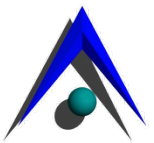
More advanced (and fun) techniques using x-rays



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Alan Goldman

IOWA STATE UNIVERSITY

More than “just diffraction”

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- **X-ray resonant magnetic scattering*****
  - Magnetic structures of neutron absorbing materials with very high resolution
- **Pump-probe experiments**
  - Dynamics on picosecond to millisecond timescales
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  - Studying mesoscopic-scale structures
- **X-ray radiography and tomography**
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- **Surface scattering**
  - Studies of both solid and liquid surfaces
- **Coherent x-ray diffraction**
  - Probing coherence effects on the atomic scale

Diffraction peak intensities

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Generally speaking:

Whereas the dimensions and symmetry of the unit cell determine peak positions, peak intensities are governed by how the atoms are arranged within the unit cell.

$$I_{hkl} \propto |F_{hkl}|^2$$

$$F_{hkl} = \sum_{j=1}^{m} N_j f_j \exp\left[2\pi i\left(hx_j + ky_j + lz_j\right)\right]$$

- where the atoms are on the atomic planes
  - this is expressed by the fractional coordinates x_j y_j z_j
- what atoms are on the atomic planes
  - the scattering factor f_j quantifies the efficiency of X-ray scattering at any angle by the group of electrons in each atom
    - The scattering factor is equal to the number of electrons around the atom at 0° θ, the drops off as θ increases
  - N_j is the fraction of every equivalent position that is occupied by atom j

Atomic scattering factors

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$$I_{hkl} \propto |F_{hkl}|^2$$

$$F_{hkl} = \sum_{j=1}^{m} N_j f_j \exp\left[2\pi i\left(hx_j + ky_j + lz_j\right)\right]$$

$$f = f_0 + f' + if''$$

Anomalous corrections for Cu

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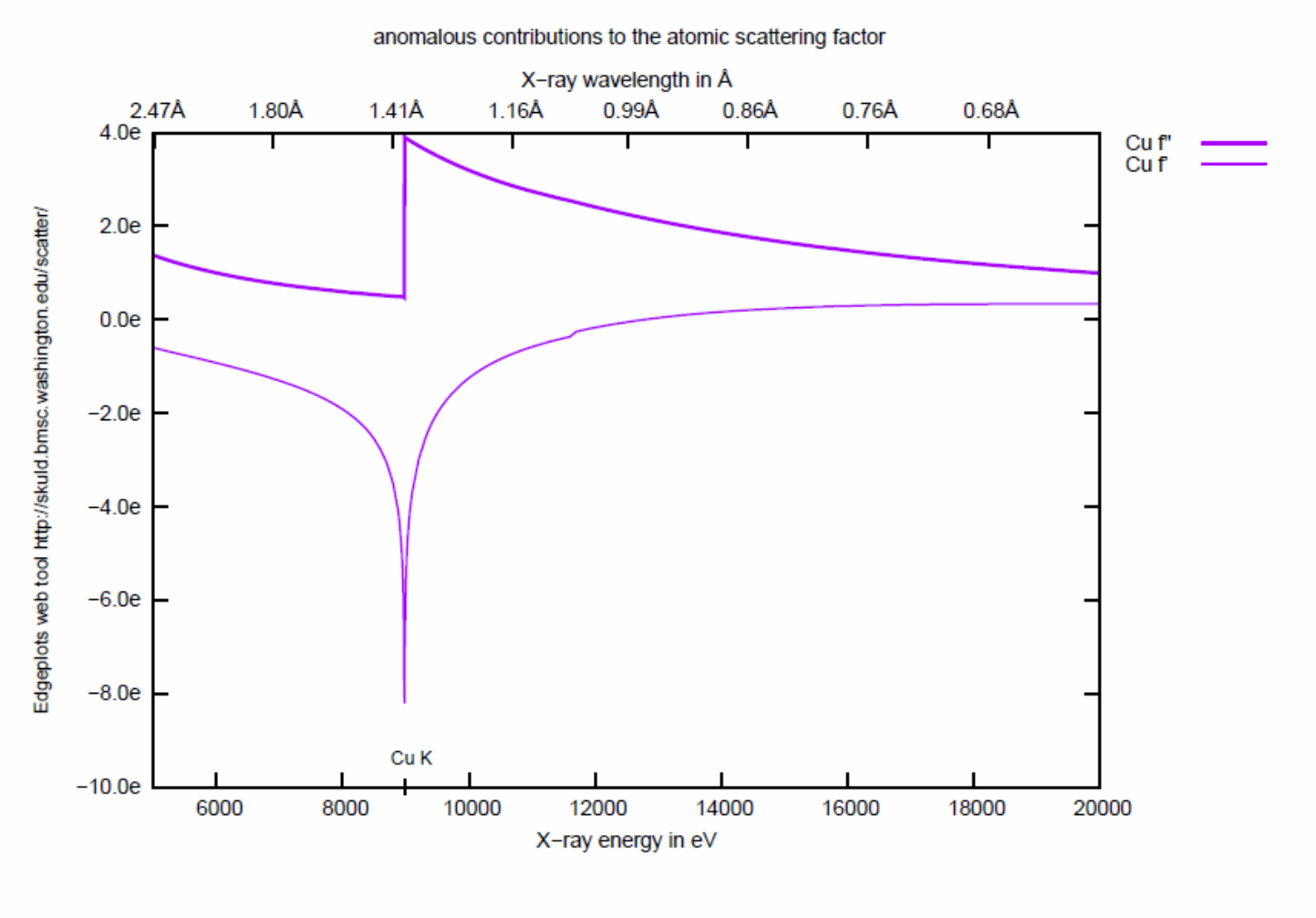

How does this help?

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- Elements close in Z have very similar values for f_0.
  - The real part of the anomalous scattering correction can change f sufficiently to resolve the different elements.
  - One approach to the “phase problem” (breaking Friedel’s Law).

X-ray Absorption Spectroscopy

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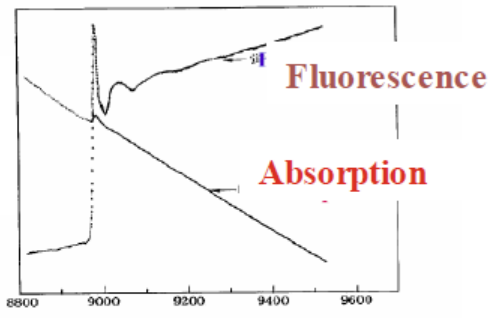
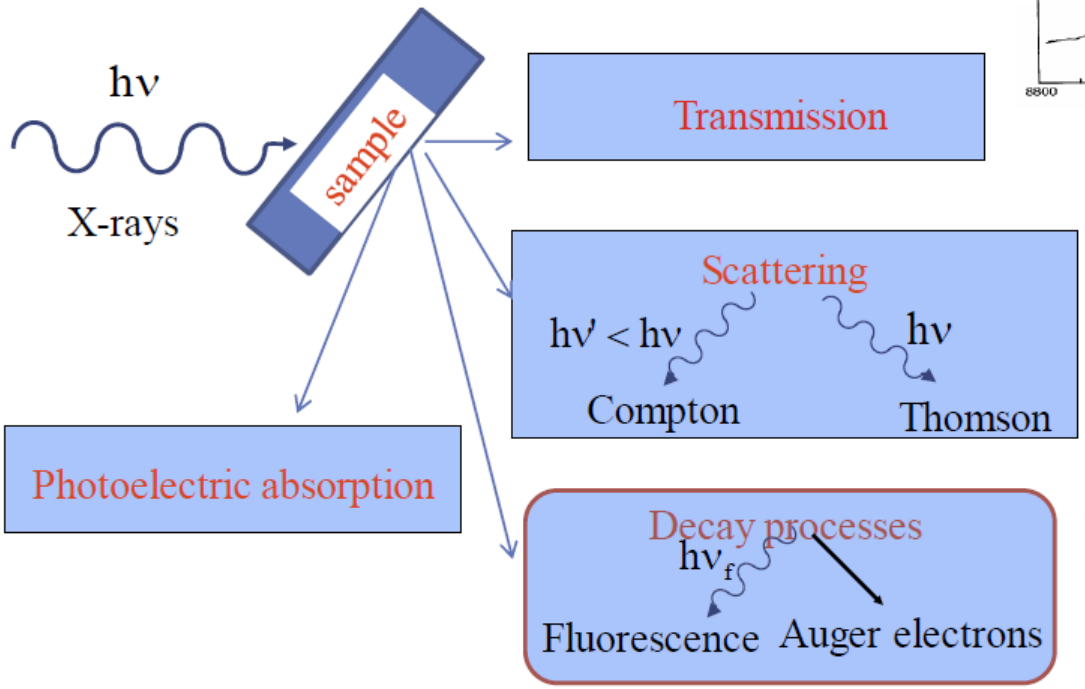
The absorption coefficient





X-ray Absorption Spectroscopy

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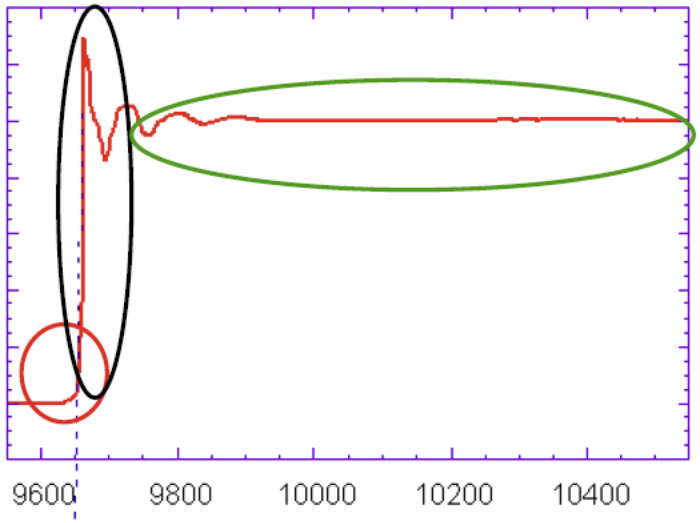

XANES and EXAFS:

- Types of Ligands
- Distances
- Coordination Number

PRE-EDGE

- Covalency
- electronic structure

XANES

- Oxidation State
- Site Symmetry

X-ray Absorption Spectroscopy

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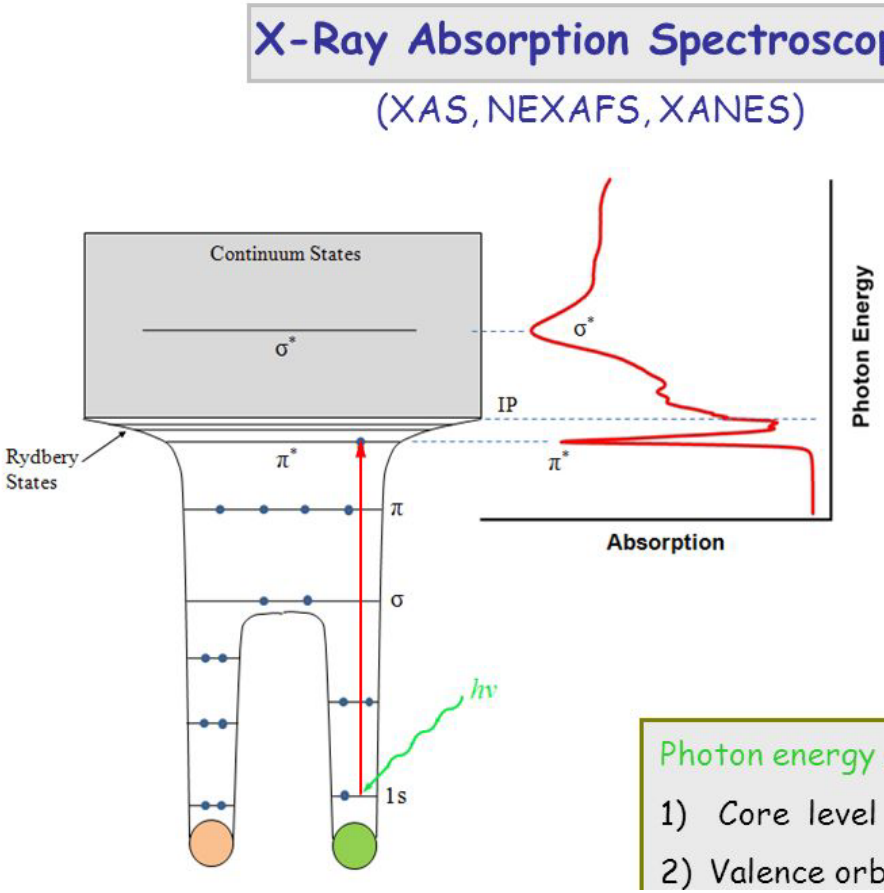

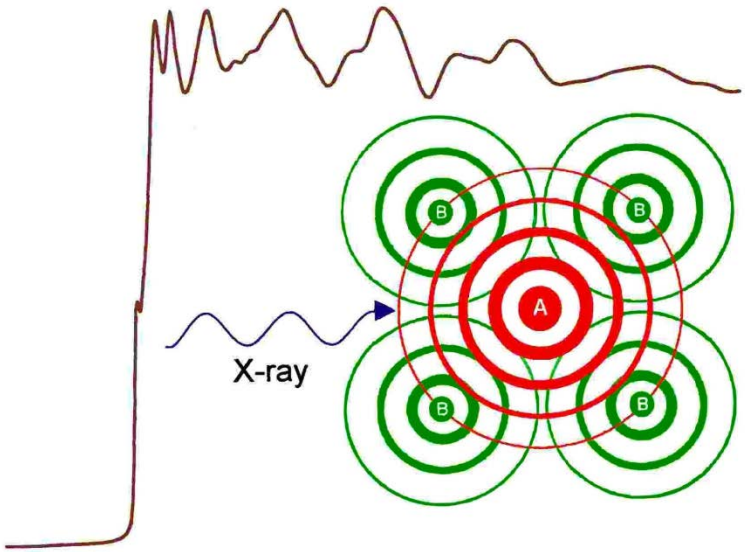

Photon energy $h\nu$ related to:

1) Core level $\Rightarrow$ Element

2) Valence orbital $\Rightarrow$ Bonding

X-ray Absorption Spectroscopy

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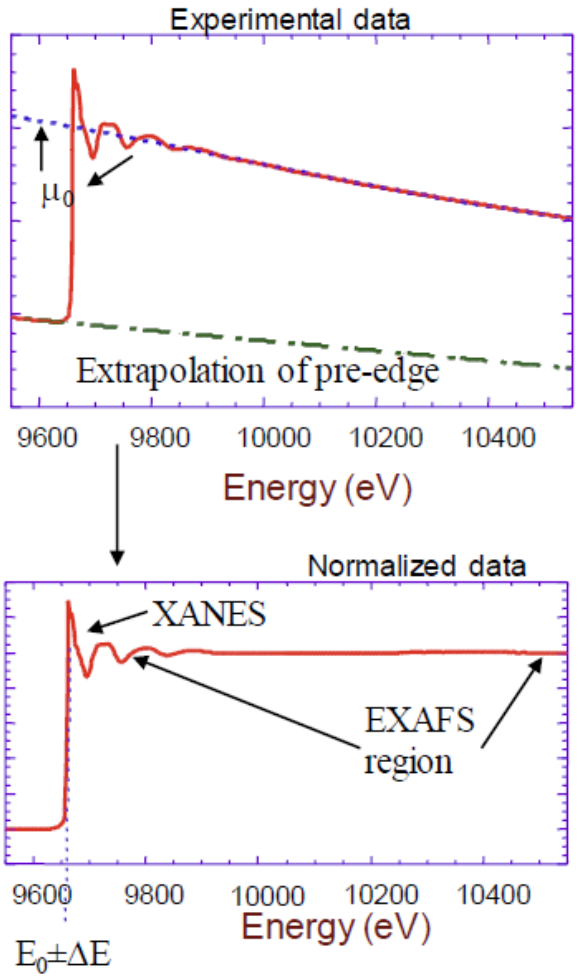

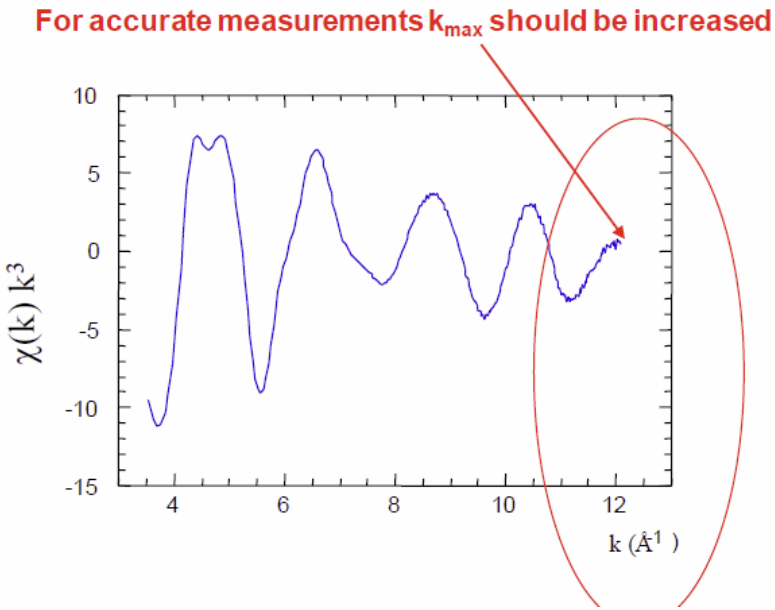

$$\chi(k) = \sum_j \frac{N_j S_0^2}{kR_j^2} F_j(k) e^{-2R_j/\lambda_j(k)} e^{-2k^2\sigma_j^2} \sin\left[2kR_j + \Phi_j(k)\right]$$

X-ray Magnetic Circular Dichroism

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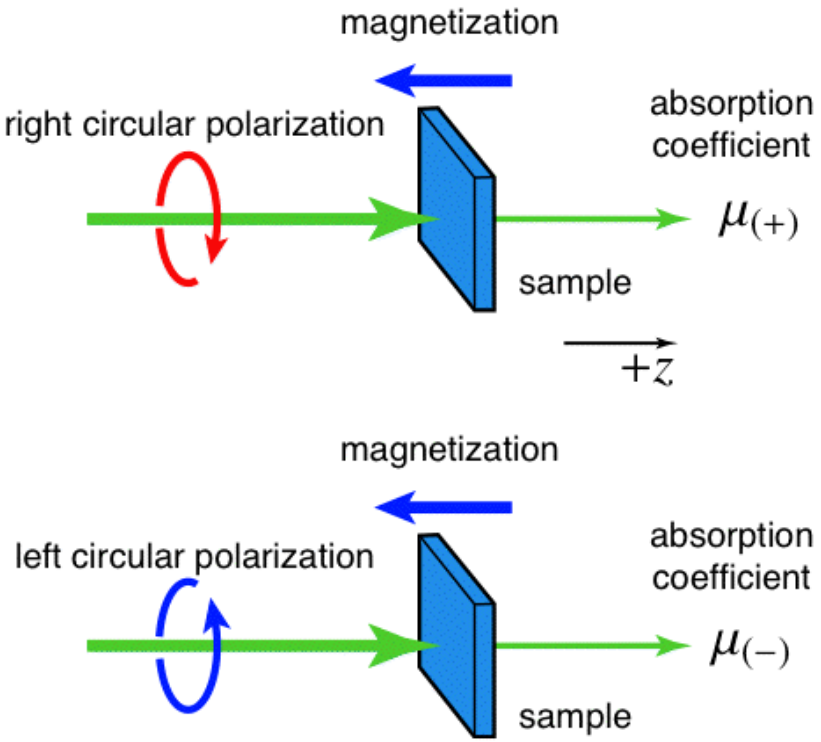
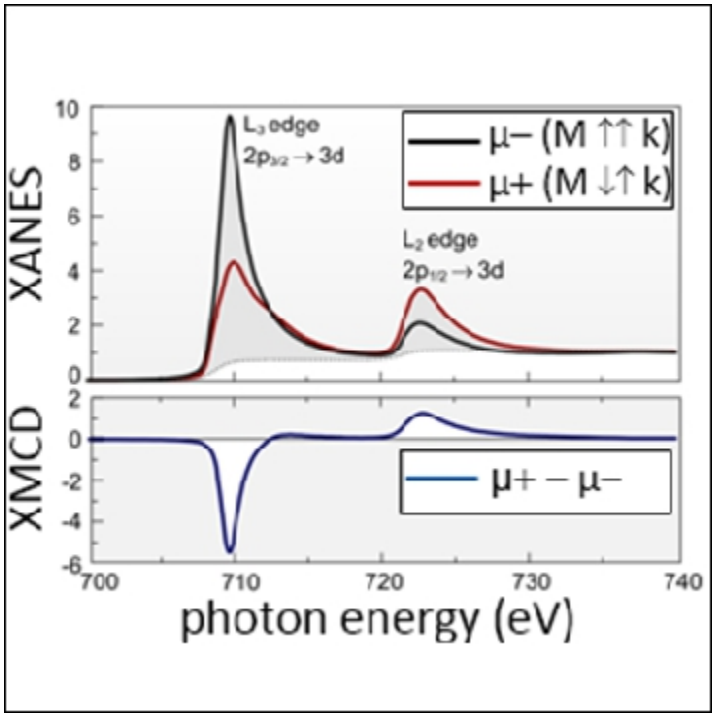
For Ferromagnetic Materials:



X-ray magnetic circular dichroism (XMCD)

$$\Delta\mu = \mu_{(+)} - \mu_{(-)}$$



X-ray Magnetic Circular Dichroism

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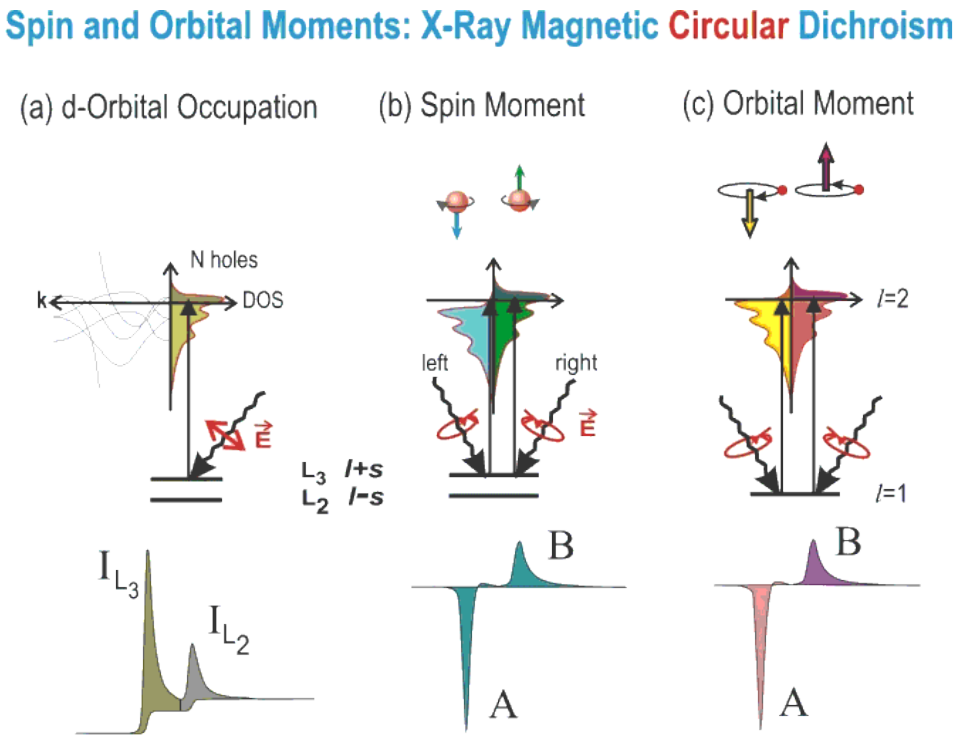

Fig. 2: Electronic transitions in conventional L-edge x-ray absorption (a), and x-ray magnetic circular x-ray dichroism (b,c), illustrated in a one-electron model. The transitions occur from the spin-orbit split 2p core shell to empty conduction band states. In conventional x-ray absorption the total transition intensity of the two peaks is proportional to the number of d holes (first sum rule). By use of circularly polarized x-rays the spin moment (b) and orbital moment (c) can be determined from linear combinations of the dichroic difference intensities A and B, according to other sum rules

Element and orbital specific magnetic susceptibility.

Different probes

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	NEUTRONS	X-RAYS	ELECTRONS
Wavelength range	0.4 - 10 Å	0.1 - 5 Å	0 .04 - 0.2 Å
Energy range	0.001 - 0.5 eV	3000 - 100000 eV	6000 - 120000 eV
Cross-section	10^{-25} barns	10^{-25} Z^2 barns	~10^{-22} barns
Penetration depth	~ cm	~ μm	~ nm
Typical flux	10^{11} s^{-1} m^{-2}	10^{24} s^{-1} m^{-2}	10^{26} s^{-1} m^{-2}
Beam size	mm-cm	μm-mm	nm-μm
Typical sample	Any bulk sample	Small crystals, powders, surfaces	Surfaces, thin films, grains, gases
Techniques	**Diffraction** Inelastic scattering Reflectivity	Diffraction Photon absorption Photoemission Inelastic scattering	Microscopy Diffraction Emission spectroscopy EELS
Phenomena	**Magnetic/crystal structures** collective excitations (phonons, spin waves) electronic excitations (crystal-field, spin-orbit)	Crystal structures, electronic transitions (photoemission, absorption),	microstructure crystal structures electronic transitions

X-ray Resonant Magnetic Scattering

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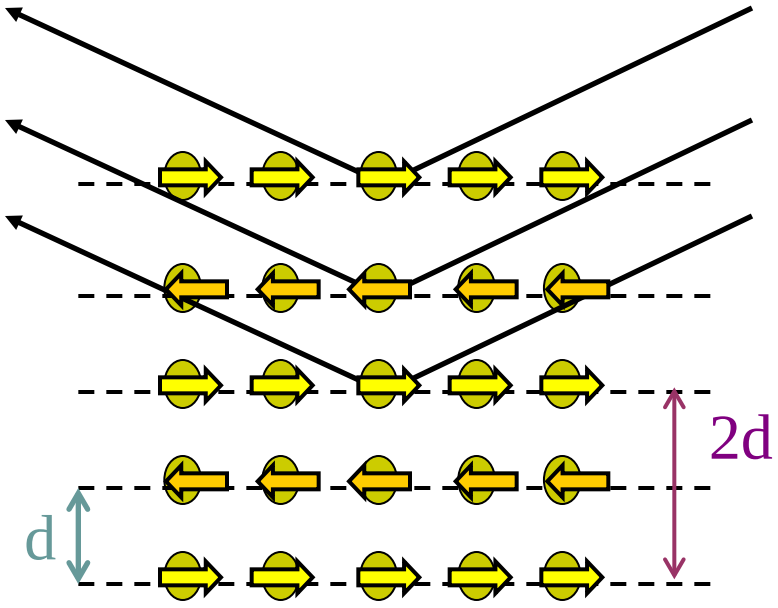
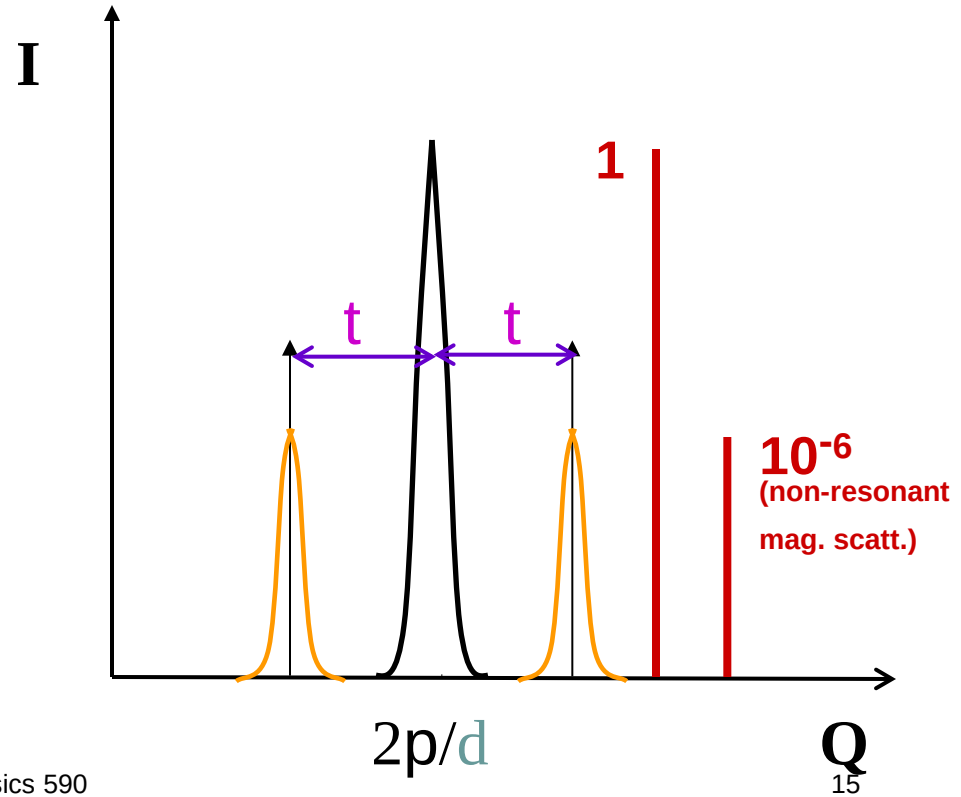
$Q_{Bragg}=2p/d$

$t = 2p/2d$





Why Bother?

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- Many of the technologically important RE compounds contain neutron opaque elements.
- Superior reciprocal space (Q) resolution allows more detailed study … reinvestigation of “solved” structures.
- Can be used for investigations of submillimeter-sized single crystals.
- Resonant magnetic scattering occurs at well-defined energies specific to elements of interest -- probe local magnetism.
- Studies of magnetic surfaces and interfaces.

Absorption of neutrons

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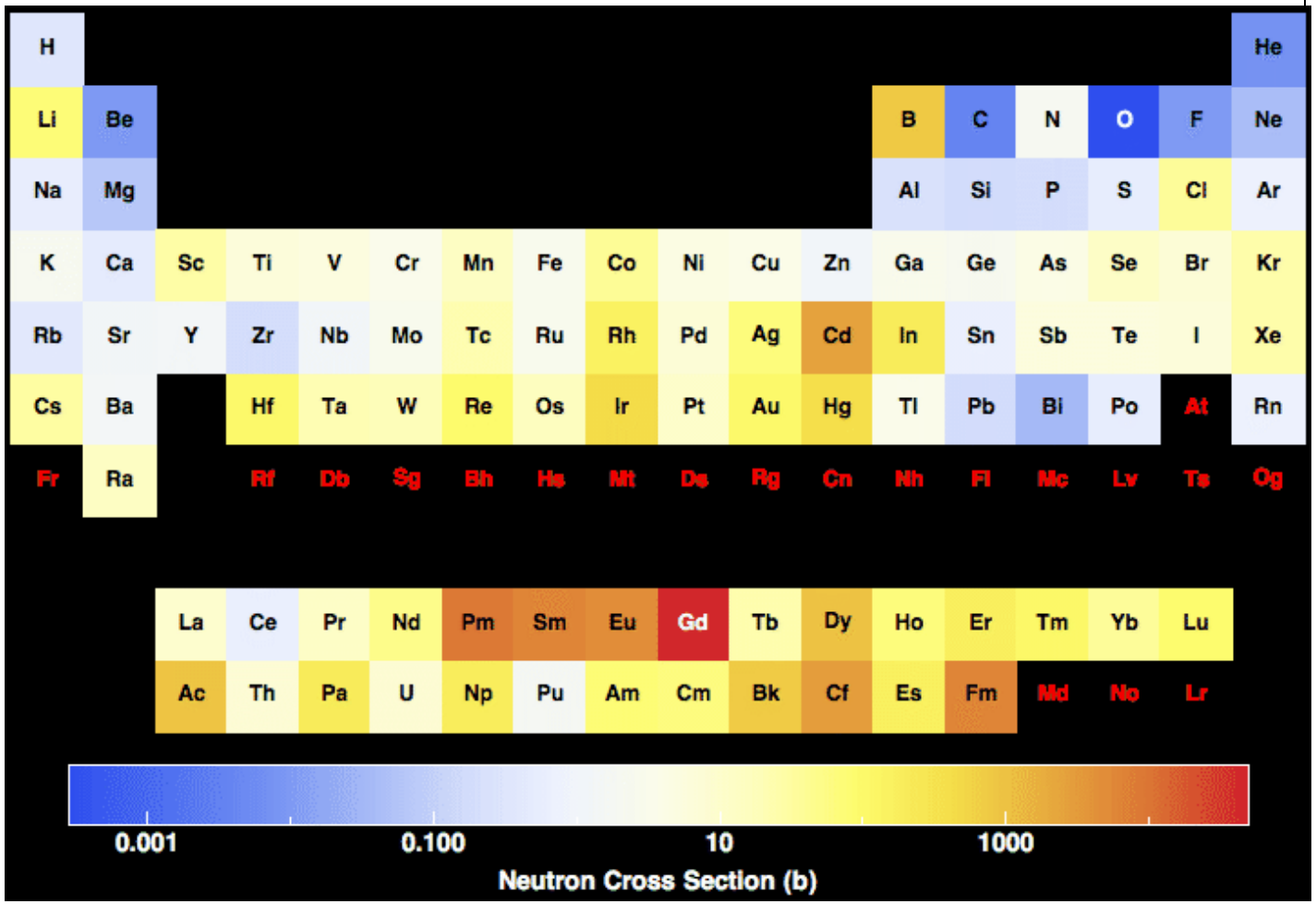

X-ray Resonant Magnetic Scattering

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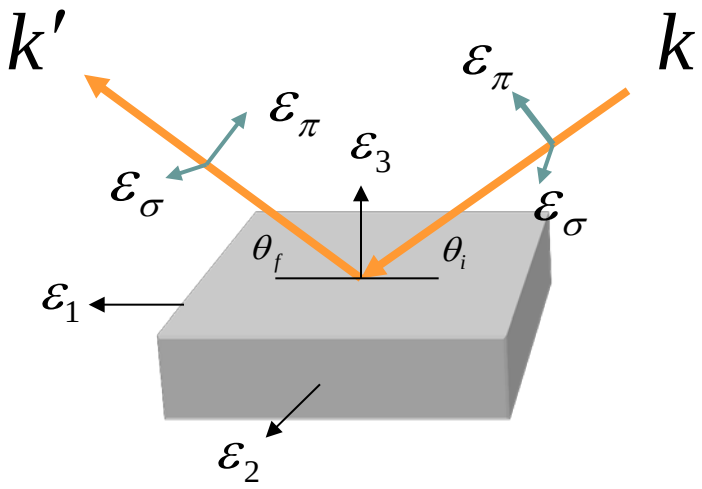

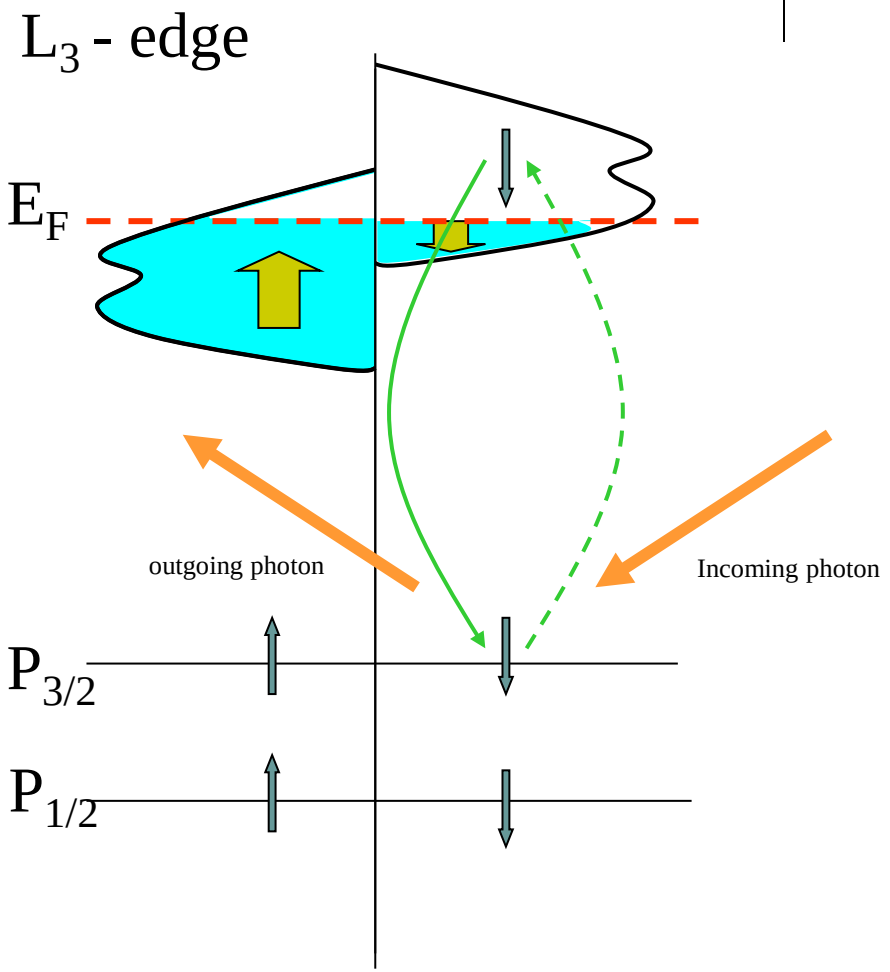

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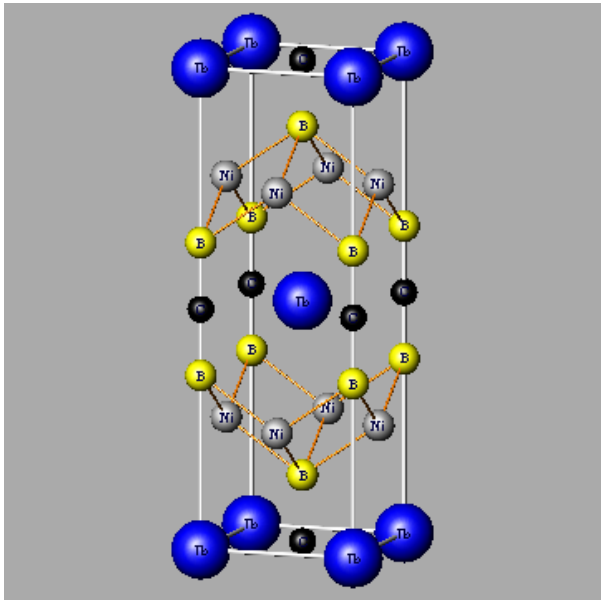

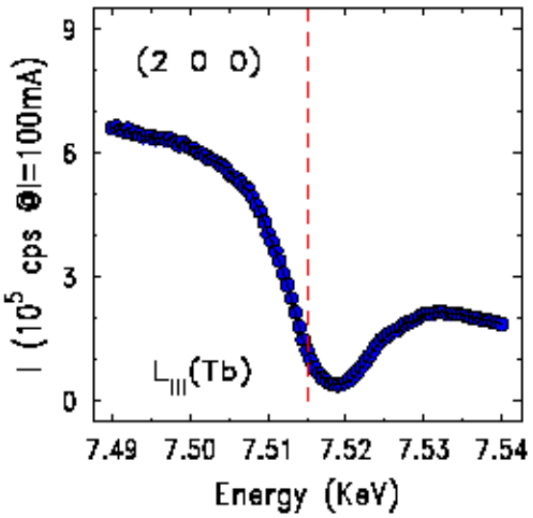

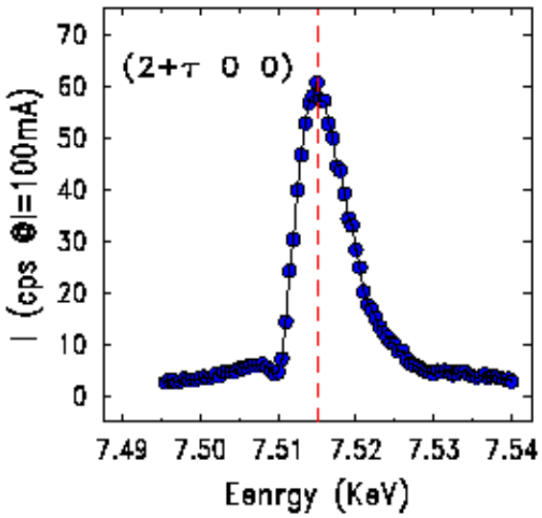

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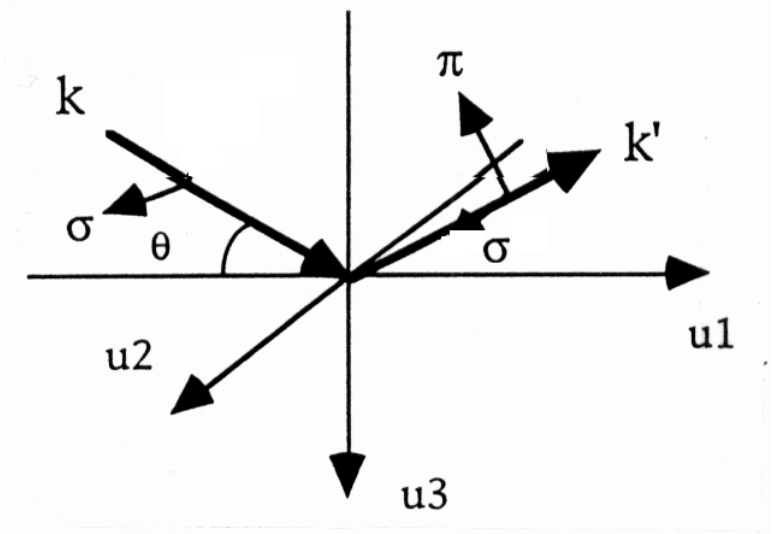

Non-resonant: $d\sigma/d\Omega \propto [S_2 \sin\Theta]^2$ (outgoing σ- pol.)

$\propto [2\sin^2\Theta * \cos\Theta\{(L_1+S_1) + S_3\sin\Theta\}]^2$ (outgoing π- pol.)

Resonant (Dipole): $d\sigma/d\Omega \propto 0$ (outgoing σ- pol.)

$\propto -z_1\cos\Theta + z_3\sin\Theta$ (outgoing π- pol.)

Resonant (Quadrupole): Much more complicated, but can probe z_1, z_2, z_3

X-ray Resonant Magnetic Scattering

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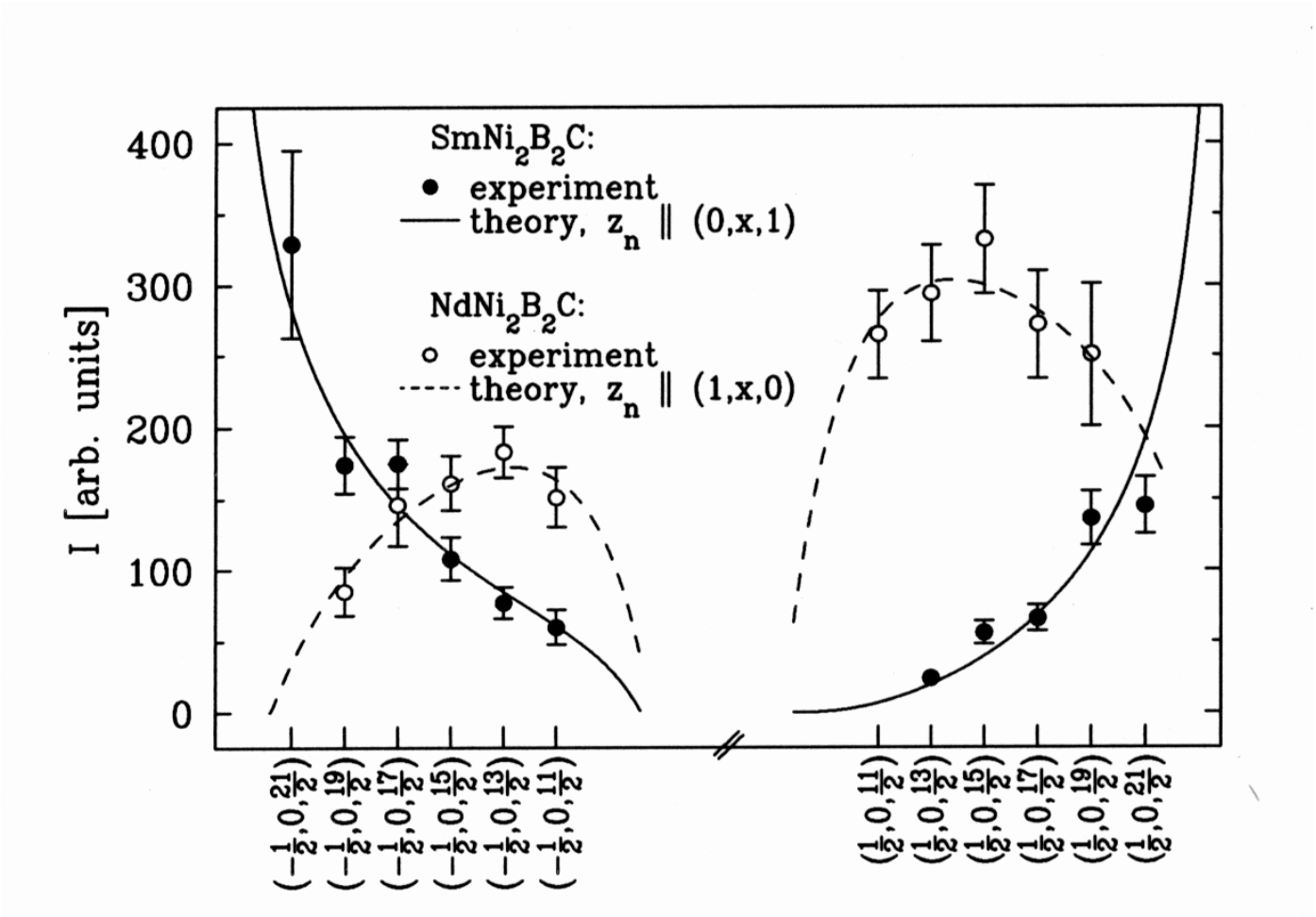

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