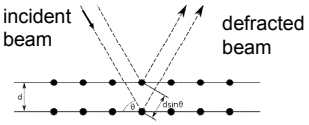
PHY 752 Solid State Physics
11-11:50 AM MWF Olin 103

Plan for Lecture 21:

- X-ray and neutron diffraction in solids (Chap. 10 in GGGPP)
  - Bragg law
  - Intensity relationships
  - Sensitivity to atomic parameters

8	Fri, 9/11/2015	Chap. 2	Group theory	#7
9	Mon, 9/14/2015	Chap. 2.4-2.7	Densities of states	#8
10	Wed, 9/16/2015	Chap. 3	Free electron model	#9
11	Fri, 9/18/2015	Chap. 4	One electron approximations to the many electron problem	#10
12	Mon, 9/21/2015	Chap. 4	One electron approximations to the many electron problem	#11
13	Wed, 9/23/2015	Chap. 4	Density functional theory	#12
14	Fri, 9/25/2015	Chap. 5	Implementation of density functional theory	#13
15	Mon, 9/28/2015	Chap. 5	Implementation of density functional theory	#14
16	Wed, 9/30/2015	Chap. 5	First principles pseudopotential methods	#15
17	Fri, 10/02/2015	Chap. 6	Example electronic structures	#16
18	Mon, 10/05/2015	Chap. 6	Ionic and covalent crystals	#17
19	Wed, 10/07/2015	Chap. 6	More examples of electronic structures	#18
20	Fri, 10/09/2015	Chap. 1-6	Review	Start exam
	Mon, 10/12/2015		No class	Take-home exam
	Wed, 10/14/2015		No class	Exam due before 10/19/2015
	Fri, 10/16/2015		Fall break -- no class	
21	Mon, 10/19/2015	Chap. 10	X-ray and neutron diffraction	#HW19
22	Wed, 10/21/2015	Chap. 10	X-ray and neutron diffraction	
	Wed, 12/02/2015		Student presentations I	
	Fri, 12/04/2015		Student presentations II	
	Mon, 12/07/2015		Begin Take-home final	

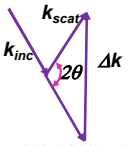
Bragg diffraction



Condition for constructive interference:

$$2d_{hkl}\sin\theta = n\lambda$$

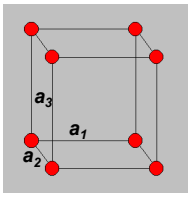
In terms of wave vectors



$$|\Delta\mathbf{k}| = 2|\mathbf{k}|\sin\theta$$

$$\frac{2\pi n}{d_{hkl}} = 2\frac{2\pi}{\lambda}\sin\theta$$

Relationship of normal distance between diffracting planes to Bravais lattice



Reciprocal lattice (modulo 2π)

$$\mathbf{b}_i = \frac{\mathbf{a}_j \times \mathbf{a}_k}{\mathbf{a}_i \cdot (\mathbf{a}_j \times \mathbf{a}_k)}$$

Note that $\mathbf{b}_i \cdot \mathbf{a}_j = \delta_{ij}$

$$d_{hkl} = \frac{1}{|h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3|}$$

Intensity profile

$$I_{hkl} = C|F_{hkl}|^2$$

$$F_{hkl} \equiv \int d^3r\, \rho(\mathbf{r}) e^{2\pi i(h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3)\cdot\mathbf{r}}$$

Comes from Born approximation describing the interaction between scattering particle and material.

$$\rho(r) = \sum_a \rho_a(\mathbf{r} - \boldsymbol{\tau}_a)$$

Atomic basis vectors:

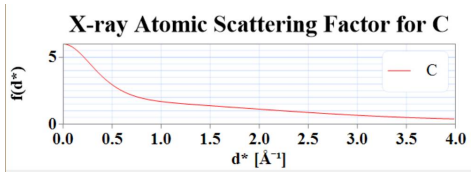
$$\boldsymbol{\tau}_a = x_a\mathbf{a}_1 + y_a\mathbf{a}_2 + z_a\mathbf{a}_3$$

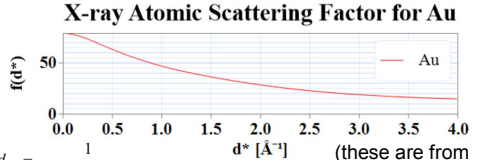
$$F_{hkl} \equiv \sum_a f^a_{hkl} e^{2\pi i(hx_a + ky_a + lz_a)}$$

$$f^a_{hkl} = \int d^3r'\, \rho_a(\mathbf{r}') e^{2\pi i(h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3)\cdot\mathbf{r}'}$$

Atomic structure factors

For X-ray scattering; Fourier transform of electronic density





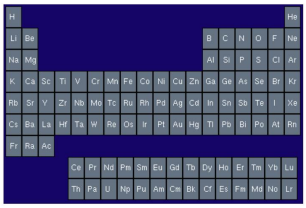
$$d_{hkl} = \frac{1}{|h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3|}$$

(these are from crystaldiffract)

Atomic structure factors

http://www.ncnr.nist.gov/resources/n-lengths/

Neutron scattering lengths and cross sections



Neutron scattering lengths and cross sections							
Isotope	conc	Coh b	Inc b	Coh xs	Inc xs	Scatt xs	Abs xs
C	---	6.6460	---	5.551	0.001	5.551	0.0035
12C	98.9	6.6511	0	5.559	0	5.559	0.00353
13C	1.1	6.19	-0.52	4.81	0.034	4.84	0.00137

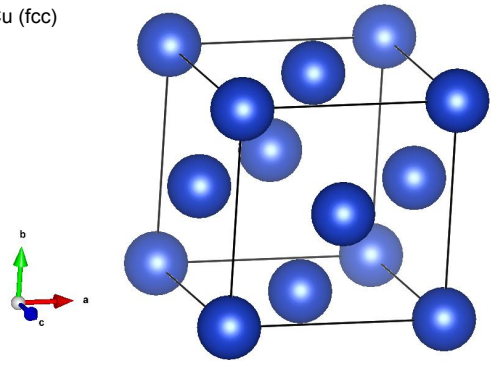
Neutron scattering lengths and cross sections							
Isotope	conc	Coh b	Inc b	Coh xs	Inc xs	Scatt xs	Abs xs
Au	100	7.63	-1.84	7.32	0.43	7.75	98.65

scattering length in 10^{-15} m

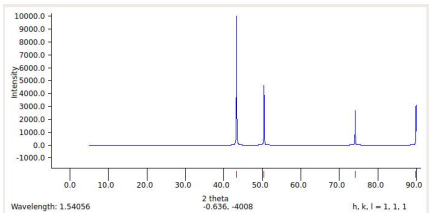
For neutrons:

$$f_{hkl}^{a} \propto b_{coh}^{a}$$

Cu (fcc)



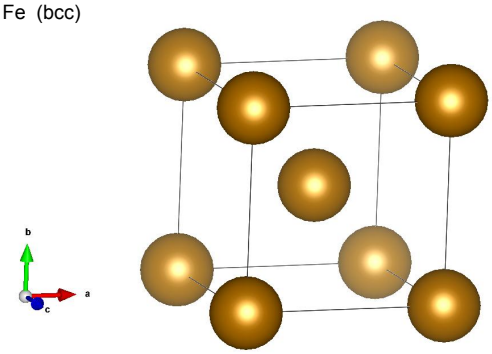
X-ray powder diffraction pattern for Cu (fcc)



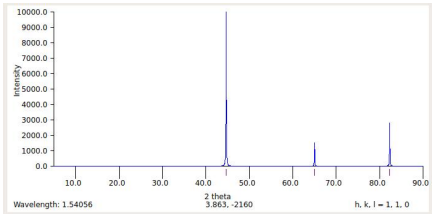
h	k	l	d-spacing	F^2	multiplicity
1	1	1	2.08715	7798.47	8
2	0	0	1.80753	6871.62	6
2	2	0	1.27811	4586.61	12
3	1	1	1.08998	3495.99	24

what is lattice constant *a?* 3.615 Angstroms

Fe (bcc)



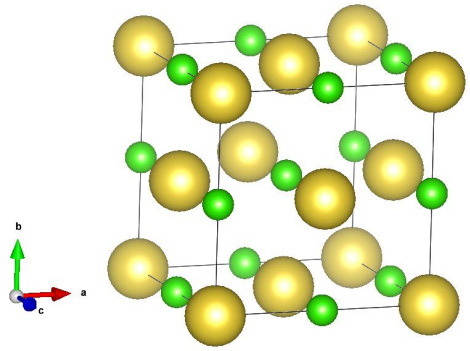
Fe (bcc)



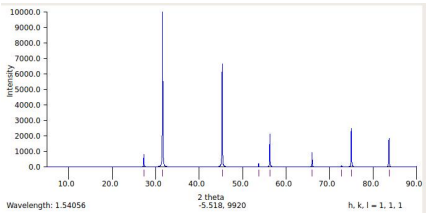
h	k	l	d-spacing	F^2	multiplicity
1	1	0	2.02692	1364.91	12
2	0	0	1.43325	931.656	6
2	1	1	1.17024	690.805	24

What is *a ?* 2.8665 Angstroms

NaCl



NaCl



h	k	l	d-spacing	F^2	multiplicity
1	1	1	3.26624	326.106	8
2	0	0	2.82865	7304.07	6
2	2	0	2.00016	5329.45	12
3	1	1	1.70574	118.02	24
2	2	2	1.63312	4222.17	8
4	0	0	1.41433	3514.4	6
3	3	1	1.29787	114.114	24
4	2	0	1.26501	3022.08	24
4	2	2	1.15479	2657.42	24

a=5.6573 Angstroms

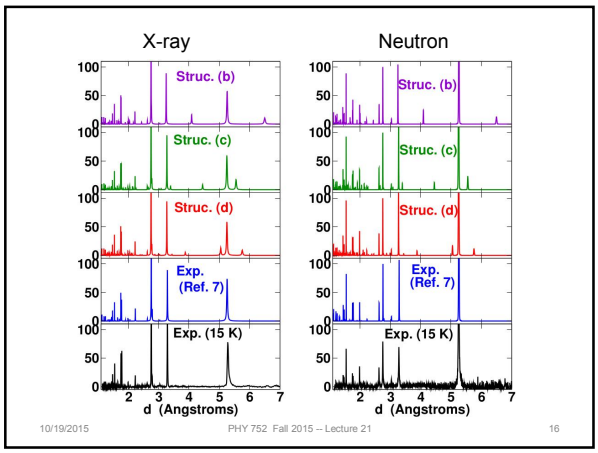
Comparison of X-ray and Neutron diffraction

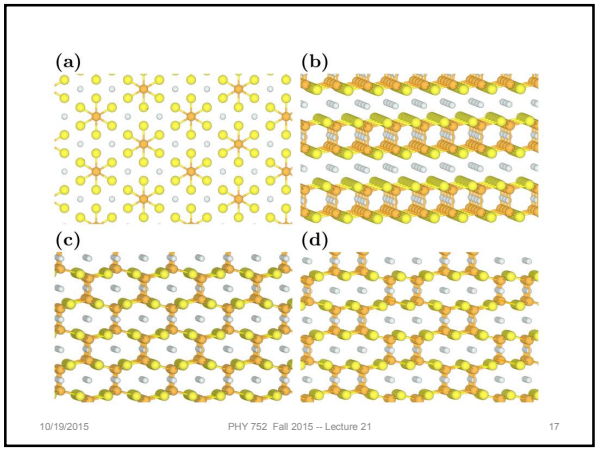
De Broglie wavelenth of neutron

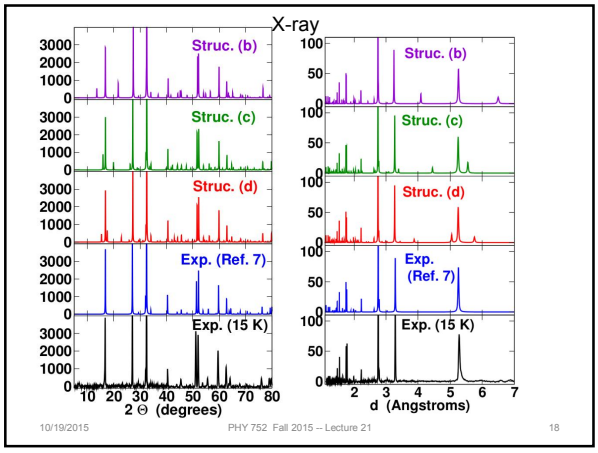
$$\lambda = \frac{h}{mv} = \frac{ht}{mL}$$

← time of flight

← path length


X-ray
Neutron
Struc. (b)
Struc. (c)
Struc. (d)
Exp. (Ref. 7)
Exp. (15 K)
d (Angstroms)


(a)
(b)
(c)
(d)


X-ray
Struc. (b)
Struc. (c)
Struc. (d)
Exp. (Ref. 7)
Exp. (15 K)
2 Θ (degrees)
d (Angstroms)

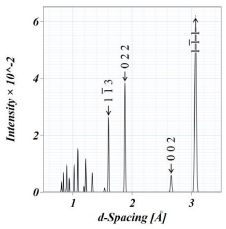
Properties of scattering particles

from pg. 61 of Marder's text

	X-rays	Neutrons	Electrons
Charge	0	0	$-e$
Mass	0	$1.67{\cdot}10^{-27}$ kg	$9.11{\cdot}10^{-31}$ kg
Typical energy	12 keV	0.02 eV	60 keV
Typical wavelength	1Å	2 Å	0.05Å
Typical attenuation length	100 μm	5 cm	1 μm
Typical atomic form factor, f	10^{-3} Å	10^{-4} Å	10 Å

Table 3.2:

1. The graph and table below shows simulated neutron diffraction data for ZnS in the zincblende structure (Fig. 2.9, pg 76-77 in GGGPP) showing the diffraction intensity versus d_{hkl} plane spacing, where the hkl Miller indices are based on the conventional cubic cell.



h	k	l	d(hkl)	I/Imax
1	1	1	3.07035	100.0%
0	0	2	2.65900	16.8%
0	2	2	1.88020	76.0%
1	1	3	1.60344	22.3%
2	2	2	1.53517	1.2%
0	0	4	1.32950	9.5%
1	3	3	1.22003	7.5%
0	2	4	1.18914	2.7%
2	2	4	1.08553	8.4%
3	3	3	1.02345	1.2%
1	1	5	1.02345	3.7%
3	-3	3	1.02345	1.2%

(a) Using the fractional atomic positions for the ZnS structure, explain the reason for at least two of the "missing" diffraction peaks.

(b) From the table of neutron diffraction peaks given below, determine the lattice constant of ZnS and compare your result with that given in GGGPP.