Structural Analysis
Part III - X-ray tools

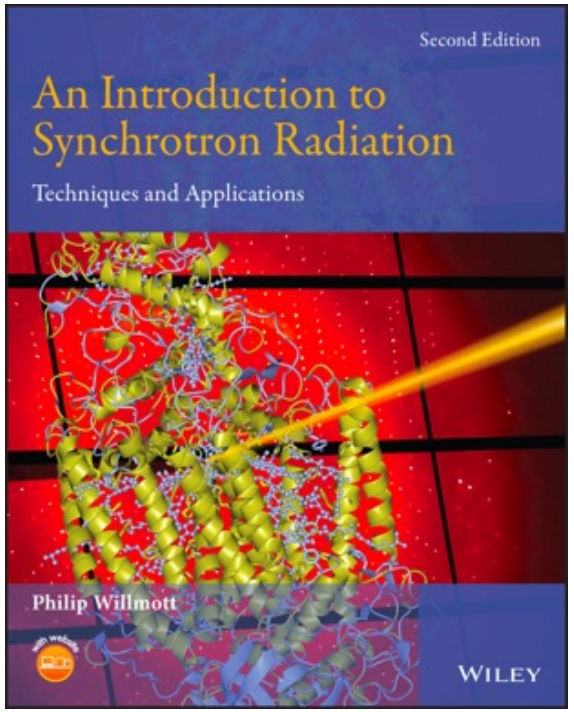
Review

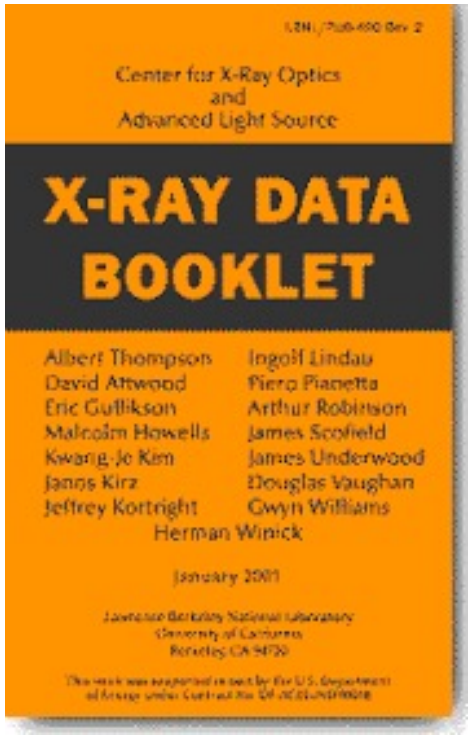
The following slides summarize the conecpts we discussed in class.

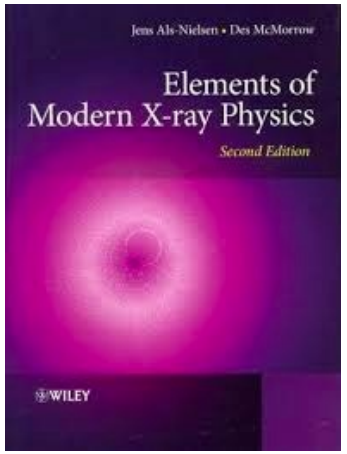
They show the key figures.

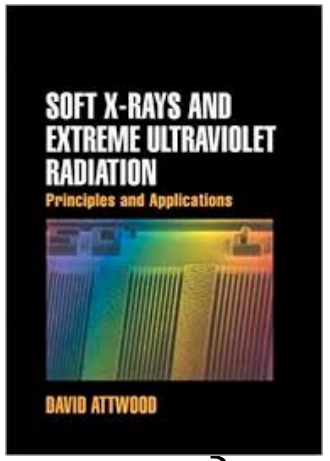
Together with the sample questions and exercises they are a guidance for your exam preparations.

Backup literature

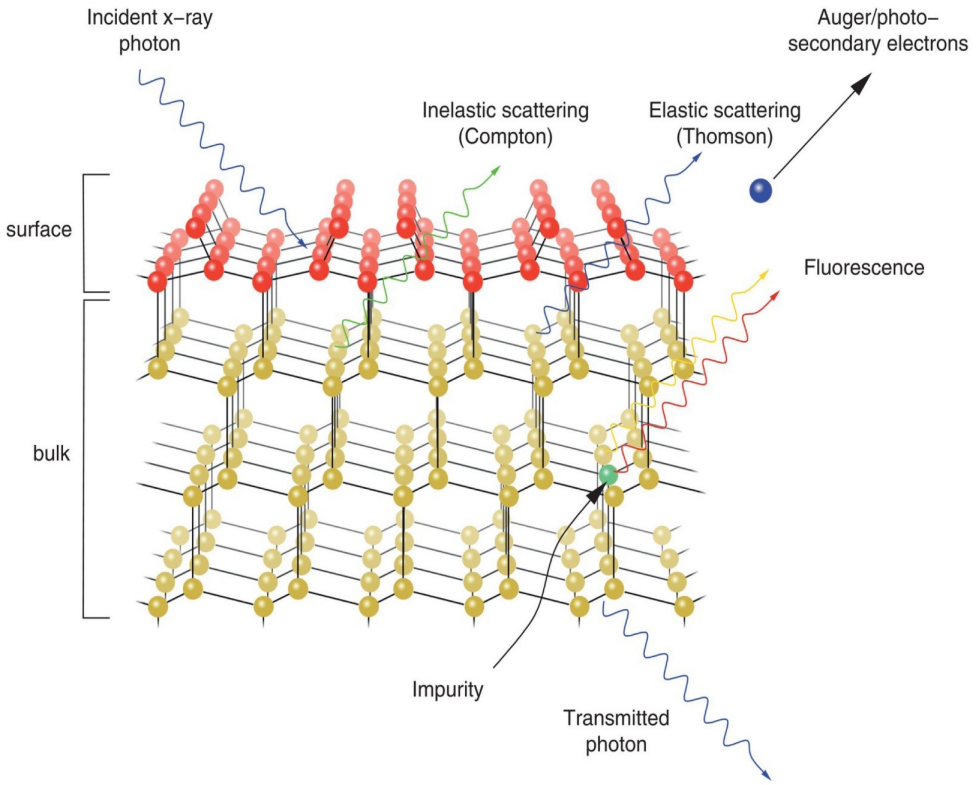








Fundamental processes for the x-ray matter interaction.



The x-ray properties of the elements

Table 1-1. *Electron binding energies, in electron volts, for the elements in their natural forms.*

Element	K 1s	L_1 2s	L_2 $2p_{1/2}$	L_3 $2p_{3/2}$	M_1 3s	M_2 $3p_{1/2}$	M_3 $3p_{3/2}$	M_4 $3d_{3/2}$	M_5 $3d_{5/2}$	N_1 4s	N_2 $4p_{1/2}$
1 H	13.6										
2 He	24.6*										
3 Li	54.7*										
4 Be	111.5*										
5 B	188*										
6 C	284.2*										
7 N	409.9*	37.3*									
8 O	543.1*	41.6*									
9 F	696.7*										
10 Ne	870.2*	48.5*	21.7*	21.6*							
11 Na	1070.8†	63.5†	30.65	30.81							
12 Mg	1303.0†	88.7	49.78	49.50							
13 Al	1559.6	117.8	72.95	72.55							
14 Si	1839	149.7*b	99.82	99.42							
15 P	2145.5	189*	136*	135*							
16 S	2472	230.9	163.6*	162.5*							
17 Cl	2822.4	270*	202*	200*							
18 Ar	3205.9*	326.3*	250.6†	248.4*	29.3*	15.9*	15.7*				
19 K	3608.4*	378.6*	297.3*	294.6*	34.8*	18.3*	18.3*				
20 Ca	4038.5*	438.4†	349.7†	346.2†	44.3 †	25.4†	25.4†				
21 Sc	4492	498.0*	403.6*	398.7*	51.1*	28.3*	28.3*				
22 Ti	4966	560.9†	460.2†	453.8†	58.7†	32.6†	32.6†				

X-ray cross sections for carbon

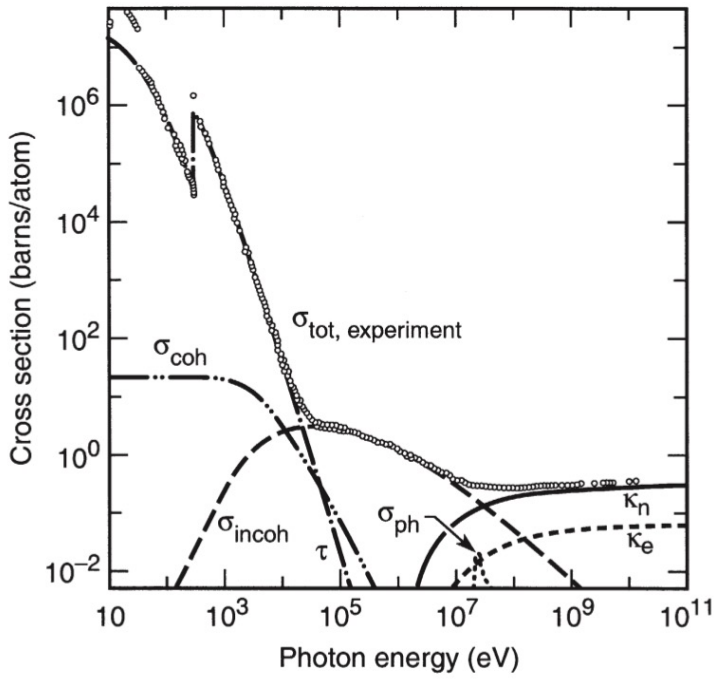
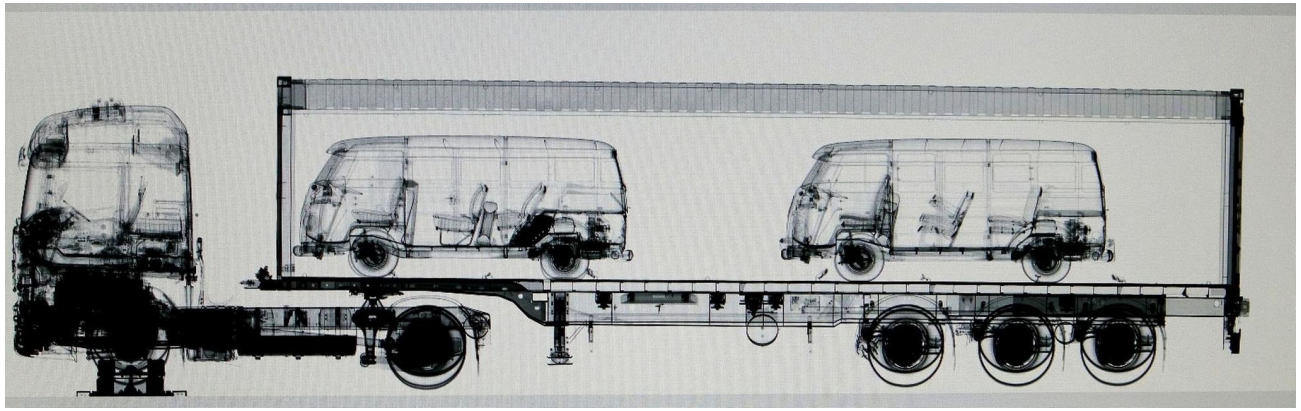
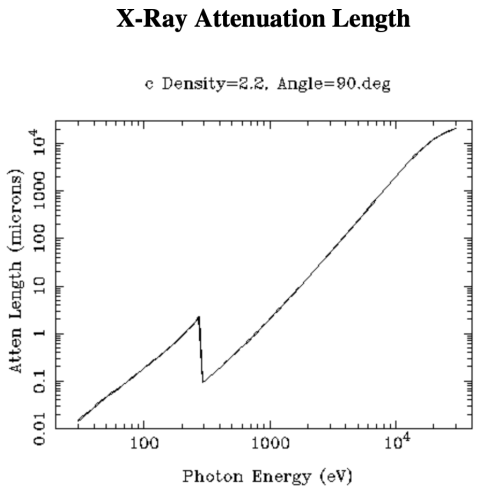
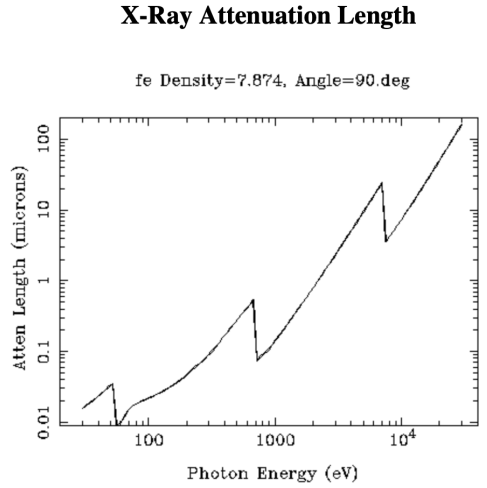


Fig. 3-1. *Total photon cross section σ_{tot} in carbon, as a*

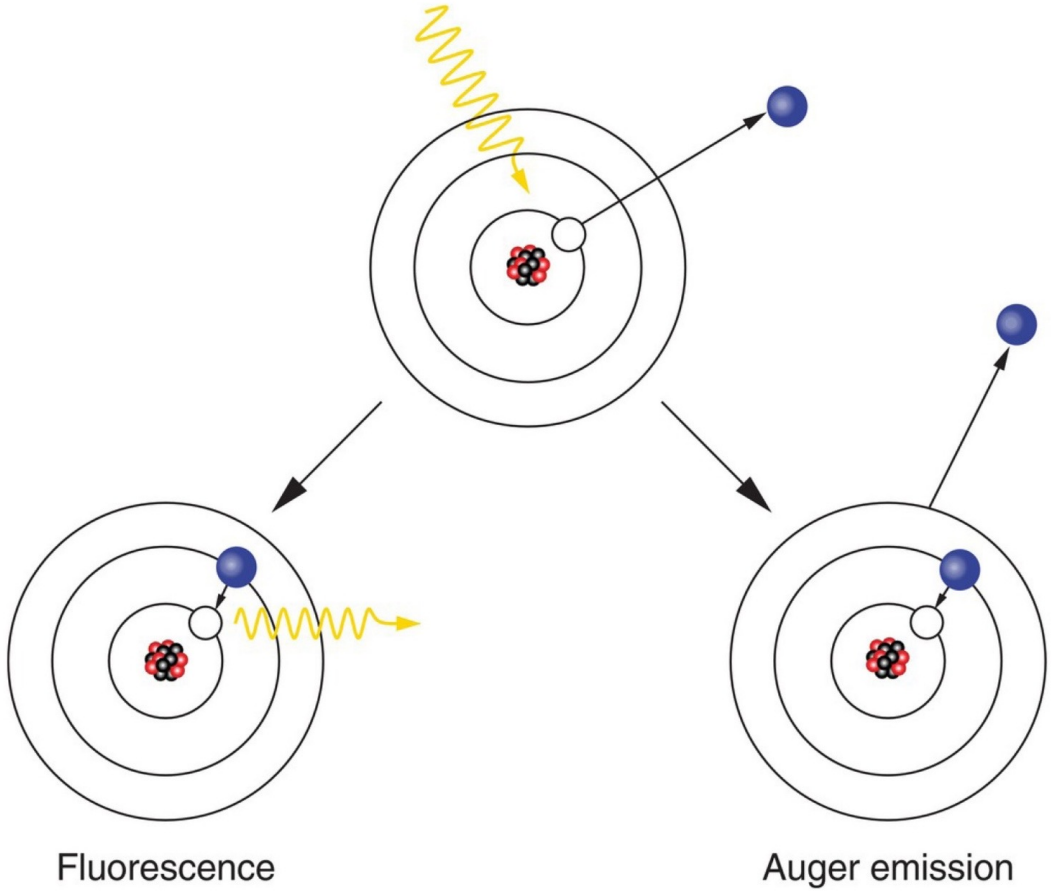
Lambert-Beer absorption law. Attenuation length.



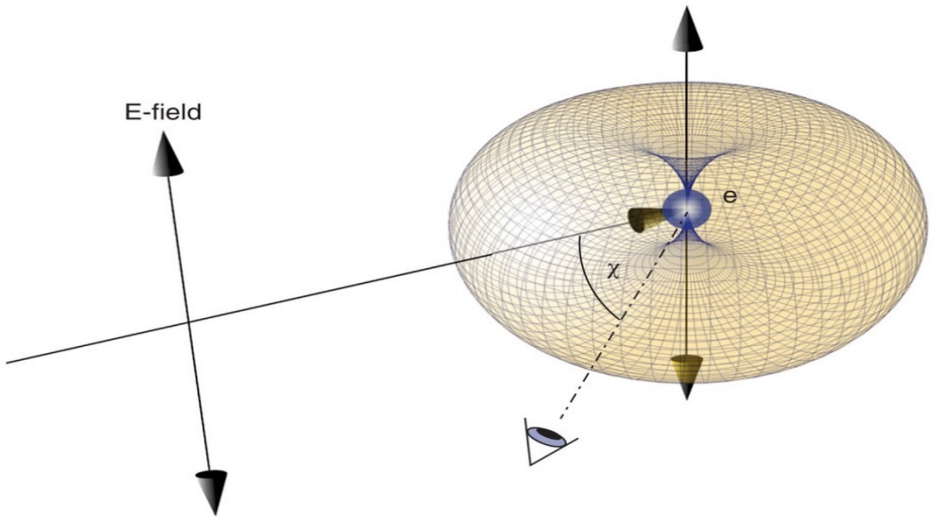


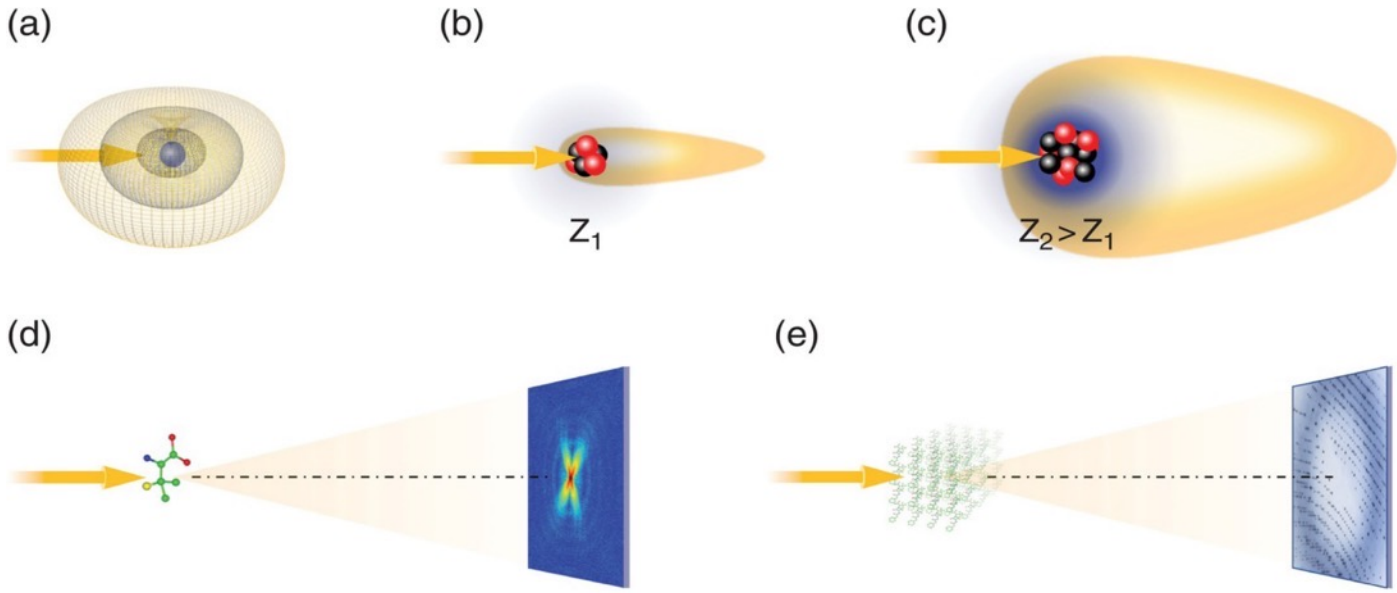


Photoabsorption and ionization. Secondary processes.

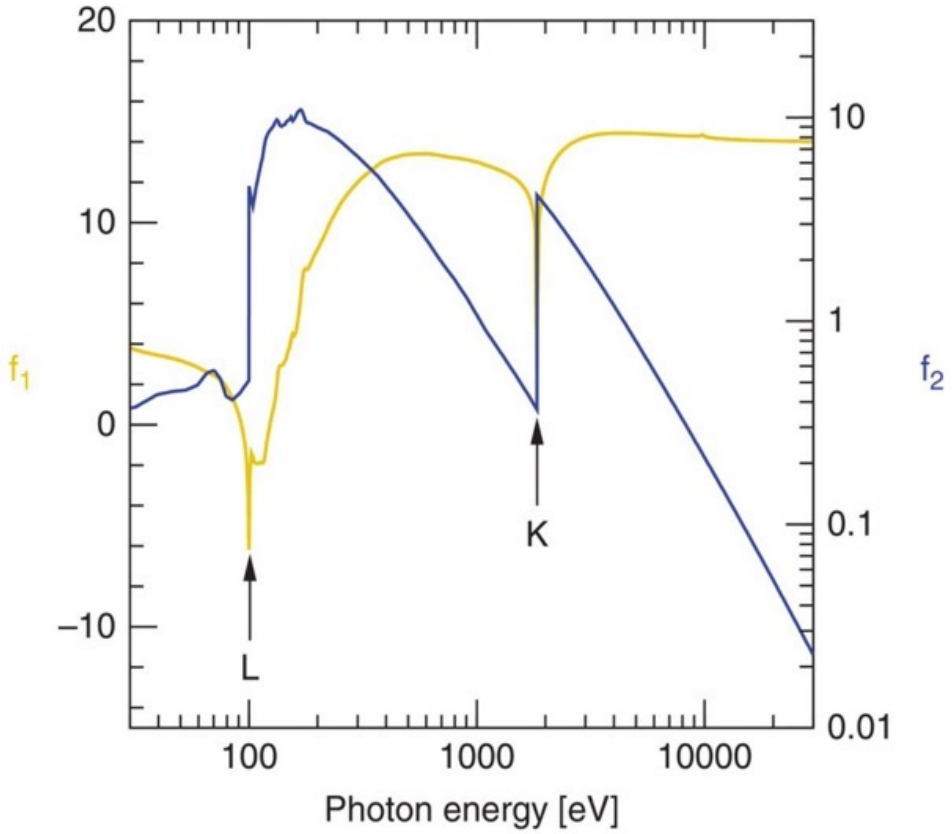


Thomson scattering and atomic form factor

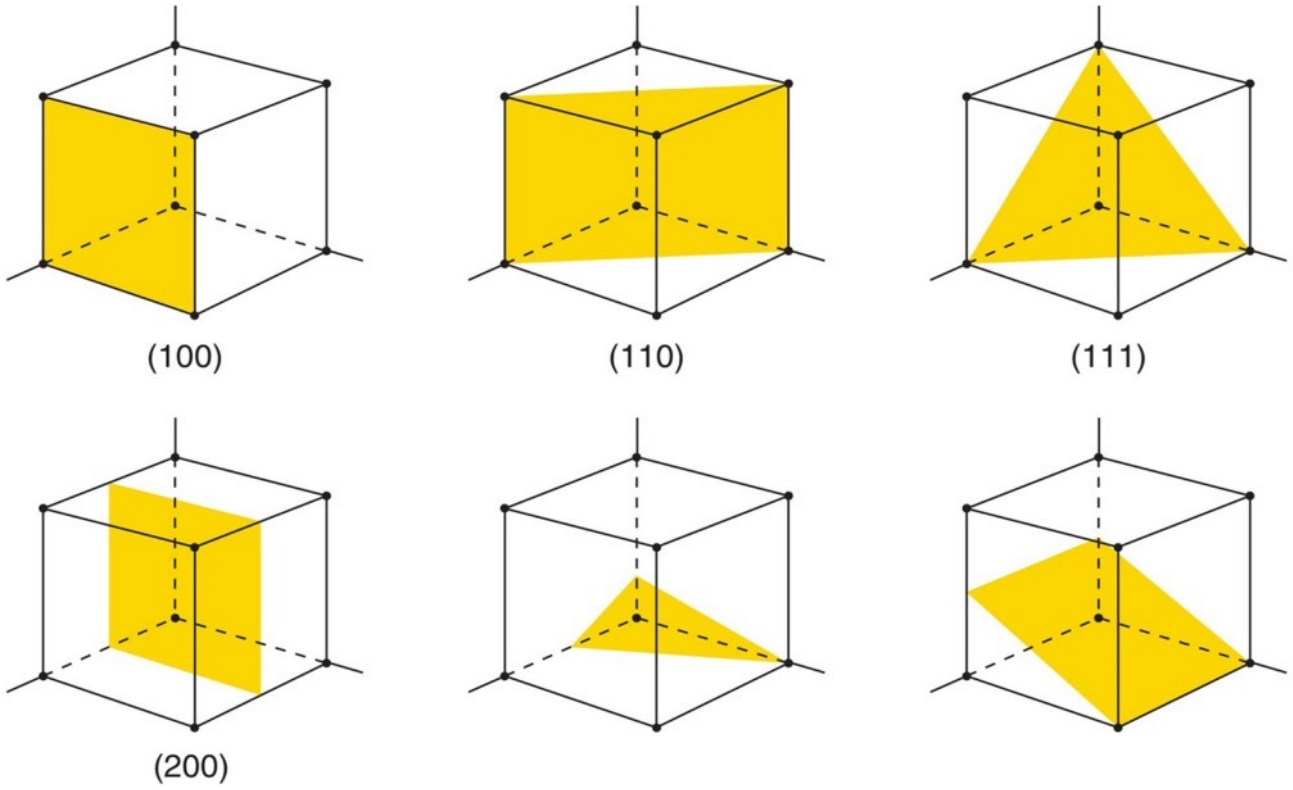




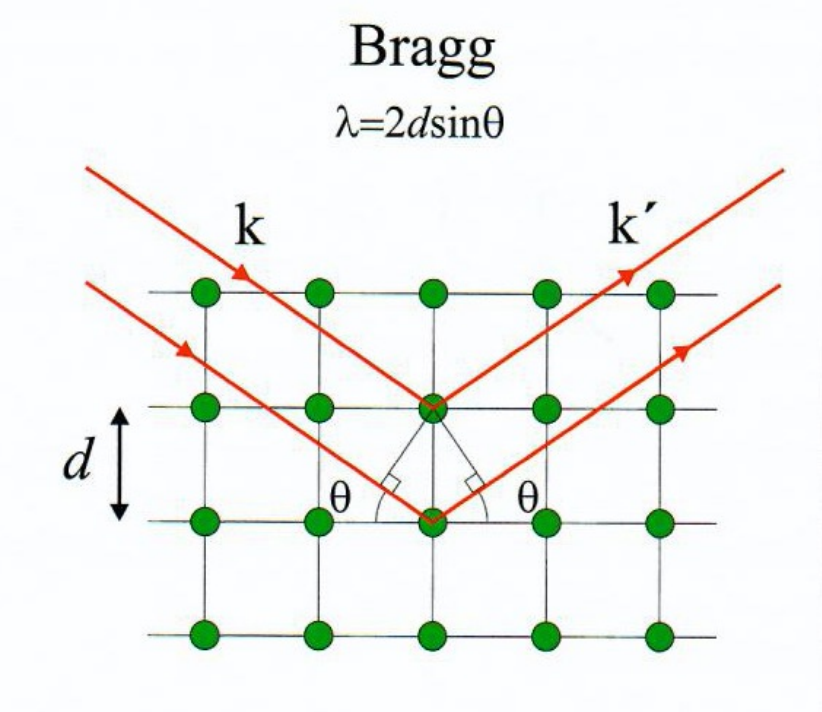
Atomic scattering factors



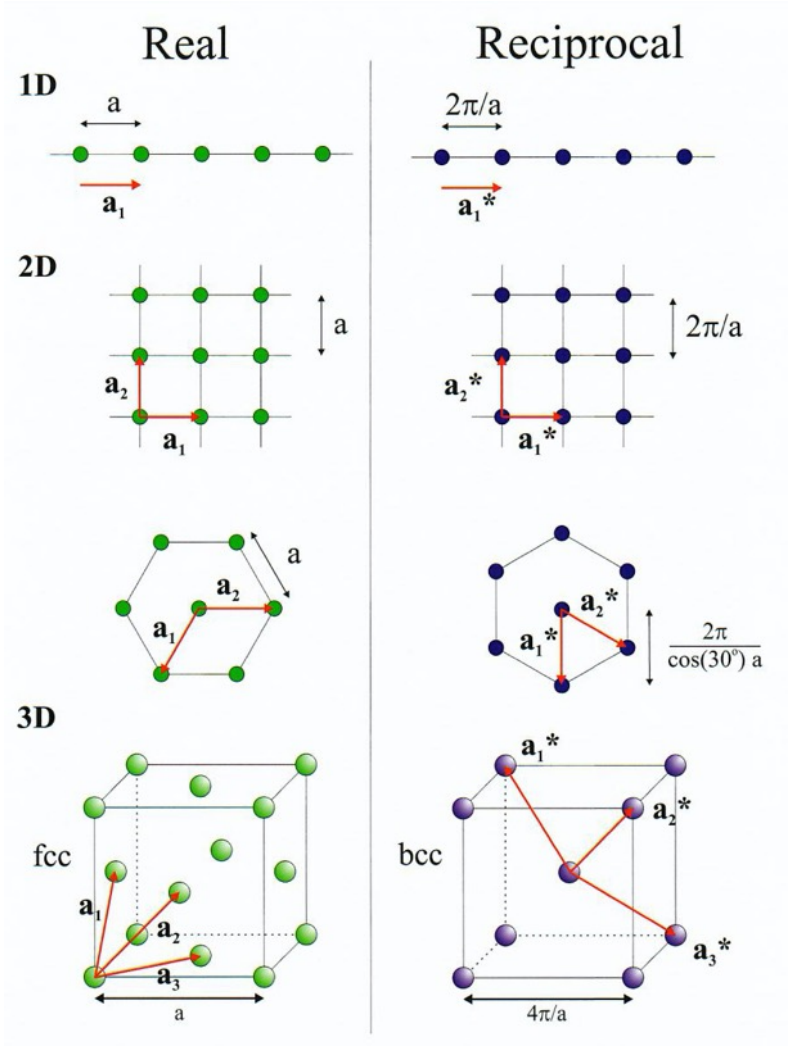
Lattice planes and Miller indices



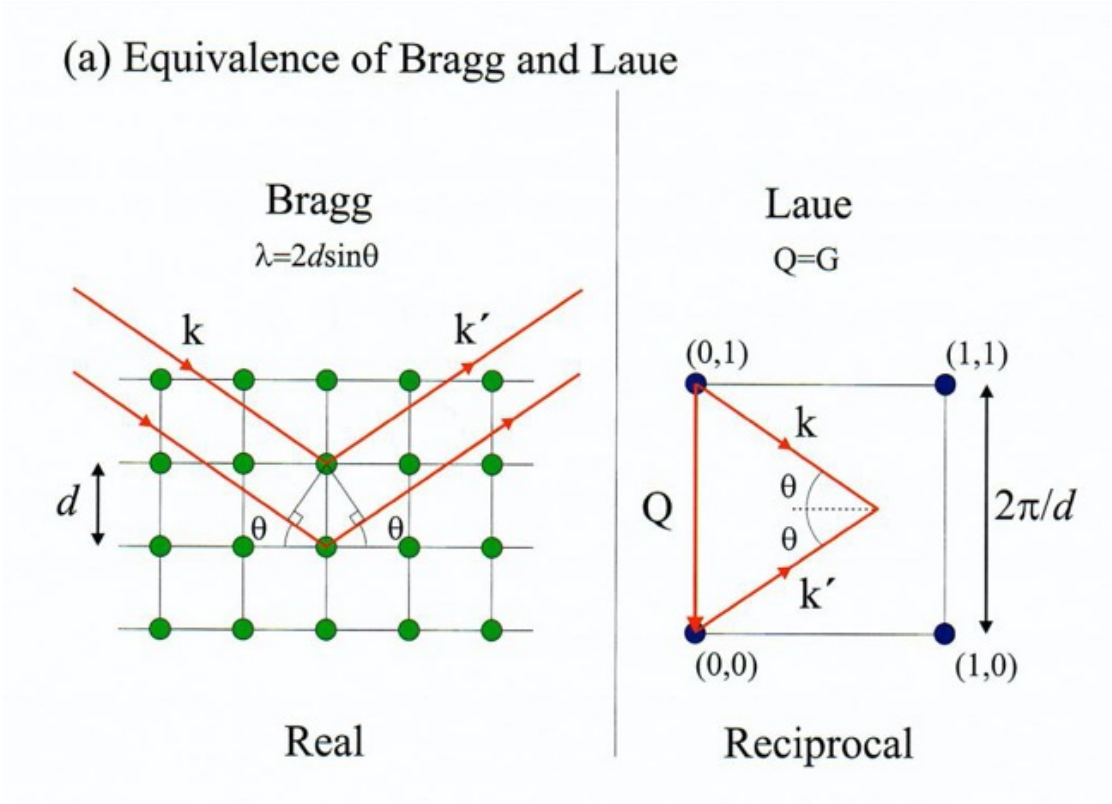
Bragg reflections



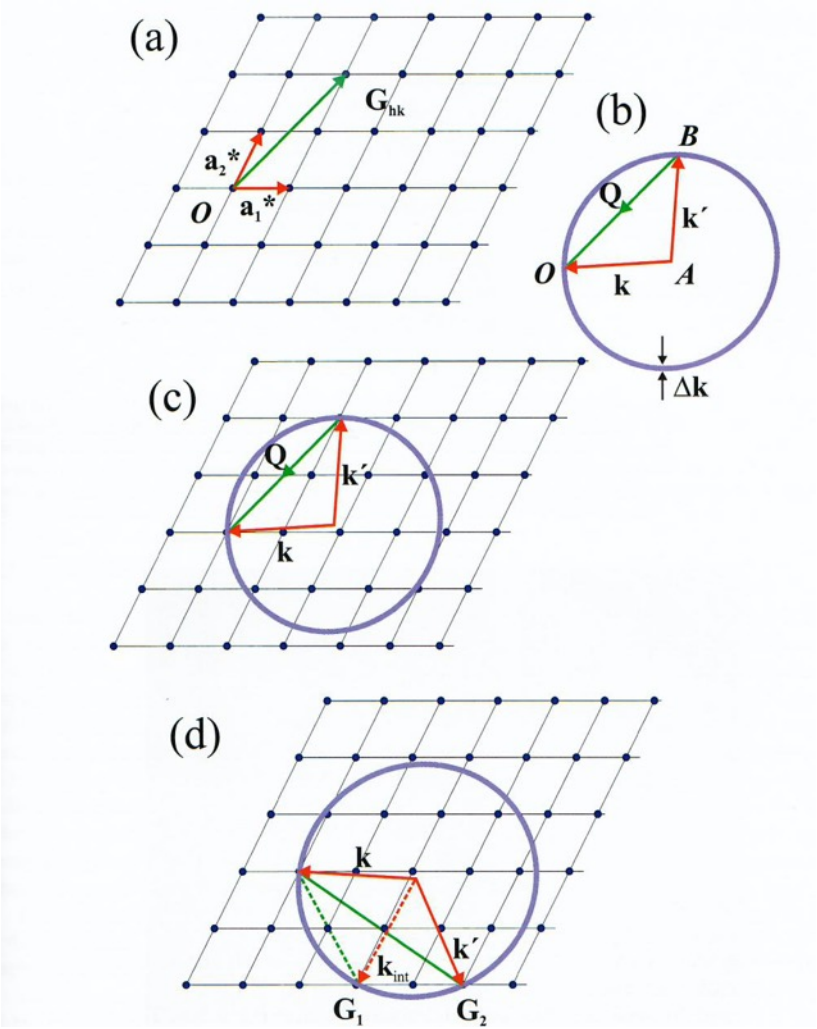
Real and reciprocal lattice



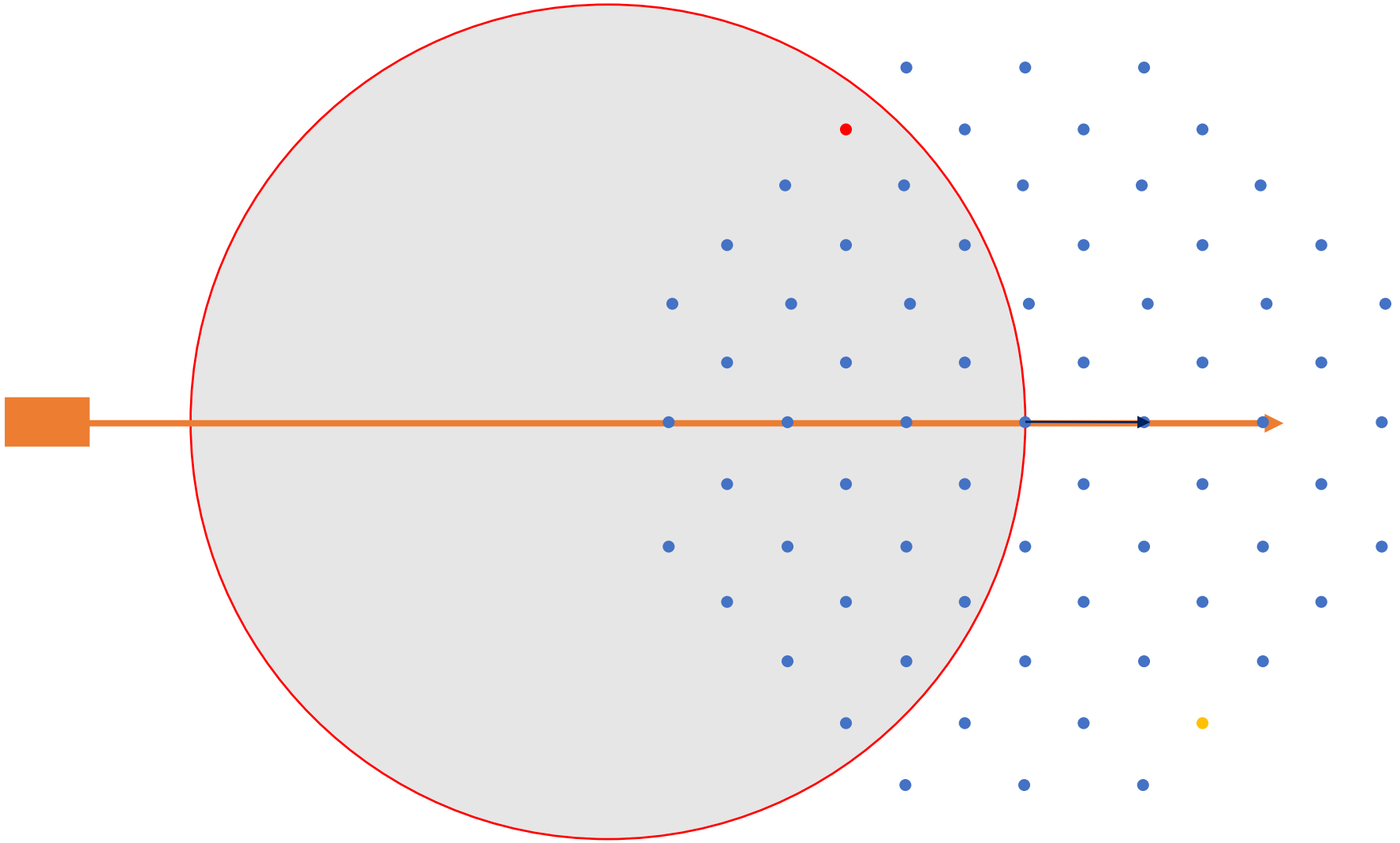
Bragg and Laue conditions



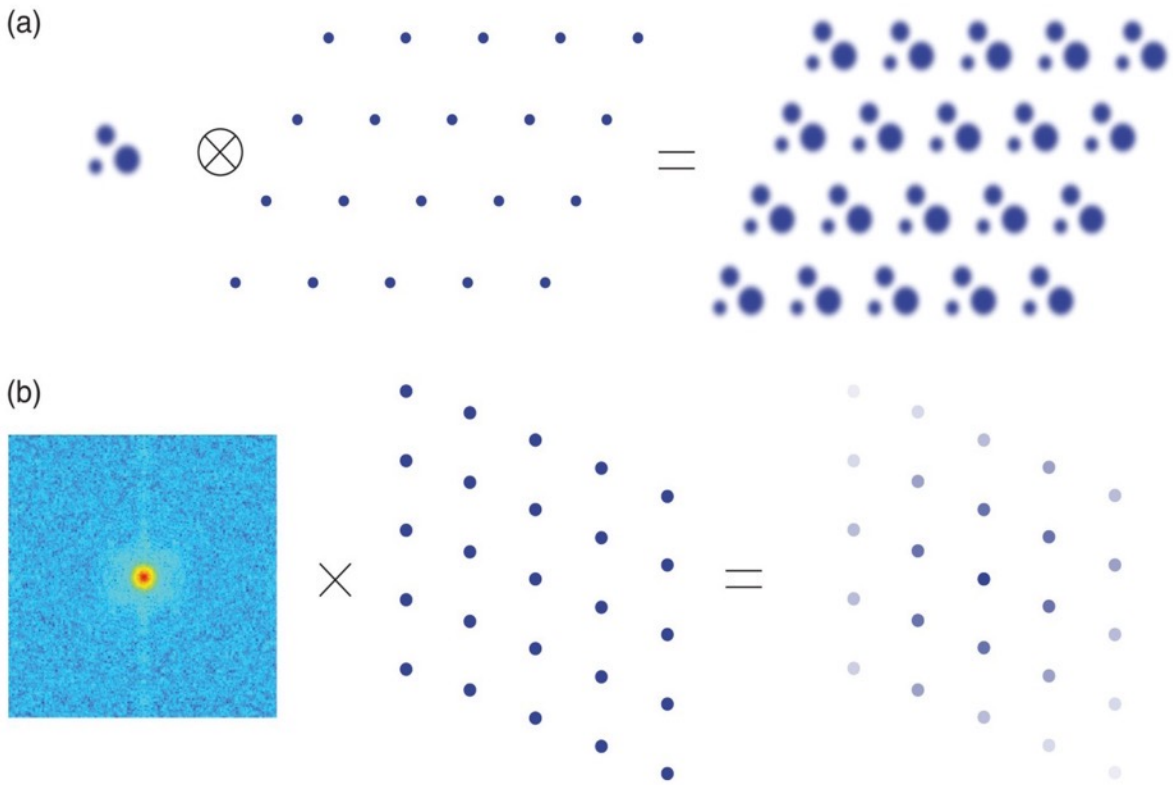
Construction of the Ewald sphere



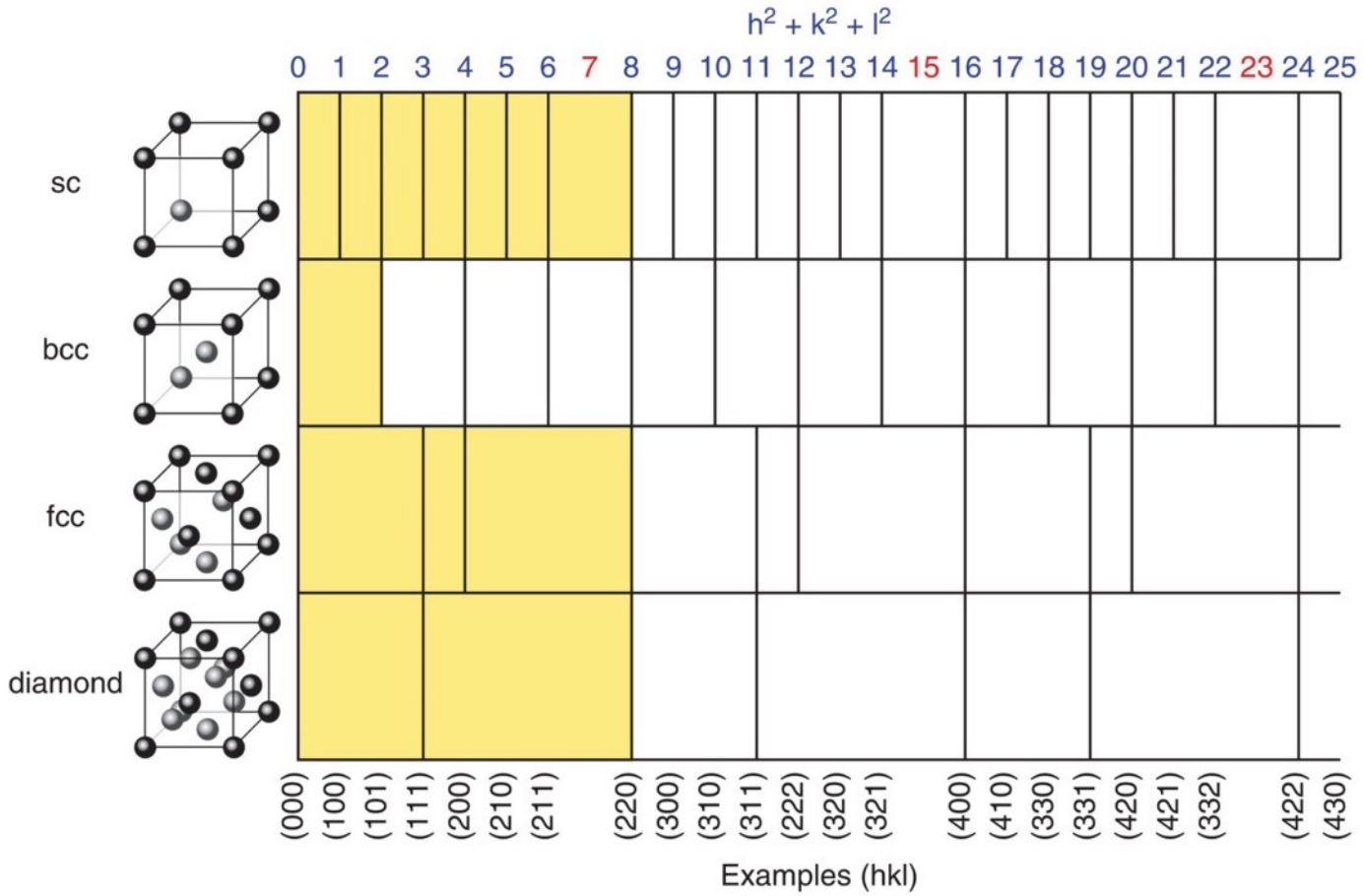
Construct diffraction experiment in Laue formalism



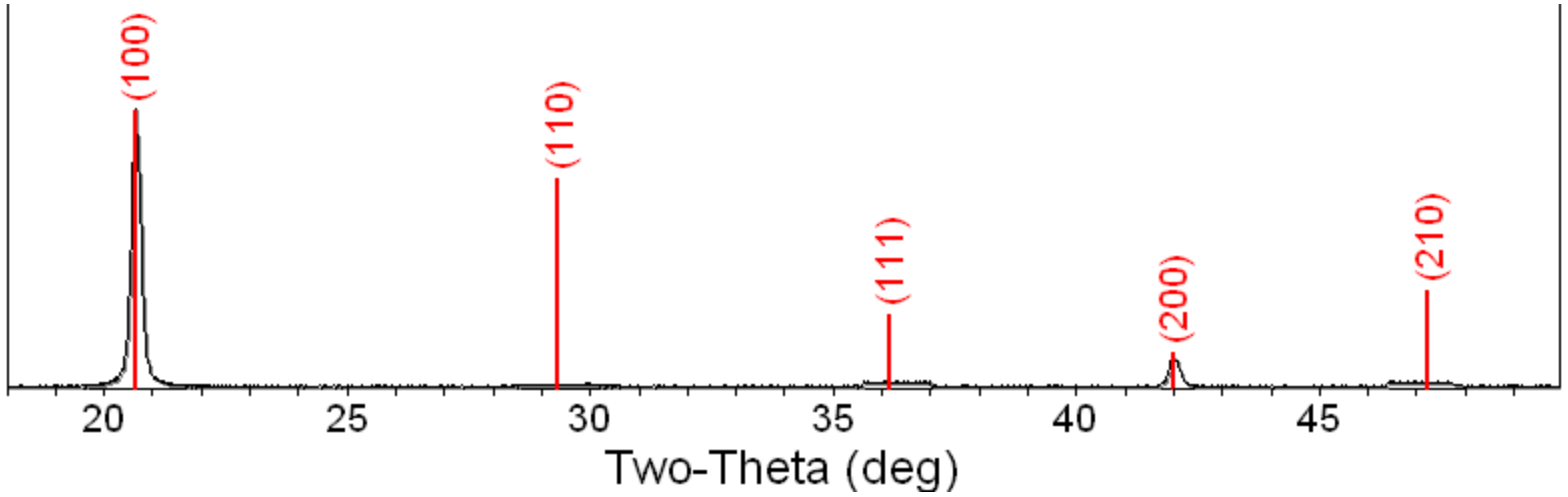
From Bragg reflections to the structure factor

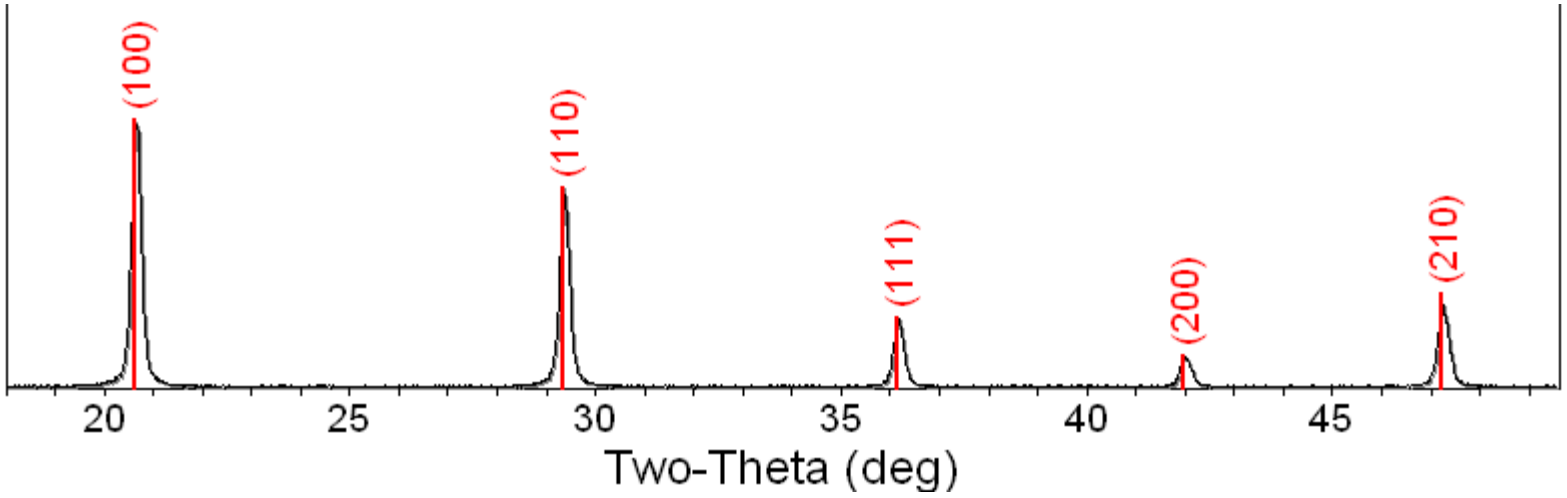


Allowed and forbidden reflections

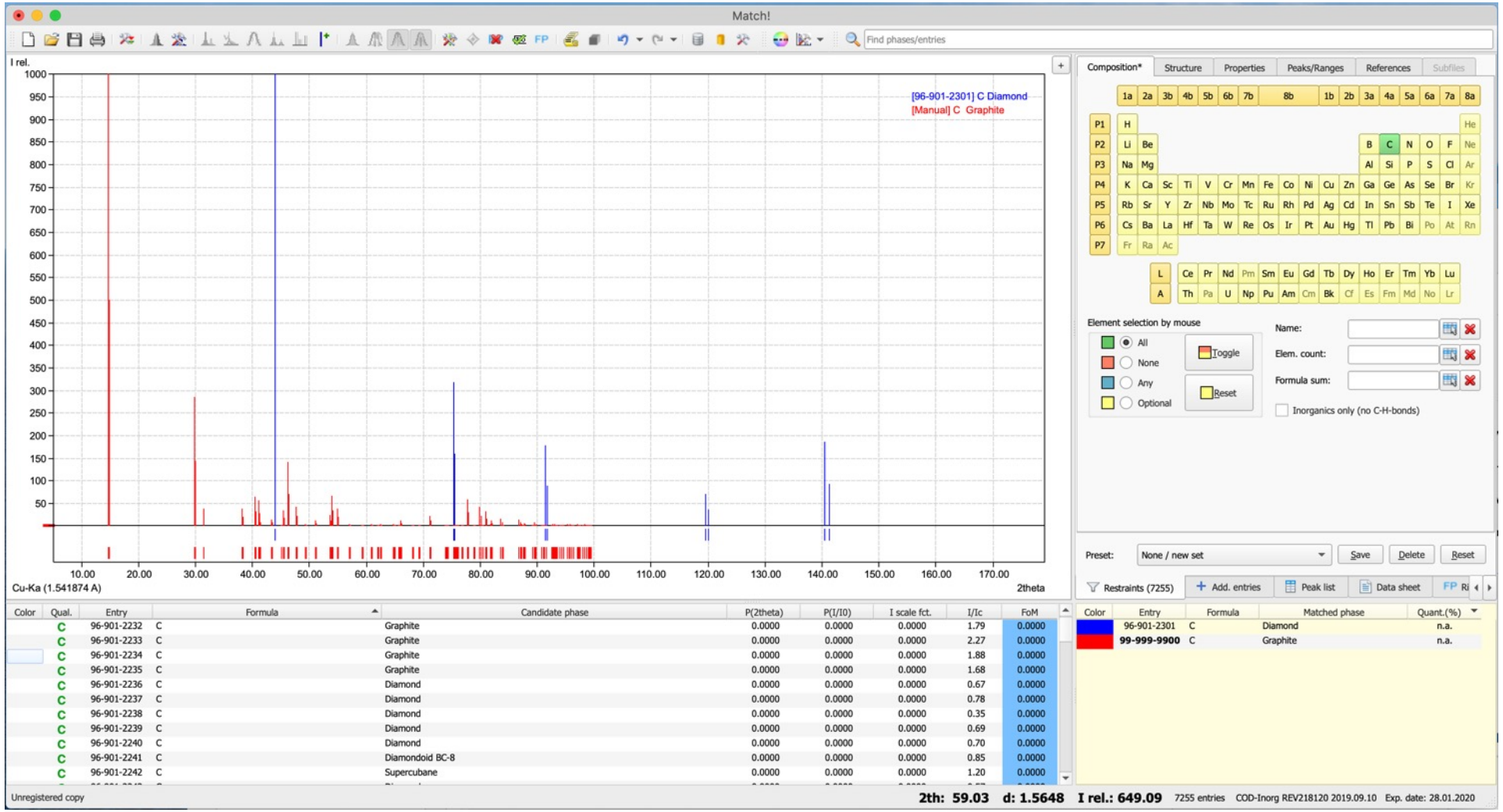


Bragg reflection from a single crystal vs powder diffraction



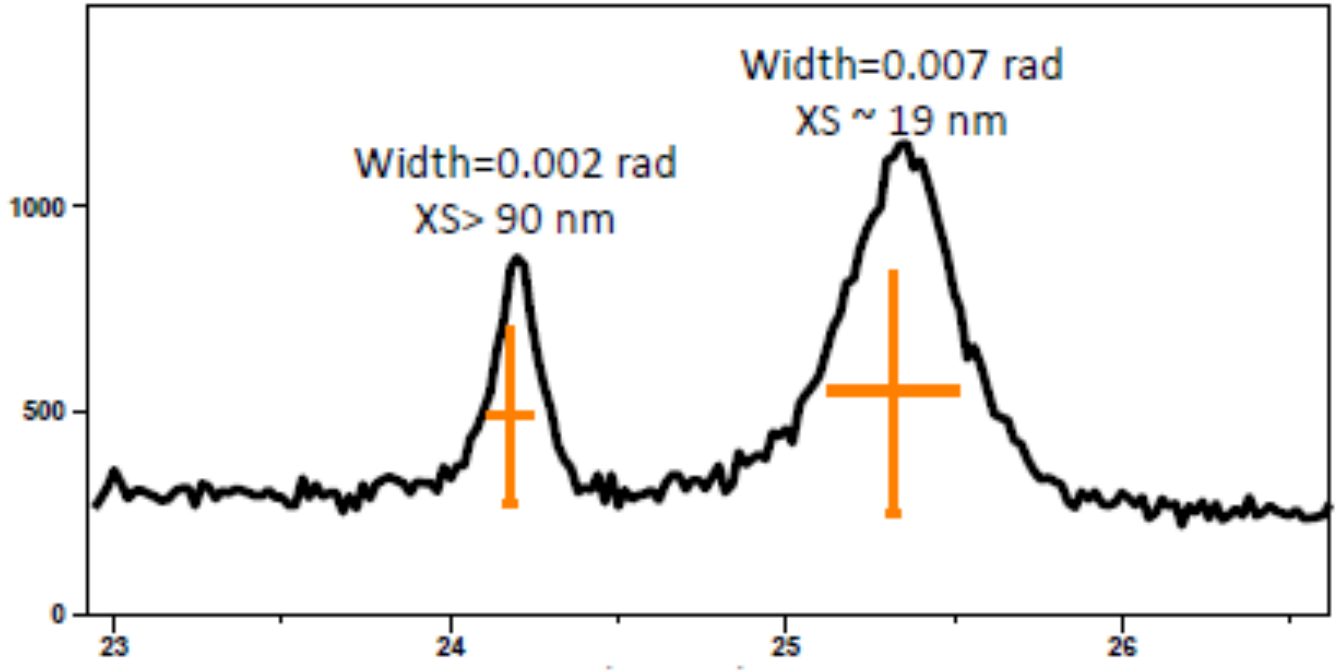


Powder diffraction for structural analysis



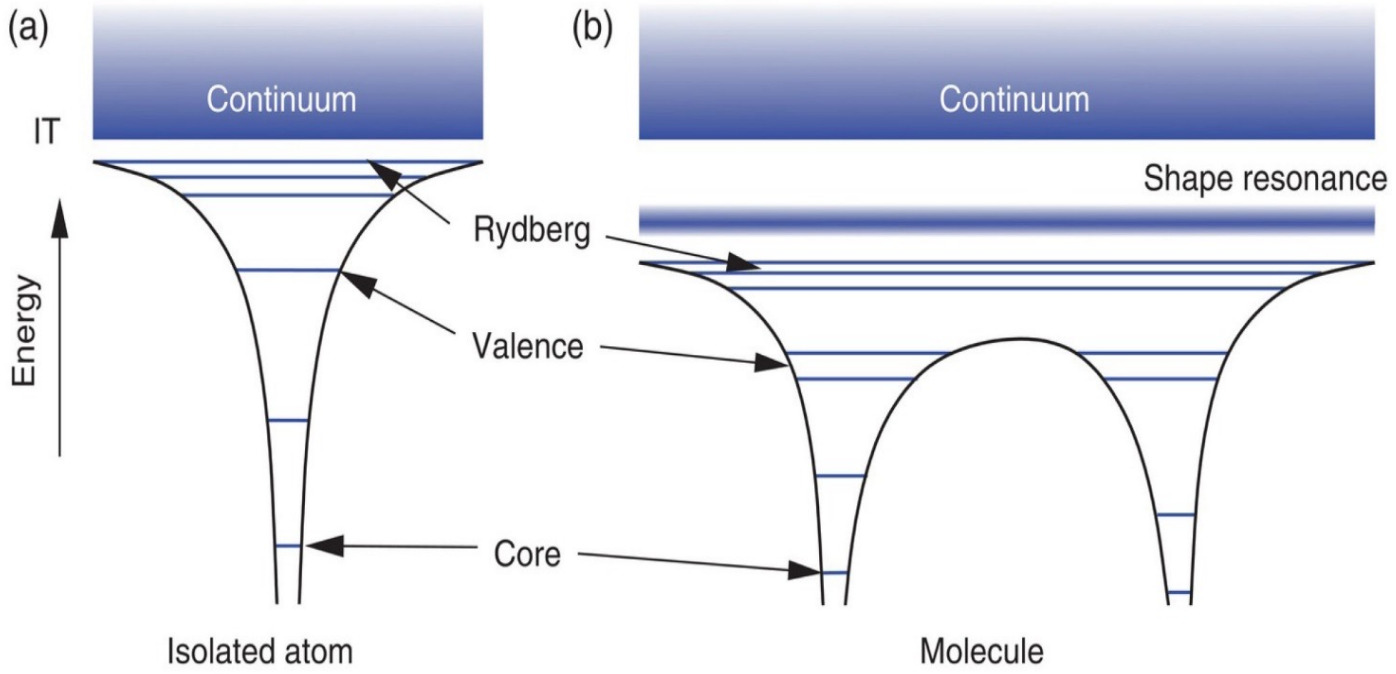
Debye-Scherrer equation

The diffraction peak width may contain microstructural information

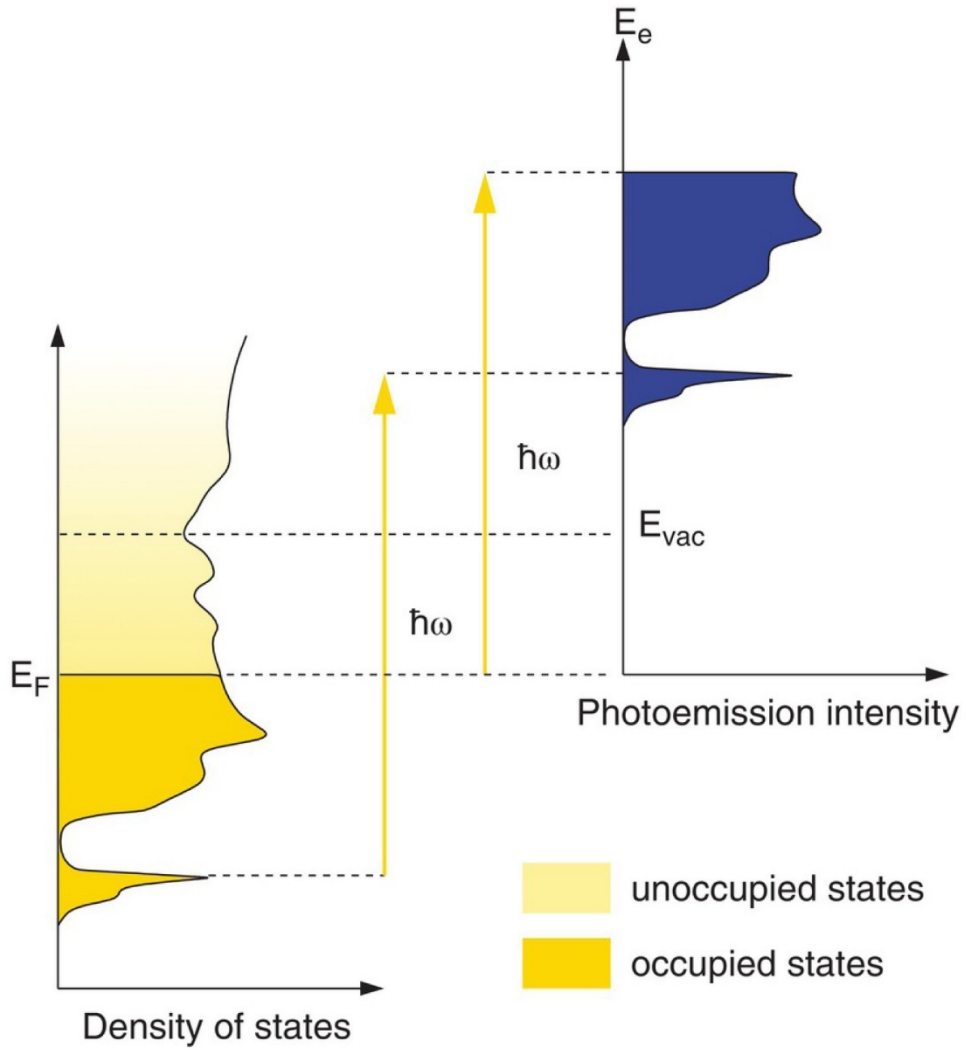


$$\text{Size} = \frac{K\lambda}{Width * \cos\theta}$$

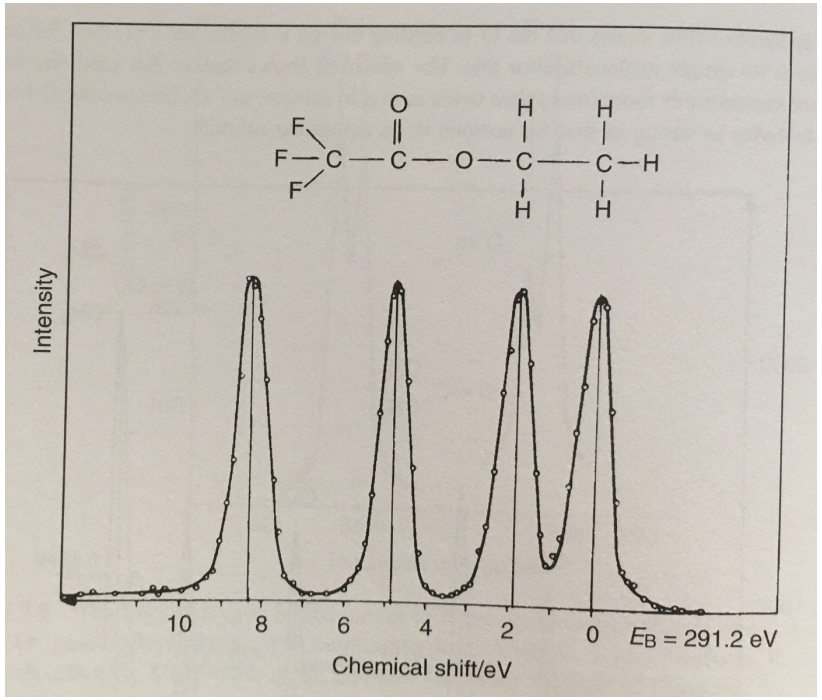
Atoms vs molecules



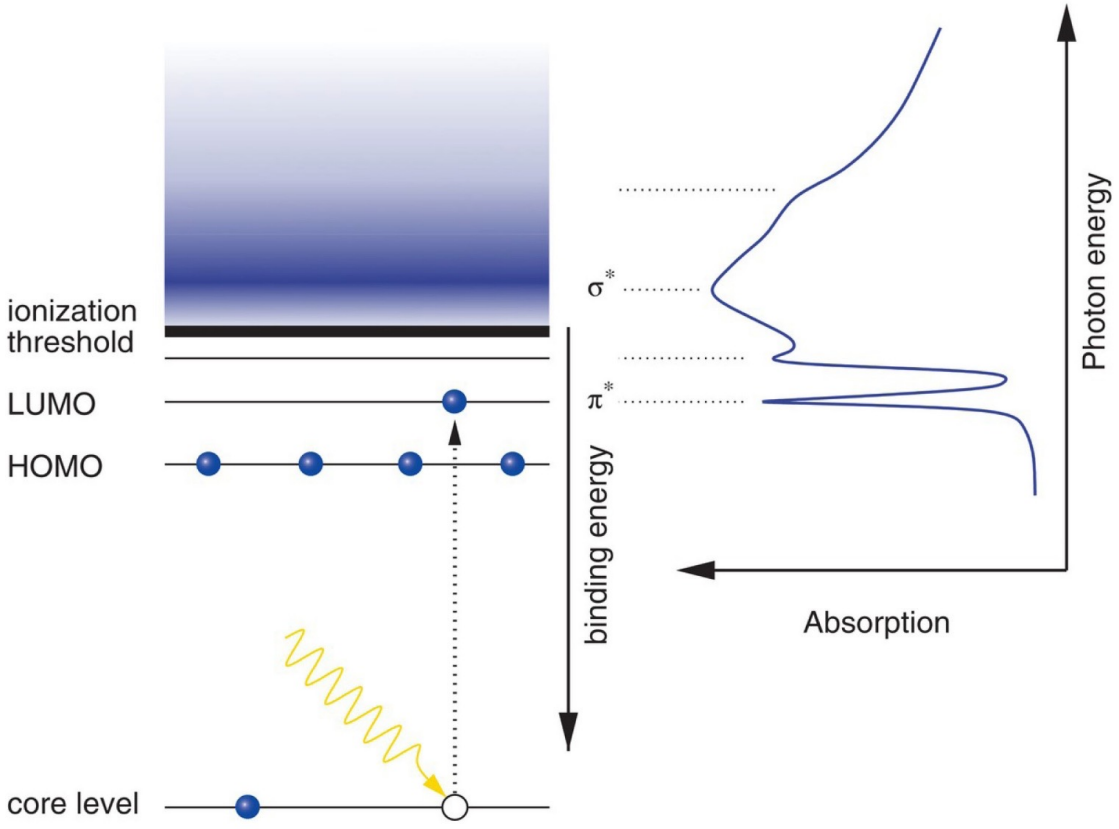
Principles of photoemission spectroscopy



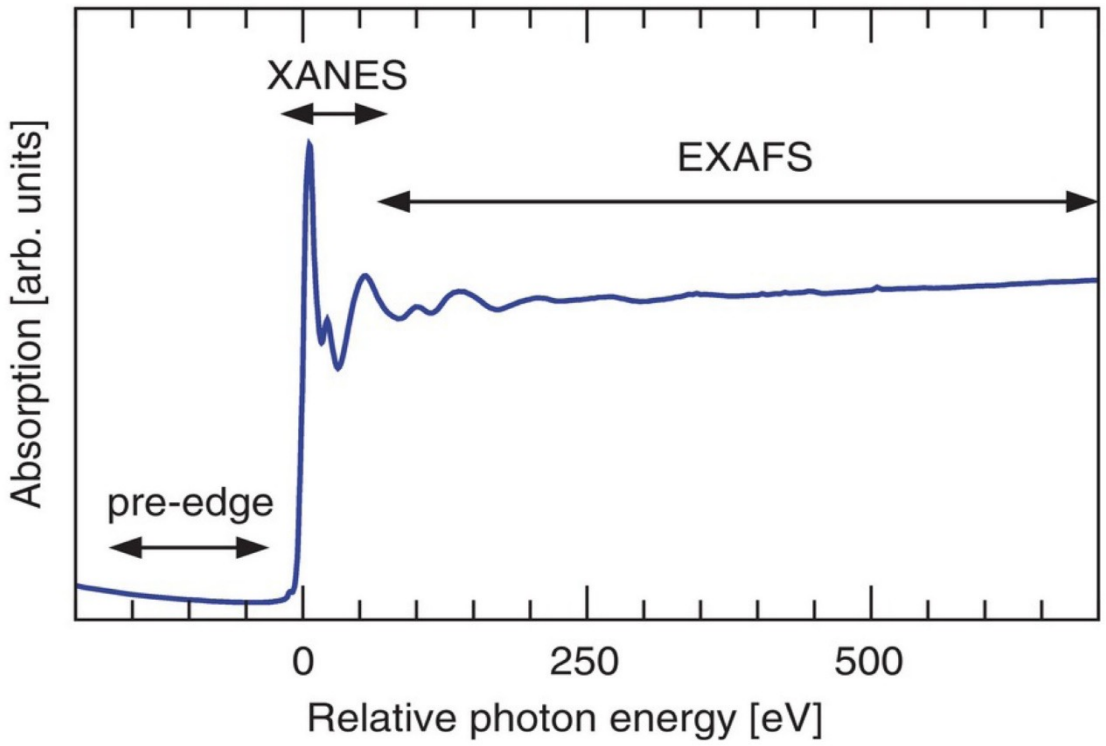
Chemical shifts in photoemission spectroscopy



Principles of X-ray absorption spectroscopy



The different regimes of x-ray absorption spectroscopy



Absorption vs Photoemission