PHY 752 Solid State Physics
11-11:50 AM MWF Olin 107

Plan for Lecture 31:

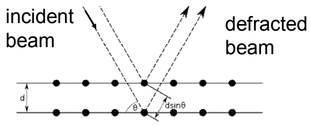
- **X-ray and neutron diffraction in solids (some material contained in Chap. 3 of Marder's text)**
  - **Bragg law**
  - **Intensity relationships**
  - **Sensitivity to atomic parameters**

20	Mon: 03/16/2015		Review Mid-term exam	#19	03/18/2015
21	Wed: 03/18/2015	Chap. 16	Electron Transport	#20	03/20/2015
22	Fri: 03/20/2015	Chap. 16	Electron Transport	#21	03/23/2015
23	Mon: 03/23/2015	Chap. 17	Electron Transport	#22	03/25/2015
24	Wed: 03/25/2015	Chap. 17 & 18	Electron Transport		
25	Fri: 03/27/2015	Chap. 18	Microscopic picture of transport	#23	03/30/2015
26	Mon: 03/30/2015	Chap. 19	Semiconductor devices	#24	04/01/2015
27	Wed: 04/01/2015	Chap. 20	Models of dielectric functions	#25	04/06/2015
	Fri: 04/03/2015	Good Friday	No class		
28	Mon: 04/06/2015	Chap. 21	Optical properties of solids	#26	04/08/2015
29	Wed: 04/08/2015	Chap. 22	Modern theory of polorization	#27	04/10/2015
30	Fri: 04/10/2015		Surface properties of solids	#28	04/13/2015
31	Mon: 04/13/2015		X-ray and neutron diffraction in solids	#29	04/15/2015
32	Wed: 04/15/2015				04/17/2015
33	Fri: 04/17/2015				04/20/2015
34	Mon: 04/20/2015				
35	Wed: 04/22/2015				
36	Fri: 04/24/2015				
	Mon: 04/27/2015		Presentations I		
	Wed: 04/29/2015		Presentations II		
	Fri: 05/01/2015		Presentations III & Take home exam		

Comment on topics

- X-ray and neutron diffraction in solids
- Low energy electron diffraction in solids
- Beyond independent electron picture -- Electron-electron interactions in the Hubbard model (Chapter 26 of your text)

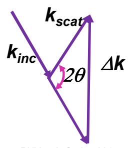
Bragg diffraction



Condition for constructive interference:

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

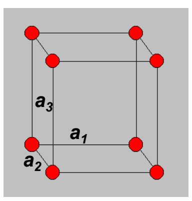
In terms of wave vectors



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

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

Relationship of normal distance between diffracting planes to Bravais lattice



Reciprocal lattice (modulo 2 π)

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

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

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

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

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:

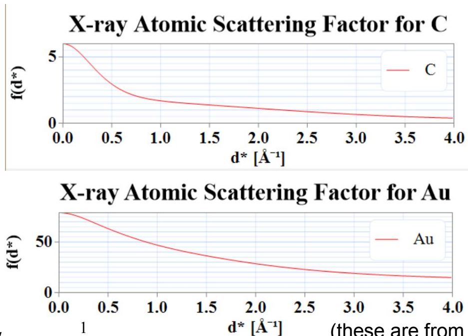
$$\boldsymbol{\tau}_a = x_a\mathbf{a}_1 + y_a\mathbf{a}_2 + z_a\mathbf{a}_3$$

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

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

Atomic structure factors

For X-ray scattering; Fourier transform of electronic density



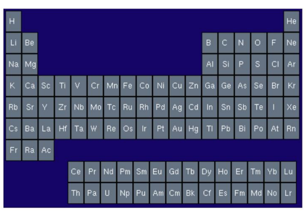
$$d_{hkl} = \frac{1}{|h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3|}$$

(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

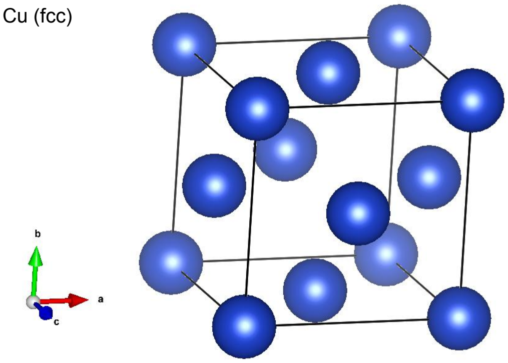
Neutron scattering lengths and cross sections							
Isotope	conc	Coh b	Inc b	Coh xs	Inc xs	Scatt xs	Abs xs
Au	100	7.63	-1.84	7.32	0.43	7.75	98.65

scattering length in 10^{-15} m

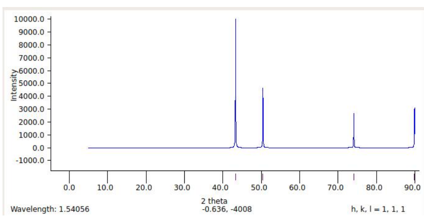
For neutrons:

$$f^a_{hkl} \propto b^a_{coh}$$

Cu (fcc)



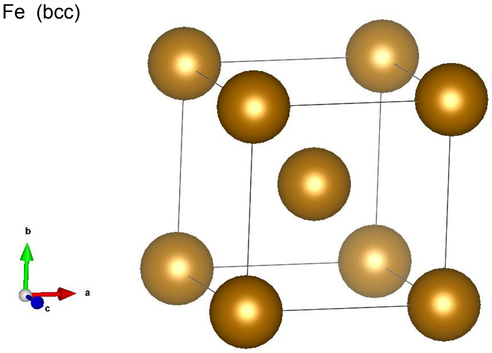
X-ray powder diffraction pattern for Cu (fcc)



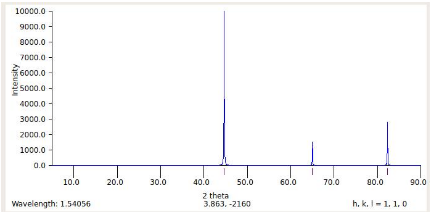
h	k	l	d-spacing	F^2	multiplicity
1	1	1	2.08715	7798.47	8
2	0	0	1.80753	6871.62	6
2	2	0	1.27811	4506.61	12
3	1	1	1.08998	3495.99	24

what is lattice constant *a?* 3.615 Angstroms

Fe (bcc)



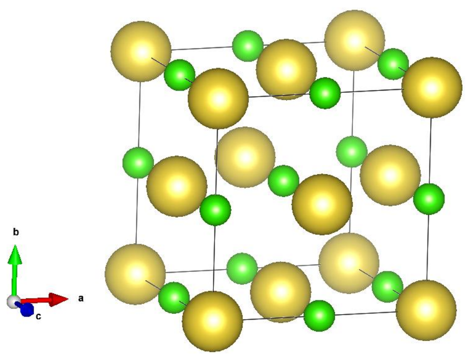
Fe (bcc)



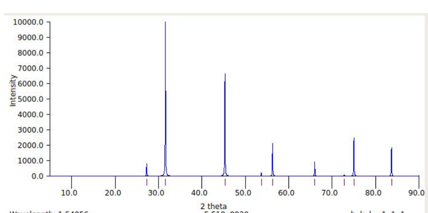
h	k	l	d-spacing	F^2	multiplicity
1	1	0	2.02692	1364.91	12
2	0	0	1.43325	931.656	6
2	1	1	1.17024	690.805	24

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

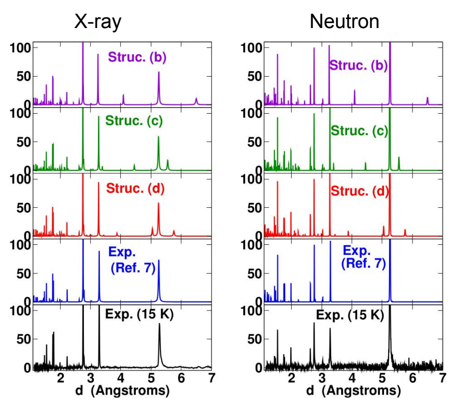
a=5.6573 Angstroms

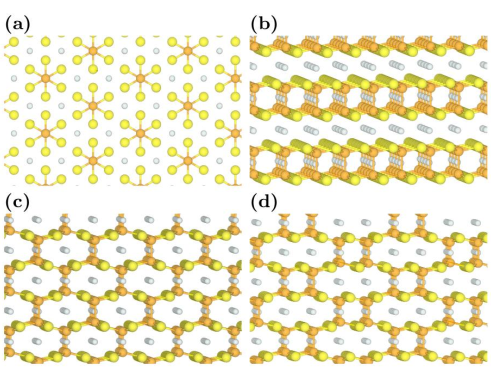
Comparison of X-ray and Neutron diffraction

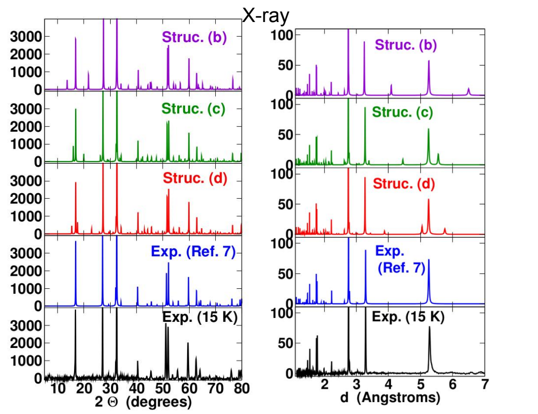
De Broglie wavelenth of neutron

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

← time of flight
← path length







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: