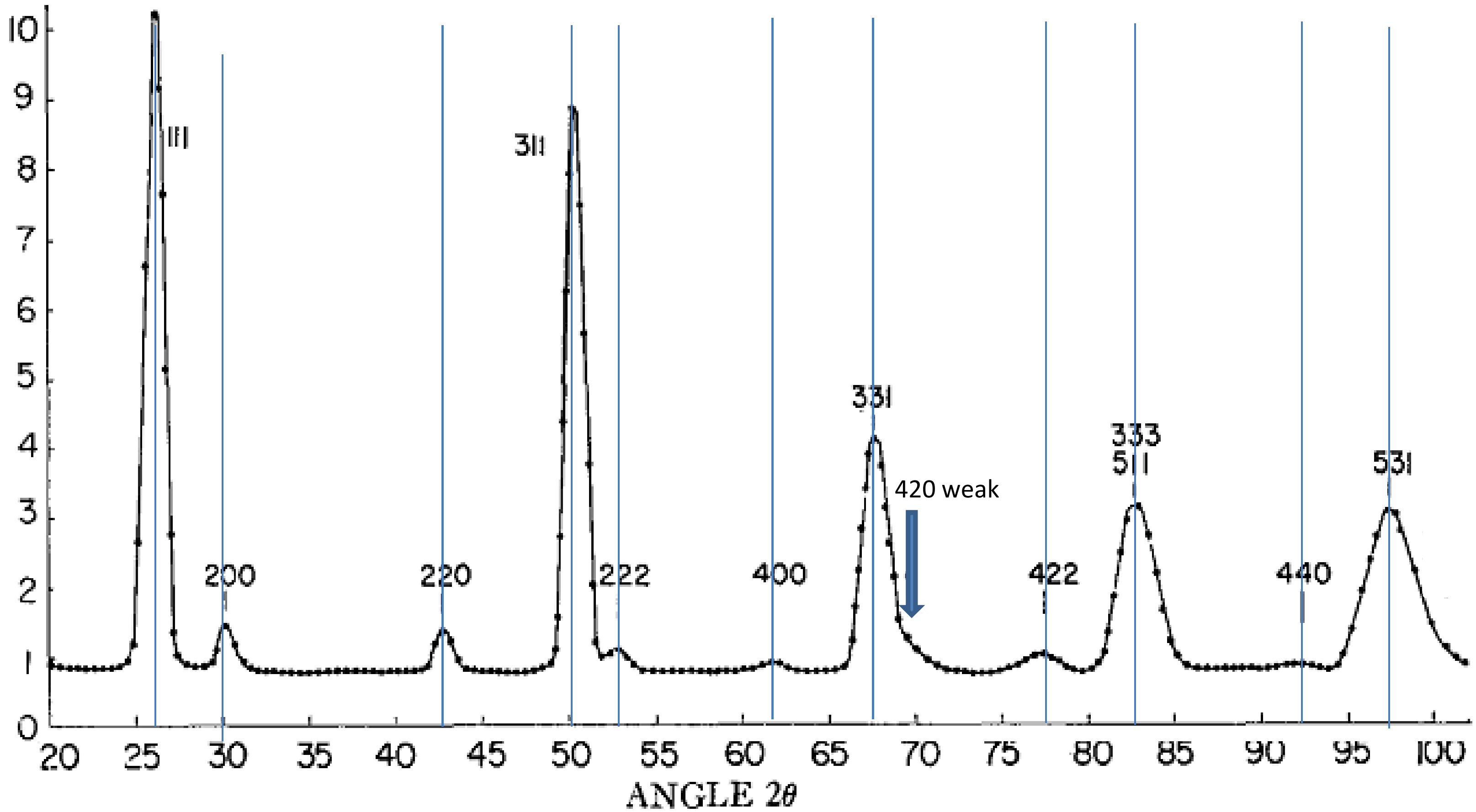
$$a^2/d^2 = h^2 + k^2 + l^2$$

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

Peak	Angle 2θ	$d = \dfrac{\lambda}{2\sin\theta}$	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 $= 4m+2$

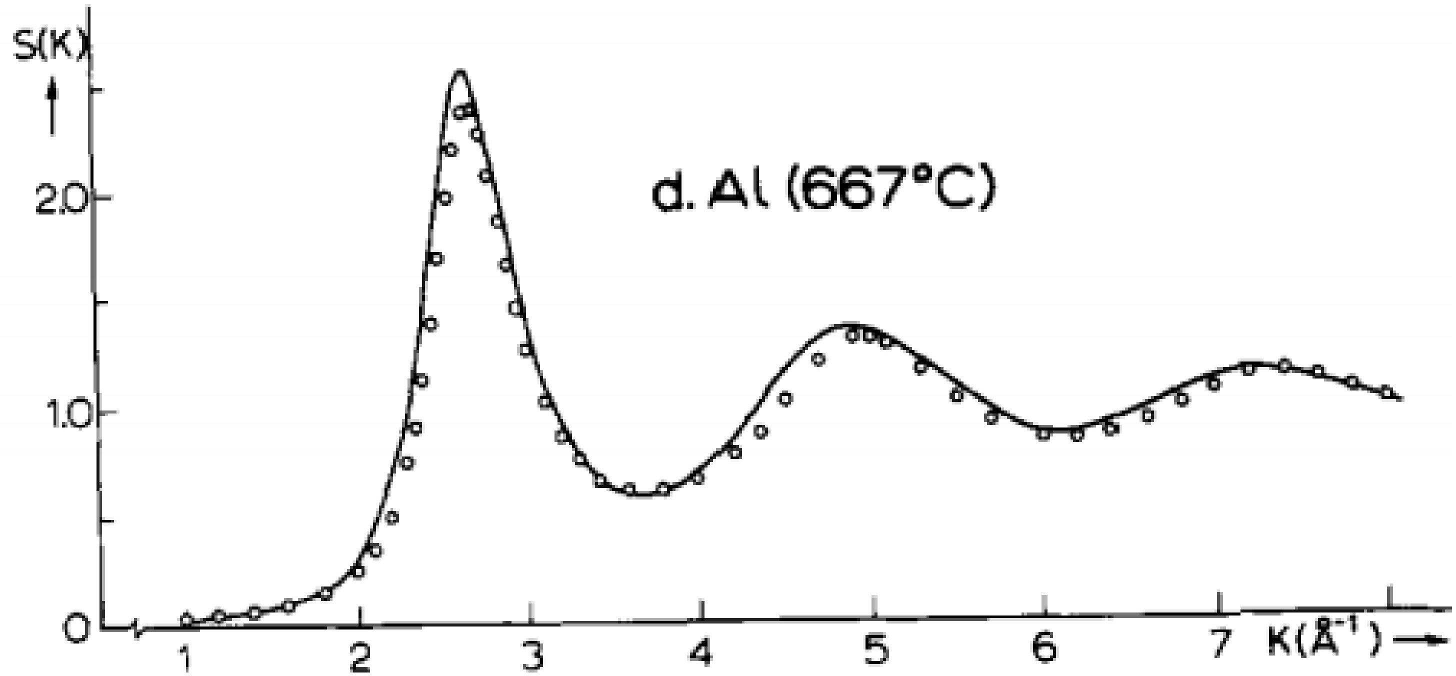
Conclude must be NaCl structure

The Rutherford-Appleton Lab in Oxfordshire

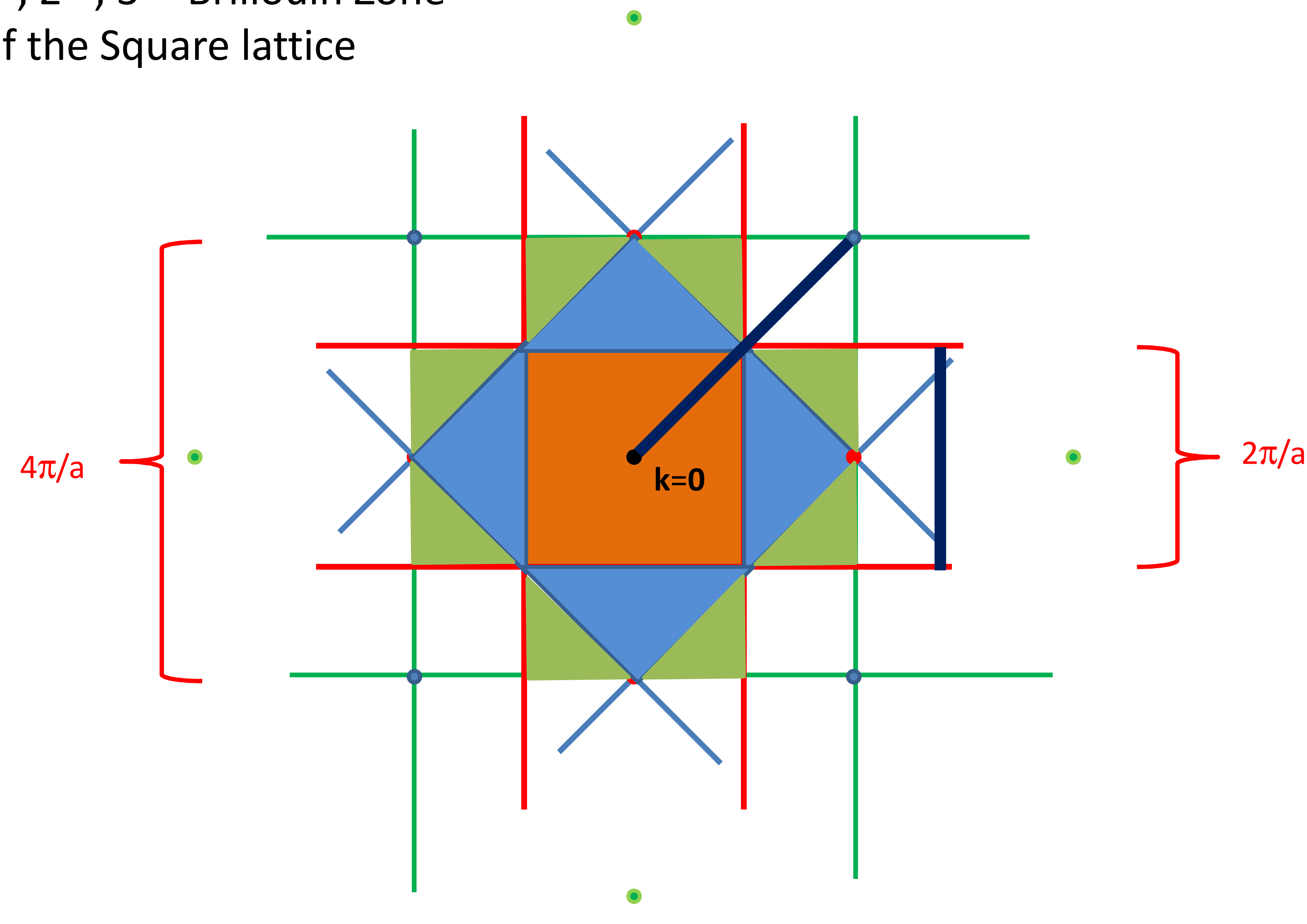
Synchrotron X-ray Source

Spallation Neutron Source

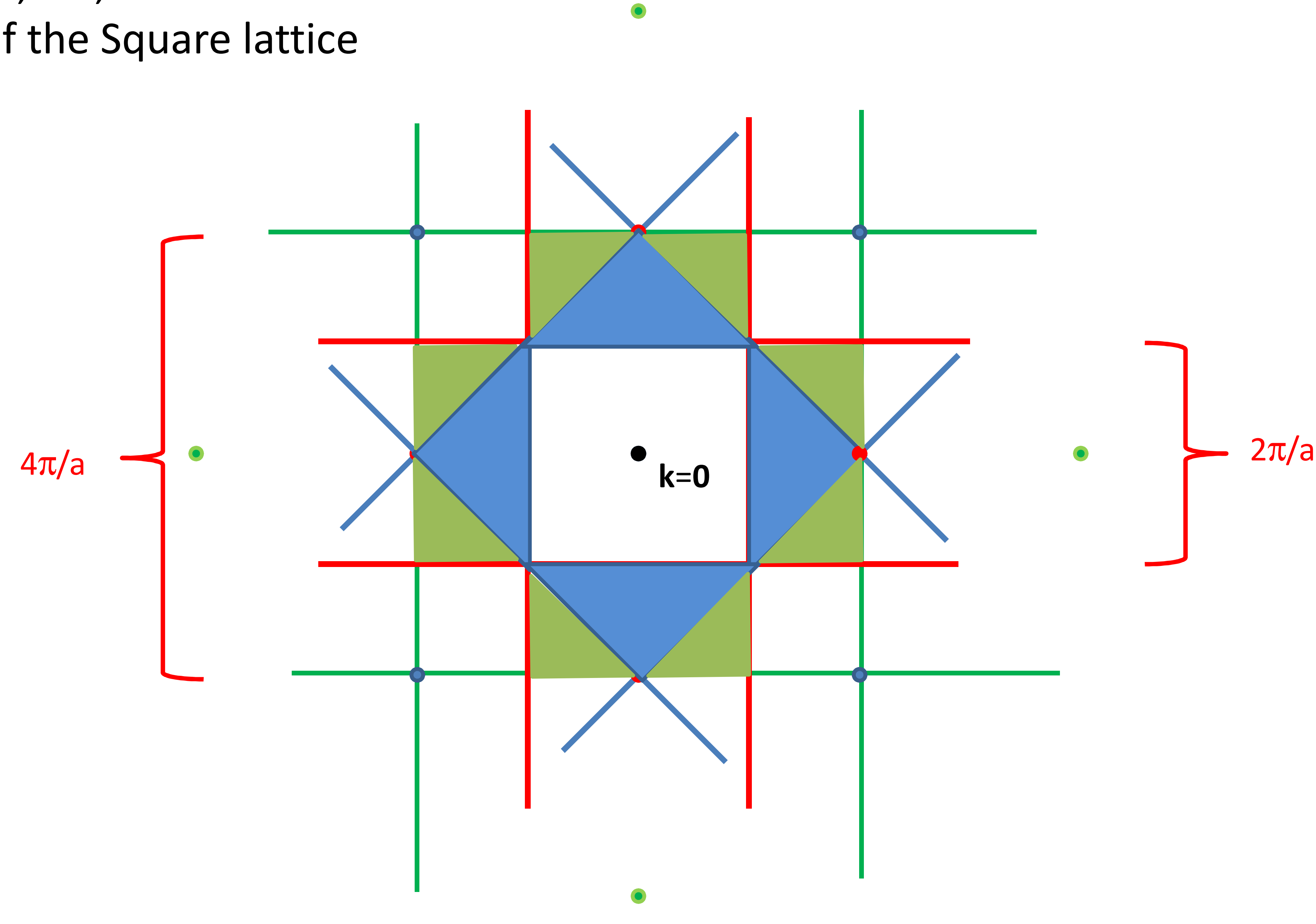
X-ray scattering on liquids
– like powder but peaks not sharp.



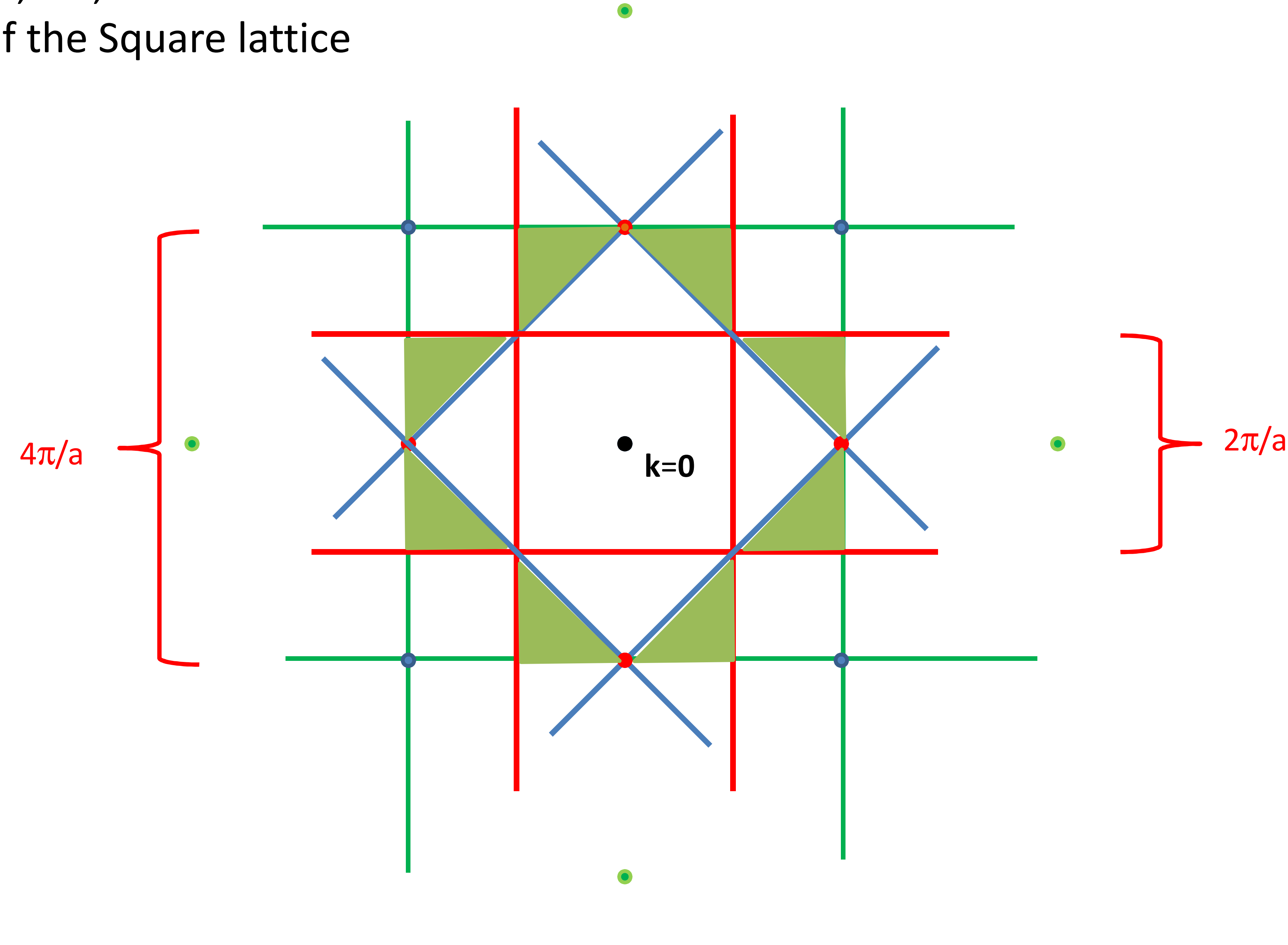
1^{st}, 2^{nd}, 3^{rd} Brillouin Zone Of the Square lattice



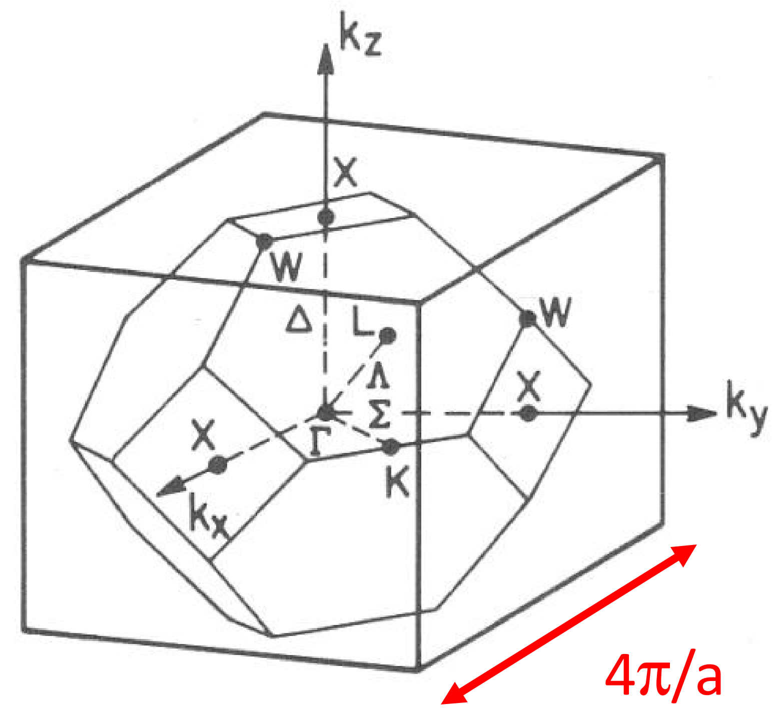
1^{st}, 2^{nd}, 3^{rd} Brillouin Zone Of the Square lattice



1st, 2nd, 3rd Brillouin Zone
Of the Square lattice



1st Brillouin Zone of an FCC lattice
=same shape as Wigner Seitz
cell of a BCC lattice



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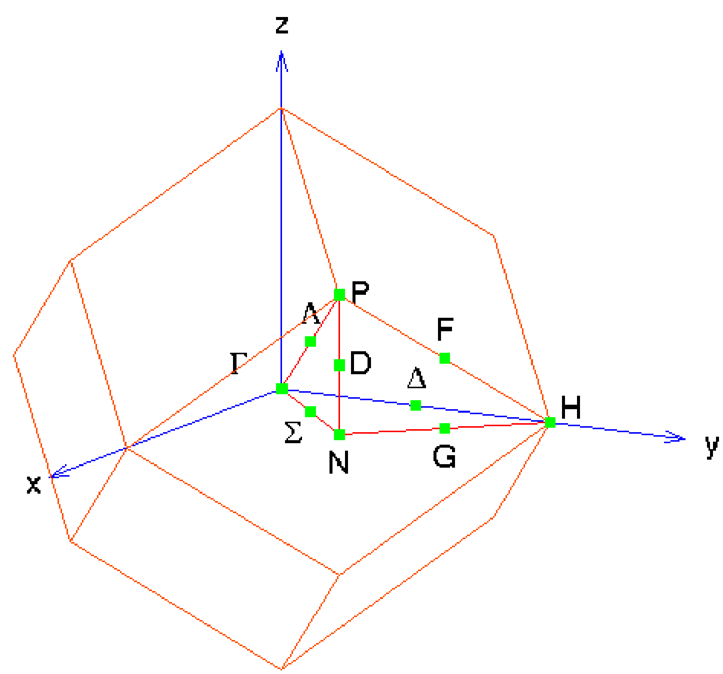
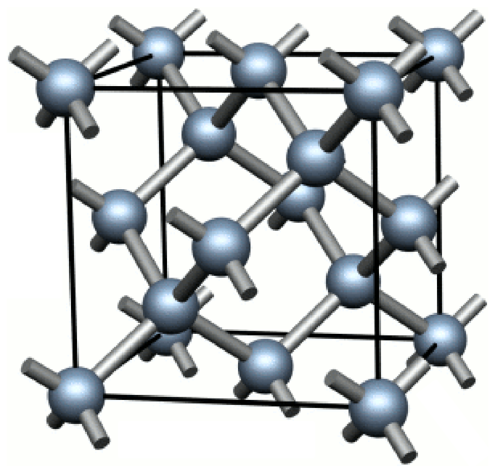
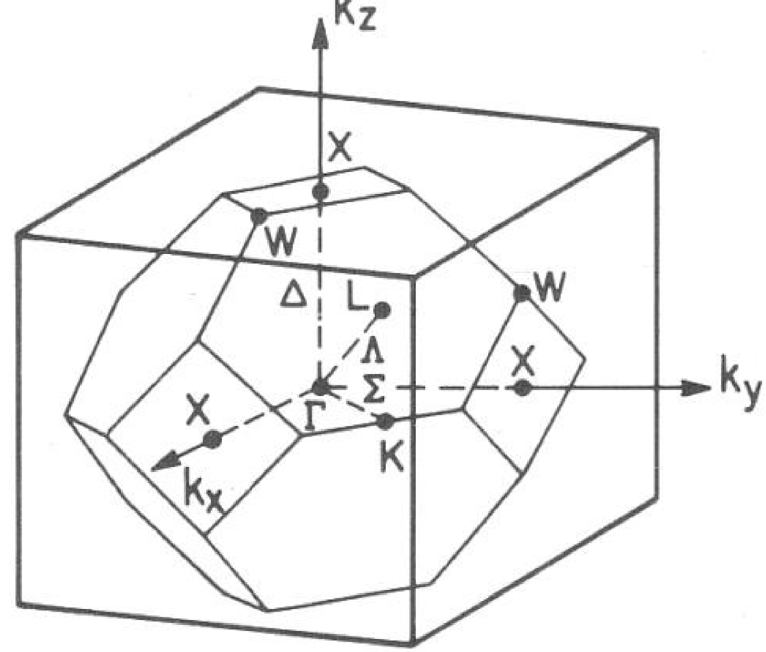
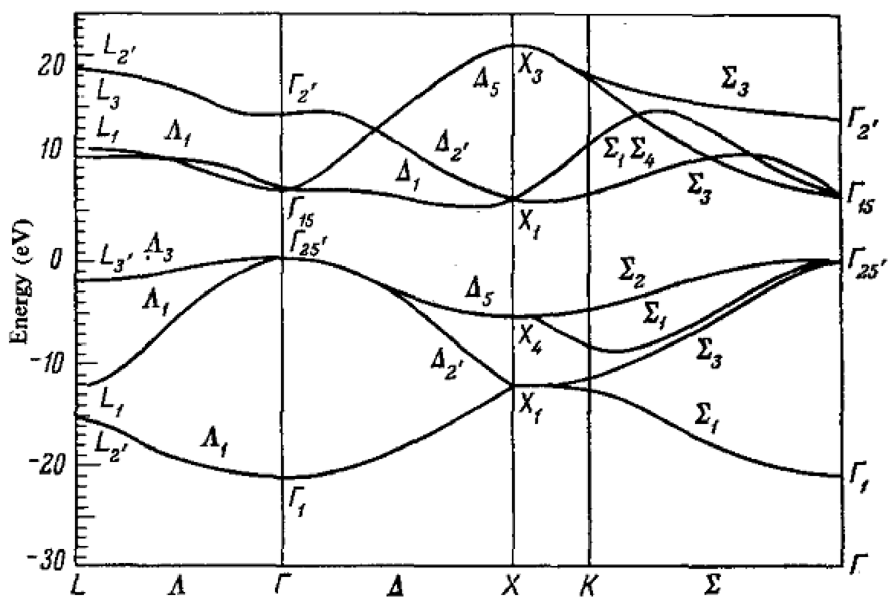


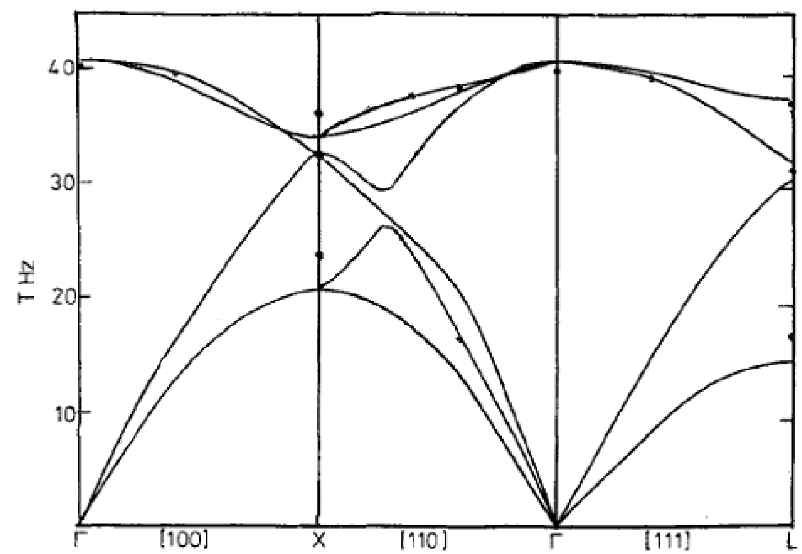
Diamond = FCC with a 2-atom basis
C @ [0,0,0]   and C @ [¼, ¼, ¼]







Diamond Electronic Band Structure



Diamond Phonon Spectrum