Today's outline - October 26, 2021

Today's outline - October 26, 2021

- Dumond diagrams & monochromators

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- Photoelectric absorption

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Reading Assignment: Chapter 7.2-3

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- Photoelectric absorption
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Reading Assignment: Chapter 7.2-3

Homework Assignment #05:
Chapter 5: 1,3,7,9,10
due Tuesday, November 02, 2021

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- Dumond diagrams & monochromators
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- X-ray absorption spectroscopy

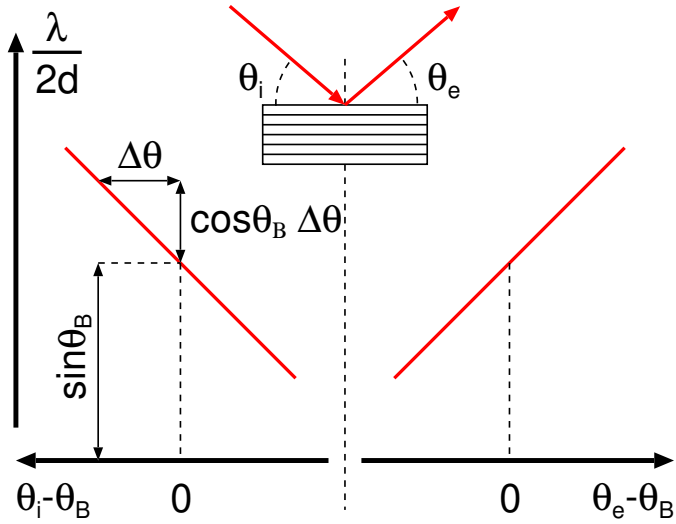
Reading Assignment: Chapter 7.2-3

Homework Assignment #05:
Chapter 5: 1,3,7,9,10
due Tuesday, November 02, 2021

Homework Assignment #06:
Chapter 6: 1,6,7,8,9
due Tuesday, November 16, 2021

Dumond diagram: no Darwin width

Transfer function of an optical element parametrized by angle and wavelength.



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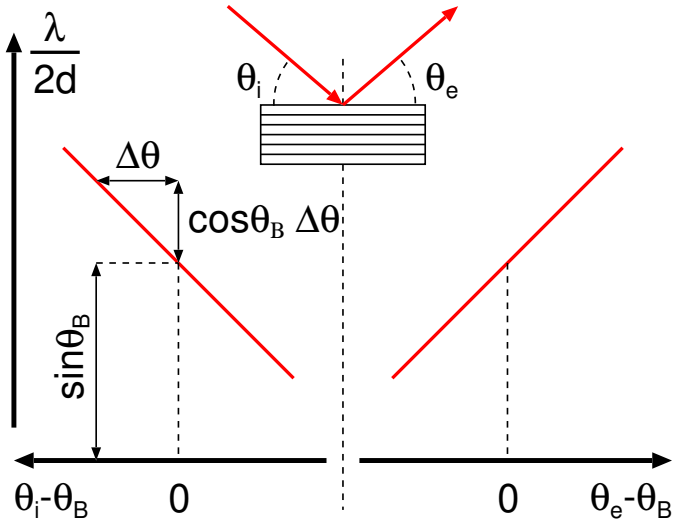

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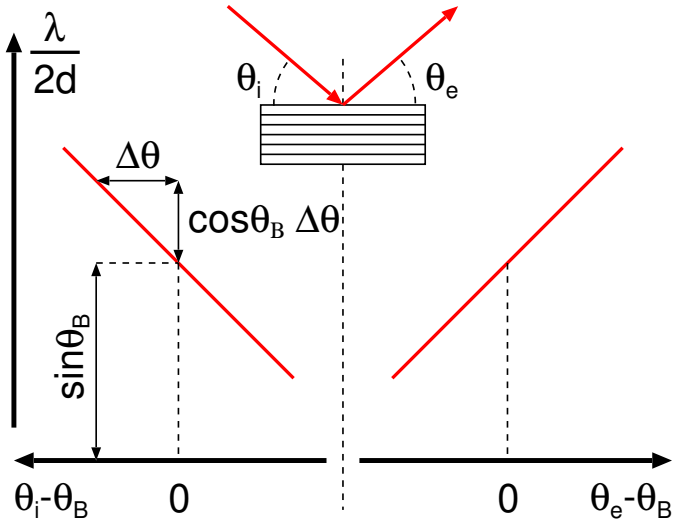
for small angular deviations $\sin\theta$ is linear with a slope of $\cos\theta_B$



Dumond diagram: no Darwin width

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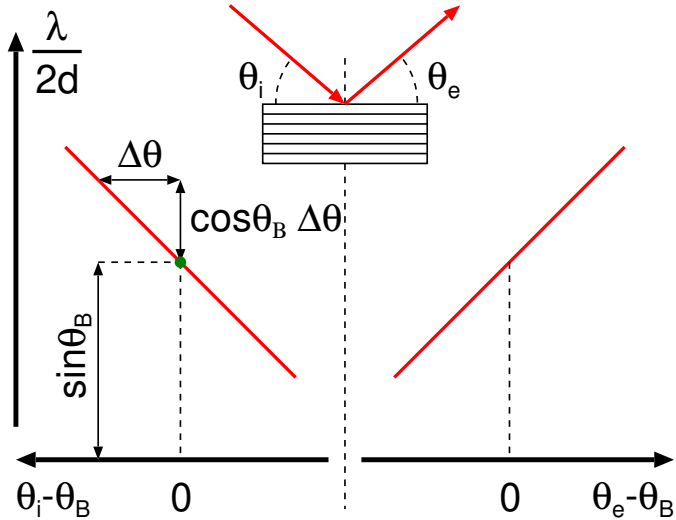
non-zero diffracted beam only for points on the line



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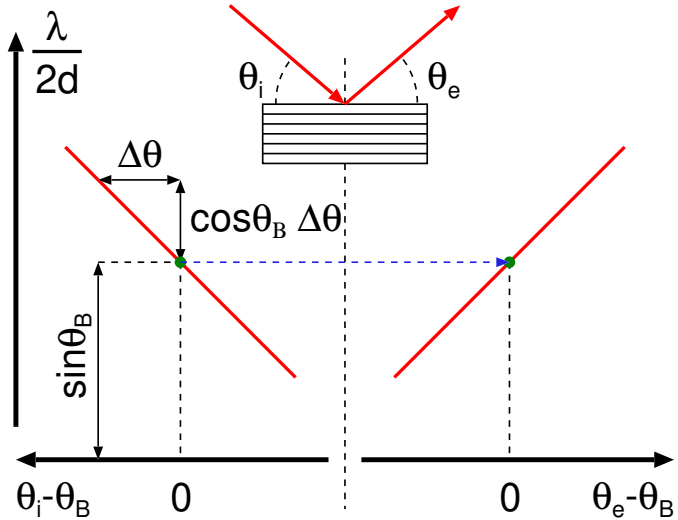
Transfer function of an optical element parametrized by angle and wavelength. Here Darwin width is ignored.

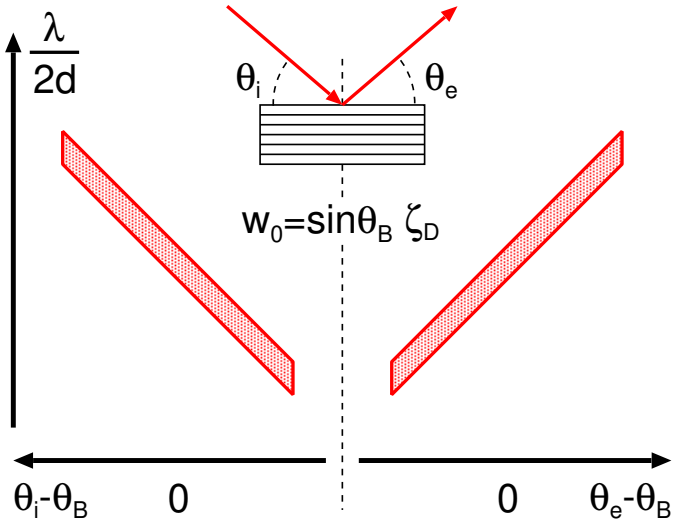
for small angular deviations $\sin\theta$ is linear with a slope of $\cos\theta_B$

non-zero diffracted beam only for points on the line

a horizontal line transfers input to output beam characteristics

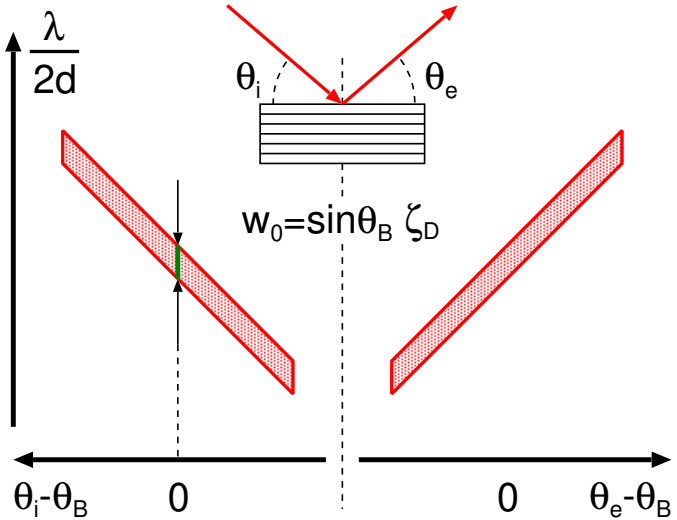


Dumond diagram: symmetric Bragg



If Darwin width is included, the Bragg condition is represented by a box

Dumond diagram: symmetric Bragg



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for a perfectly collimated (no angular divergence) input beam, a bandwidth of radiation is accepted by the crystal

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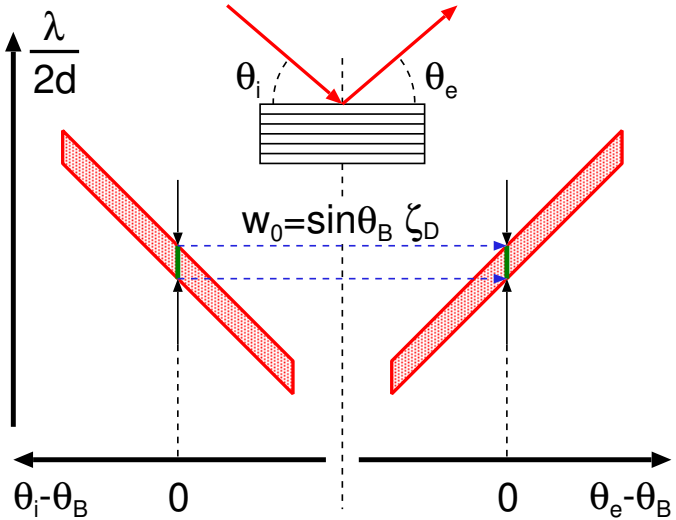
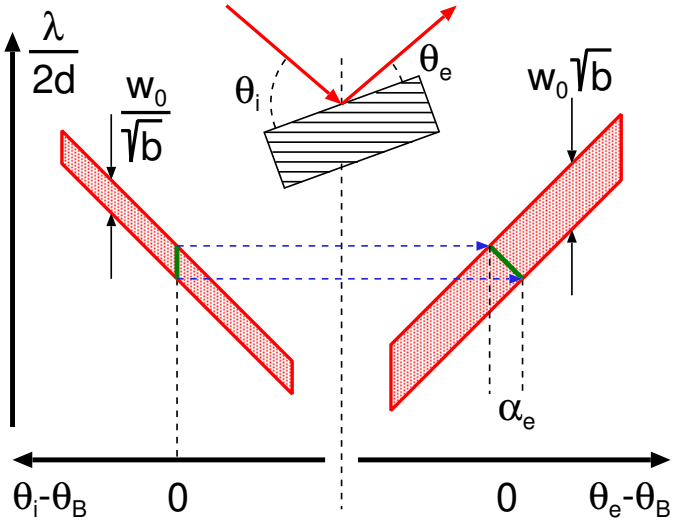


If Darwin width is included, the Bragg condition is represented by a box

for a perfectly collimated (no angular divergence) input beam, a bandwidth of radiation is accepted by the crystal

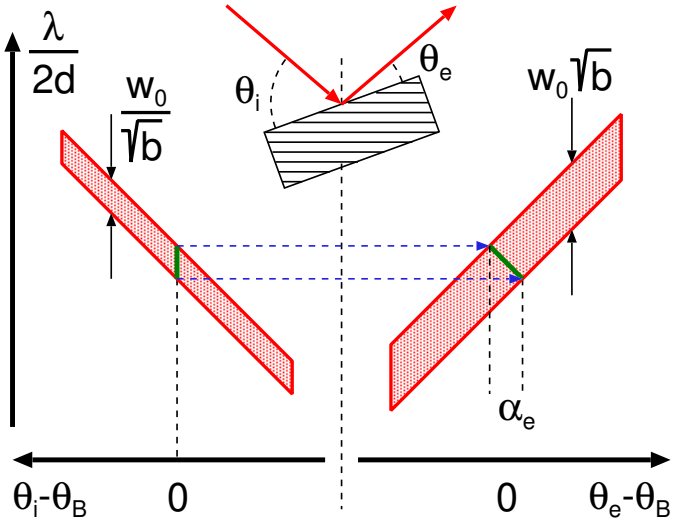
this input bandwidth is transferred to a similar output bandwidth which is also collimated

Dumond diagram: asymmetric Bragg



For an asymmetric crystal, the output beam is no longer collimated but acquires a divergence α_e

Dumond diagram: asymmetric Bragg



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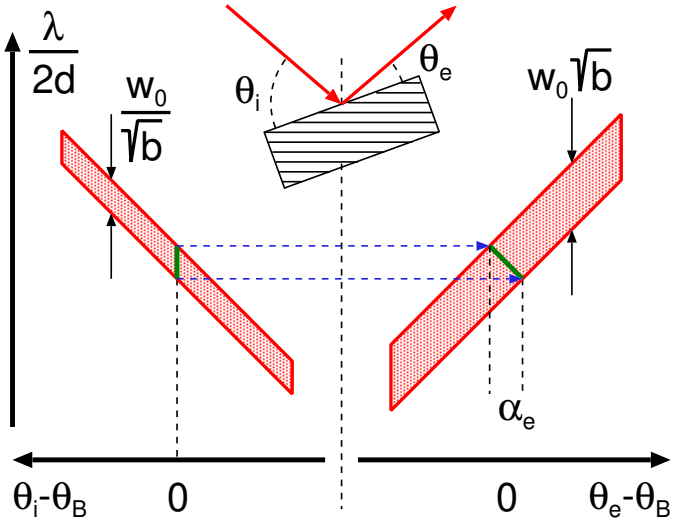
Dumond diagram: asymmetric Bragg



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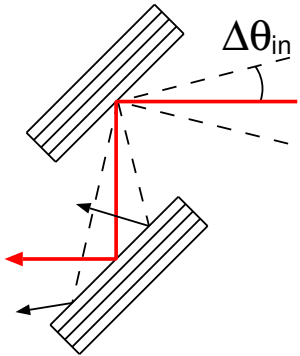
a perfectly collimated input beam transfers to an output beam that has an angular divergence which depends on the asymmetry factor *b*

this is in addition to a compression (in this case) of the beam height (Liouville's theorem!)

Double crystal monochromator: Non-dispersive



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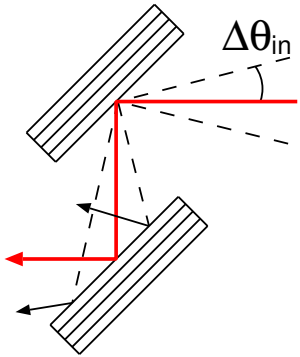

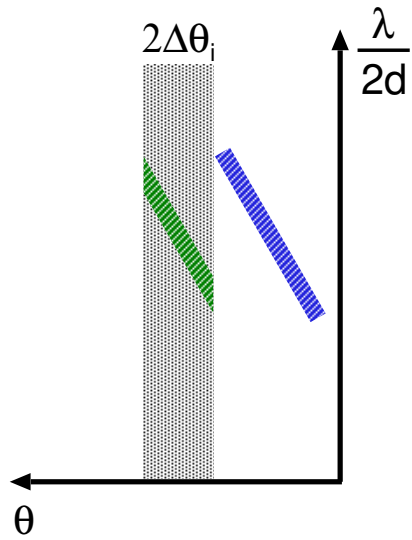

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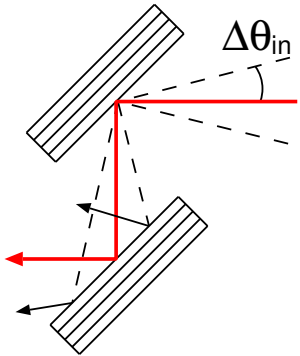

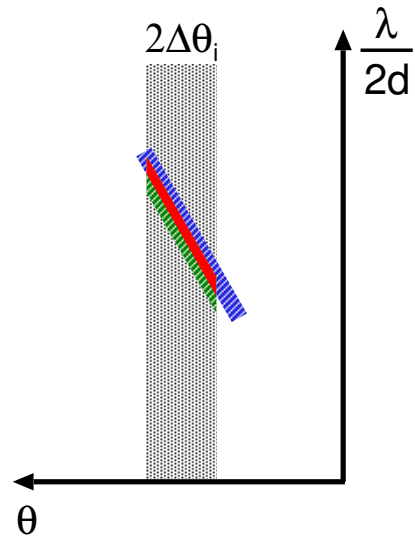

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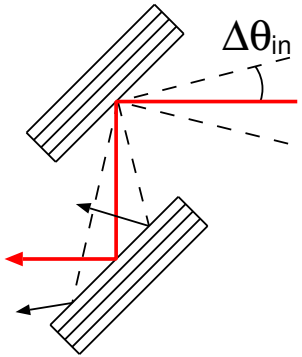

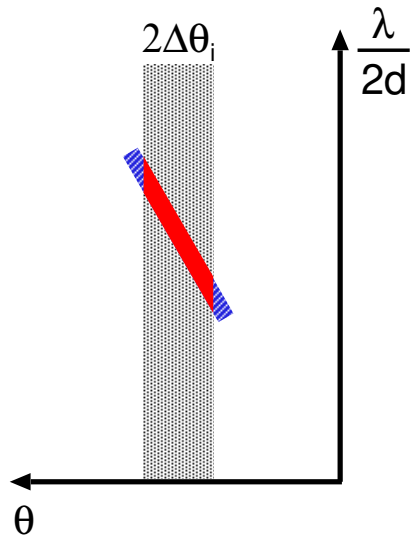

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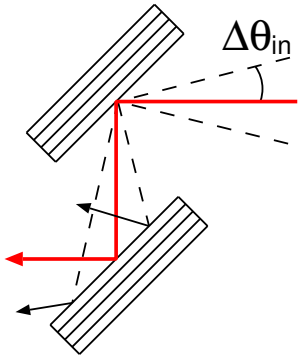

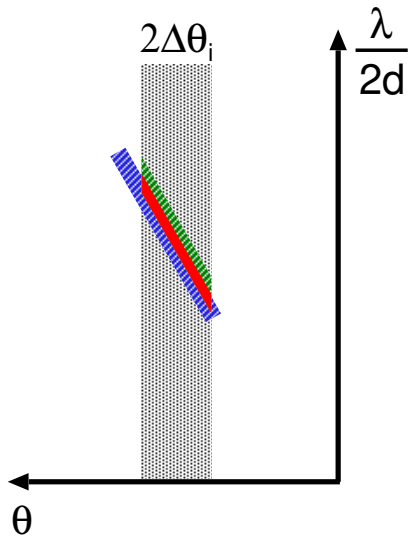

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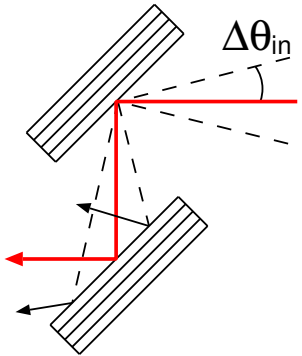
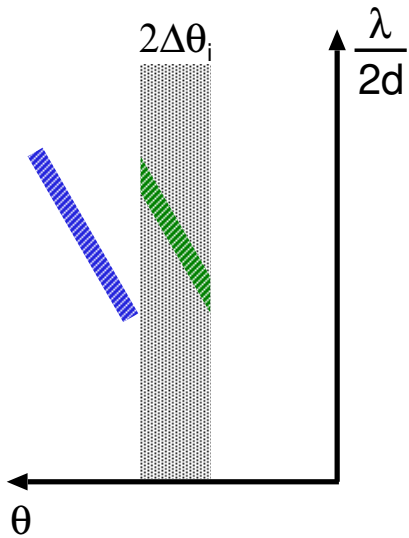
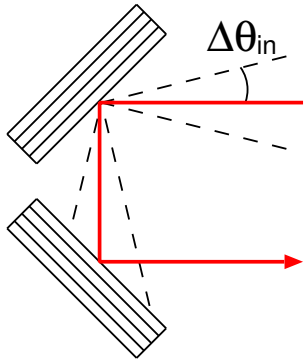




the transfer functions of the two crystals match and full bandwith and divergence is preserved, giving a triangle intensity curve

Double crystal monochromators: Dispersive



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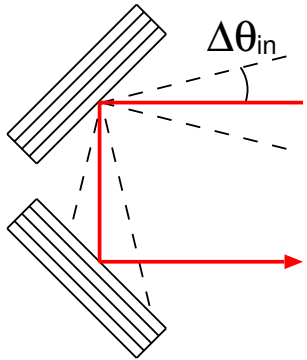

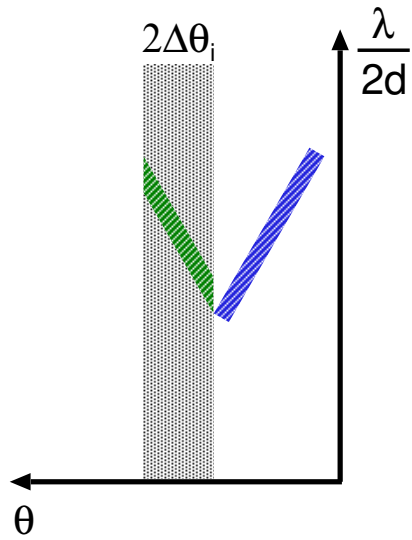

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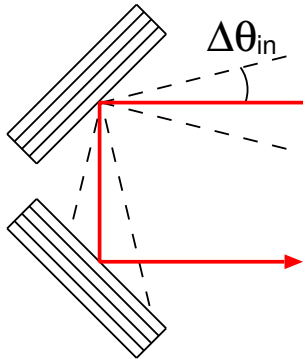

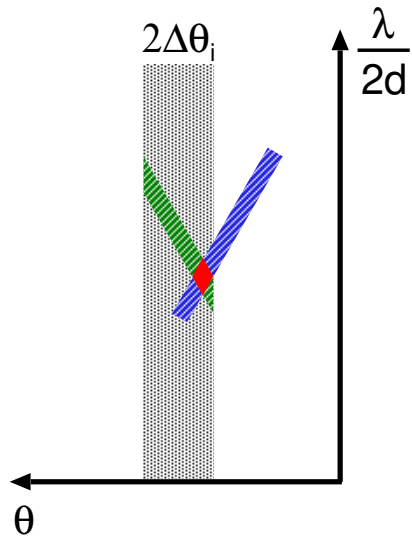

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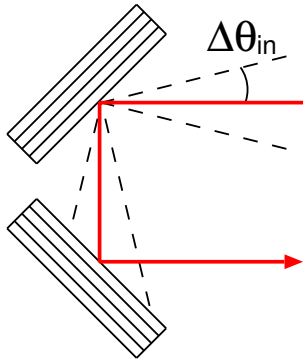

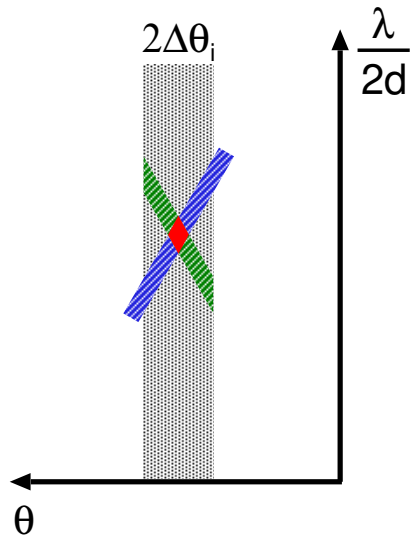

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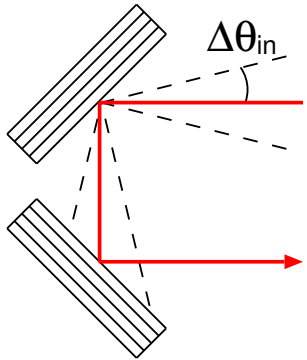

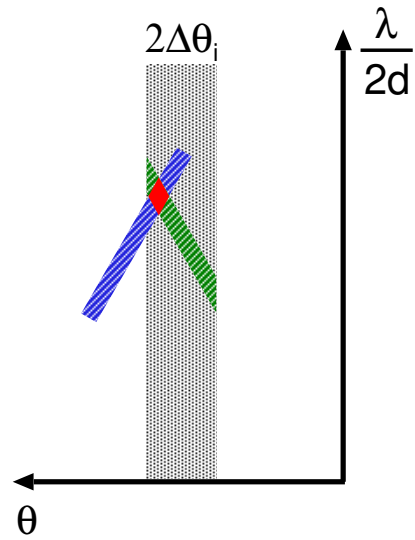

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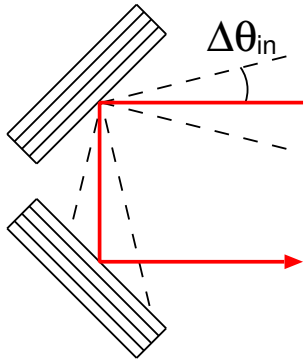
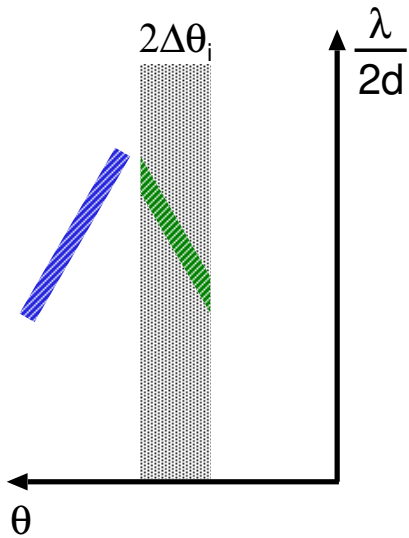
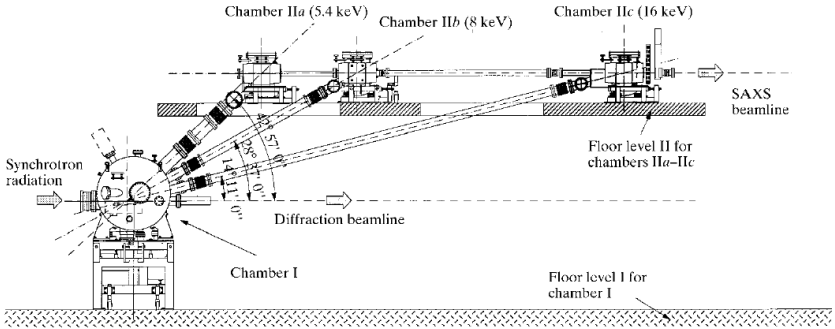




the transfer function matches only in a small energy band that varies with angle of the second crystal, mapping out the Darwin curve of the first crystal

Asymmetric monochromator at ELETTRA



"High-throughput asymmetric double-crystal monochromator of the SAXS beamline at ELETTRA," S. Bernstorff, H. Amentisch, and P. Laggner, *J. Synchrotron Rad.* **5**, 1215-1221 (1998).

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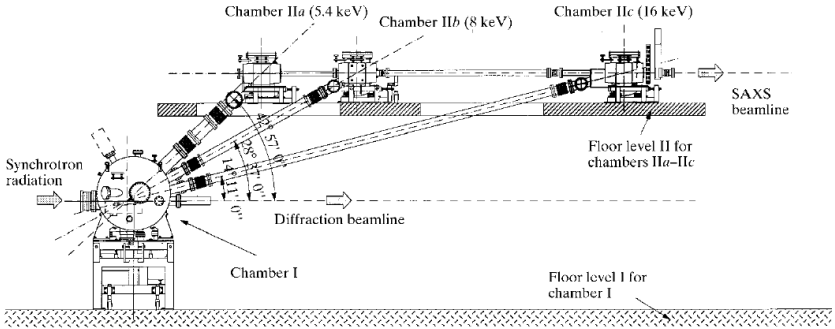

The SAXS beamline at ELETTRA has asymmetric cut crystals with 2° grazing incidence in order to spread the heat load

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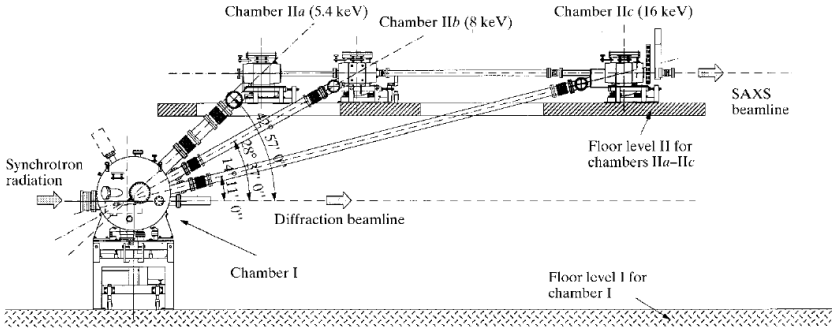

The SAXS beamline at ELETTRA has asymmetric cut crystals with 2° grazing incidence in order to spread the heat load

The three crystals are set for single energies of 5.6, 8.0, and 16 keV with a vertical displacement of 1.5 m and asymmetry parameter, b, of 0.053, 0.078, and 0.17, respectively

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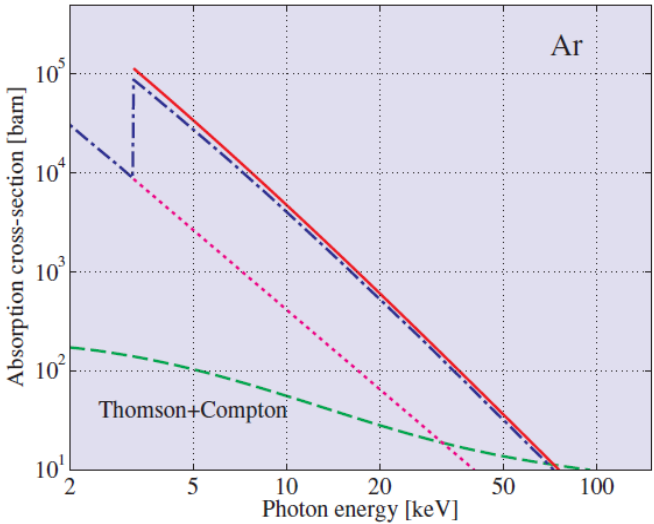
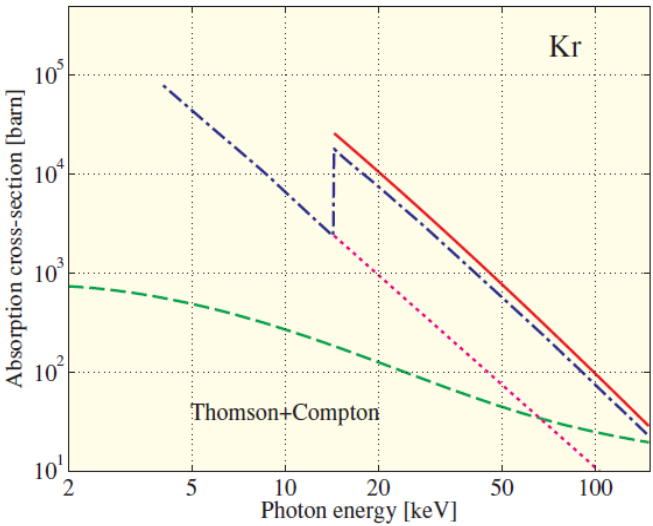
Total cross section



The total cross-section for photon "absorption" includes elastic (or coherent) scattering, Compton (inelastic) scattering, and photoelectric absorption.

Total cross section



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Characteristic absorption jumps depend on the element

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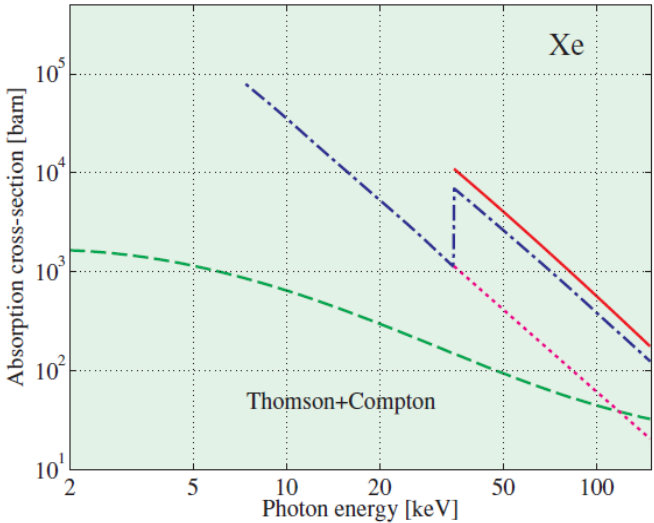

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These quantities vary significantly over many decades but can easily put on an equal footing.

Scaled absorption

$$T = \frac{I}{I_0} = e^{-\mu z}$$

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σ_a can be scaled for different elements by E^3/Z^4 and plotted together

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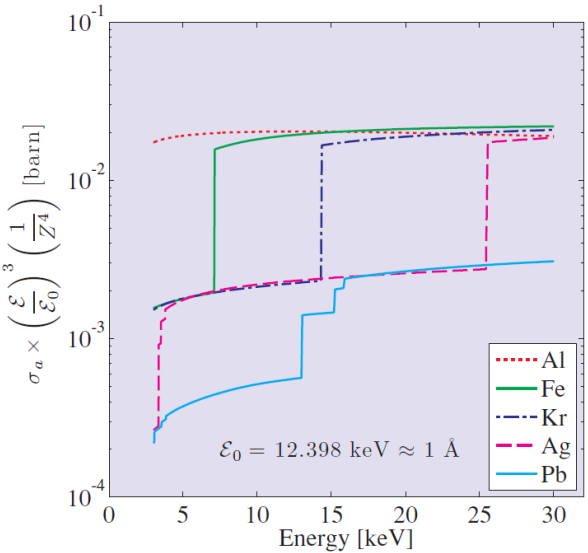
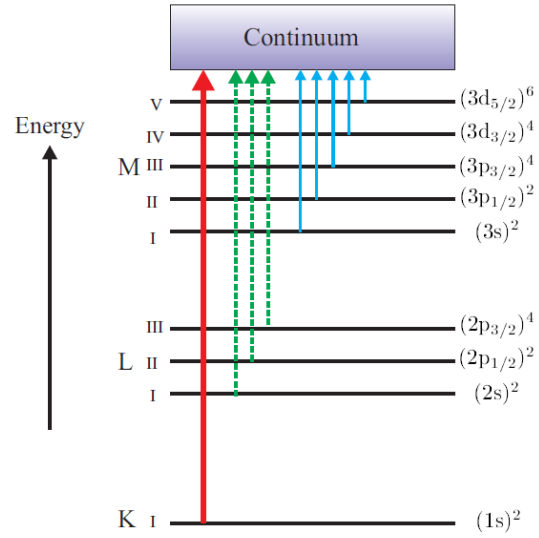
σ_a can be scaled for different elements by E^3/Z^4 and plotted together

remarkably, all values lie on a common curve above the K edge and between the L and K edges and below the L edge



Absorption edge nomenclature

The states are labeled according to the principal, orbital angular momentum, and total angular momentum quantum numbers, n, l, and j, respectively



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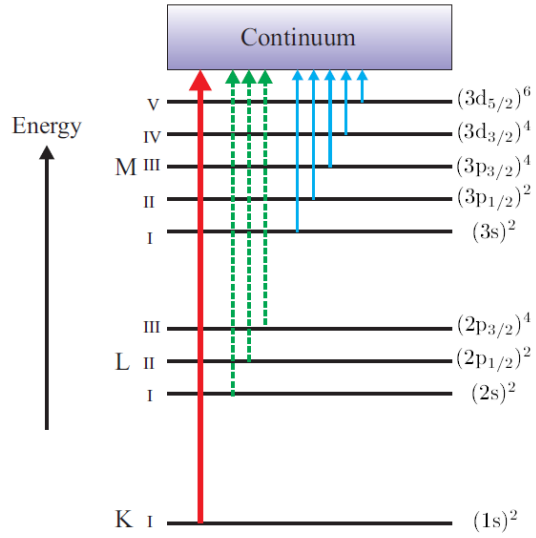

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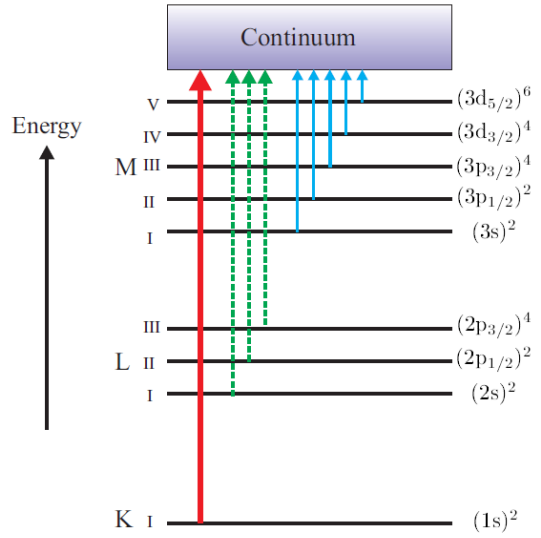

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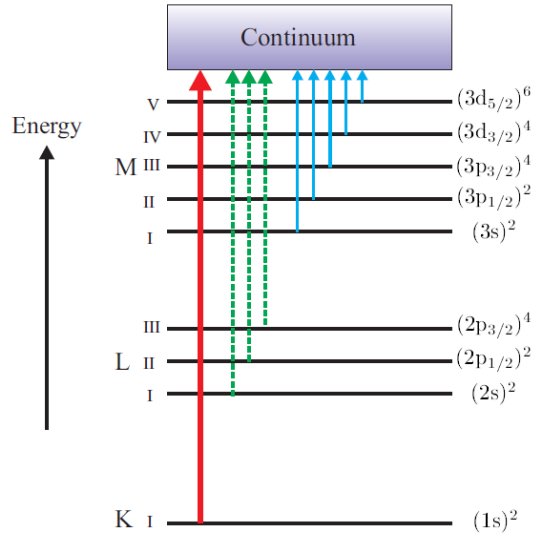
Roman numerals increase from low to high values of l and j



Dirac bra-ket notation

Photoelectric absorption and inelastic scattering are quantum phenomena which cannot be treated semi-classically as scattering can.

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Photoelectric absorption and inelastic scattering are quantum phenomena which cannot be treated semi-classically as scattering can.

Paul Dirac developed a formalism for quantum mechanics which is commonly used. One part of this formalism is a compact notation which simplifies writing expectation value integrals. We will use this "bra-ket" notation when discussing photoabsorption.

Dirac bra-ket notation

Photoelectric absorption and inelastic scattering are quantum phenomena which cannot be treated semi-classically as scattering can.

Paul Dirac developed a formalism for quantum mechanics which is commonly used. One part of this formalism is a compact notation which simplifies writing expectation value integrals. We will use this "bra-ket" notation when discussing photoabsorption.

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expectation value	$\int \psi^* Q\psi dx$	$\langle\psi \mid Q \mid \psi\rangle$	operator is applied to the right

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The first term gives absorption while the second produces Thomson scattering so we take only the first into consideration now.

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The calculation is simplified if the interaction Hamiltonian is applied to the left since the final state has only a free electron and no photon

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which is the Fourier transform of the initial state 1s electron wave function

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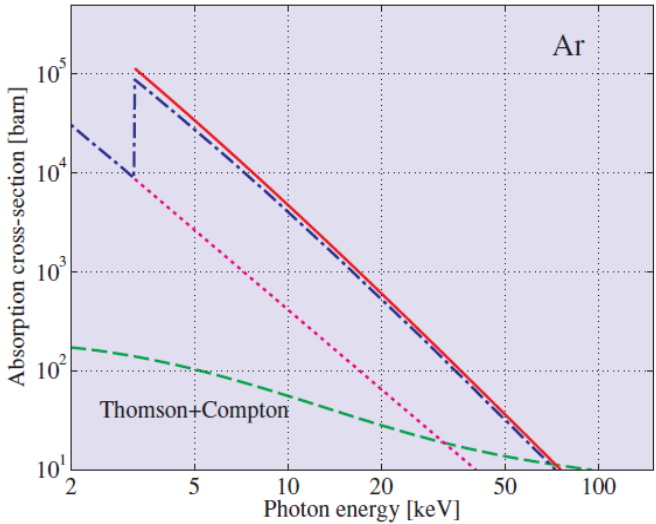
$$\sigma_a = \frac{2\pi}{\hbar c}\frac{V^2}{4\pi^3}\left(\frac{e\hbar}{m}\right)^2 \frac{\hbar}{2\epsilon_0 V^2 \omega} I_3 = \left(\frac{e\hbar}{m}\right)^2 \frac{1}{4\pi^2 \epsilon_0 c\omega} I_3$$

where the integral I_3 is given by

$$I_3 = \int \phi^2(\vec{Q}) q^2 \sin^2\theta \cos^2\varphi \delta(\mathcal{E}_f - \mathcal{E}_i) q^2 \sin\theta dq d\theta d\phi$$

Calculated cross sections



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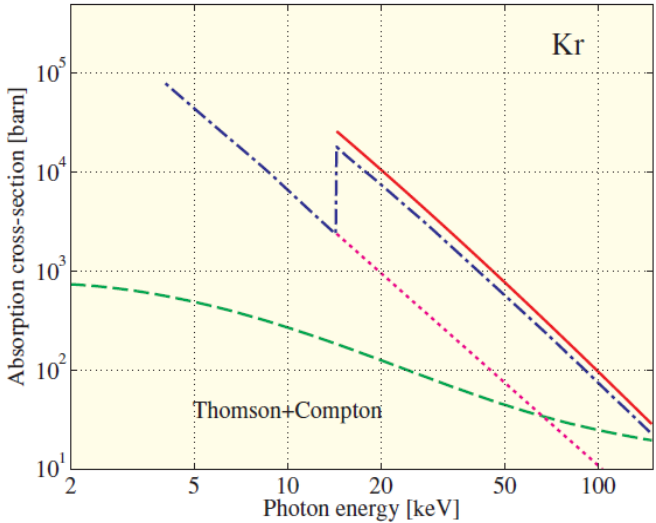

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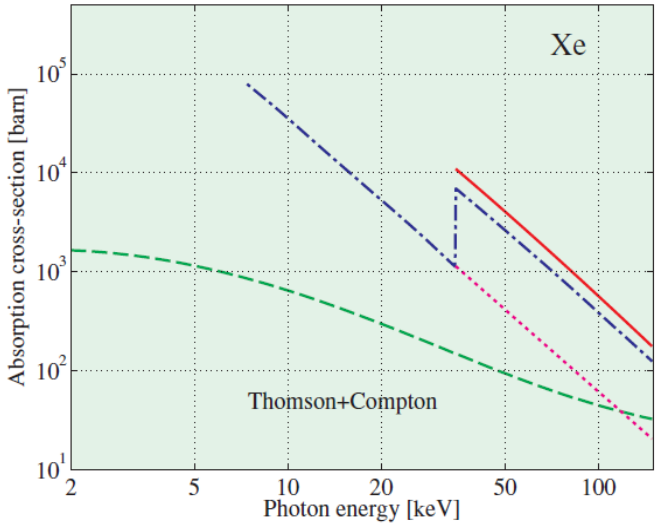

What is XAFS?

X-ray Absorption Fine-Structure (XAFS) is the modulation of the x-ray absorption coefficient at energies near and above an x-ray absorption edge. XAFS is also referred to as X-ray Absorption Spectroscopy (XAS) and is broken into 2 regimes:

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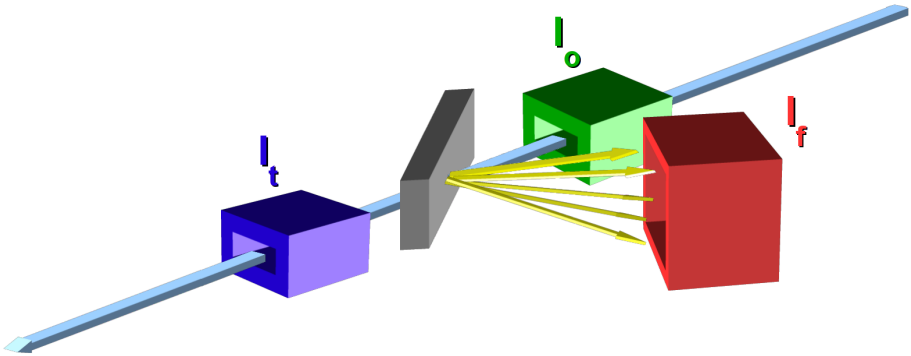
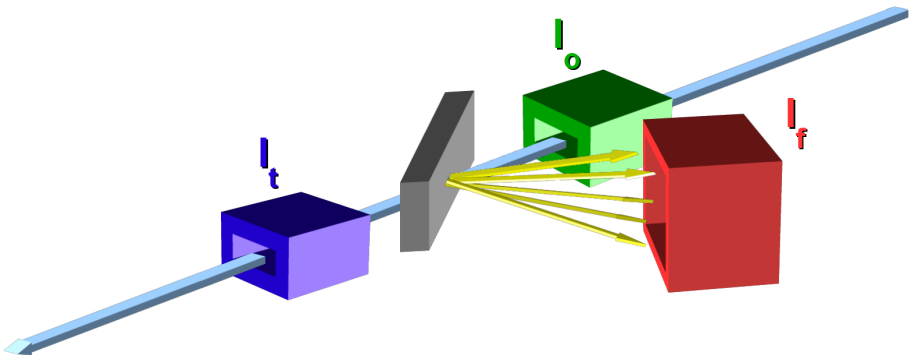
- has minimal sample requirements

The EXAFS experiment



The EXAFS experiment

I_o = incident intensity



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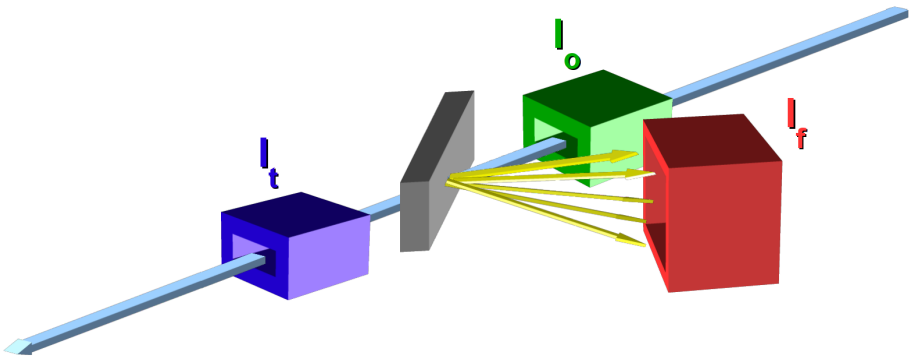

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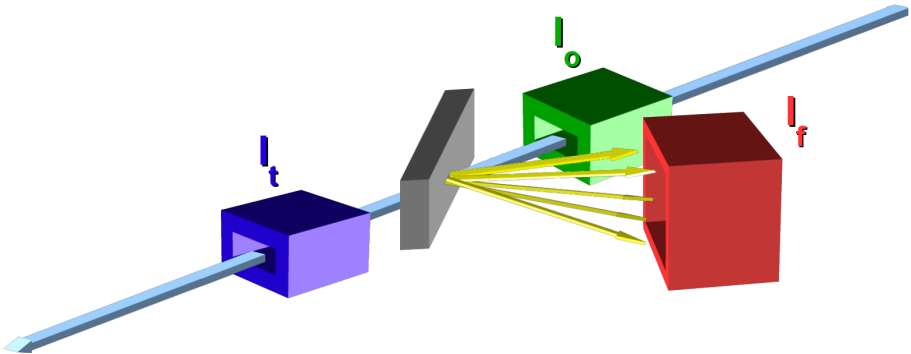

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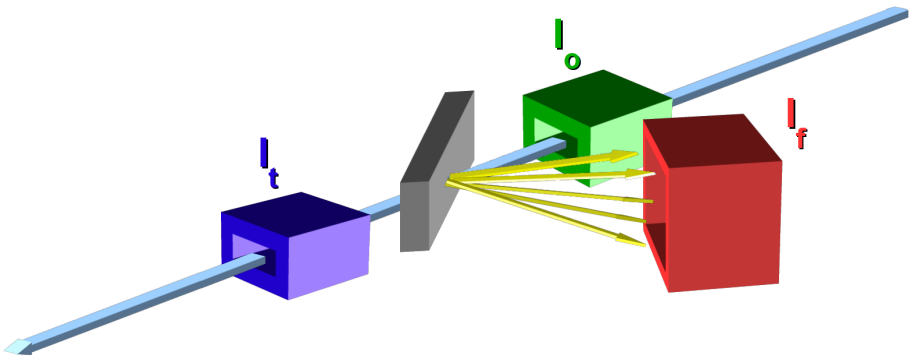

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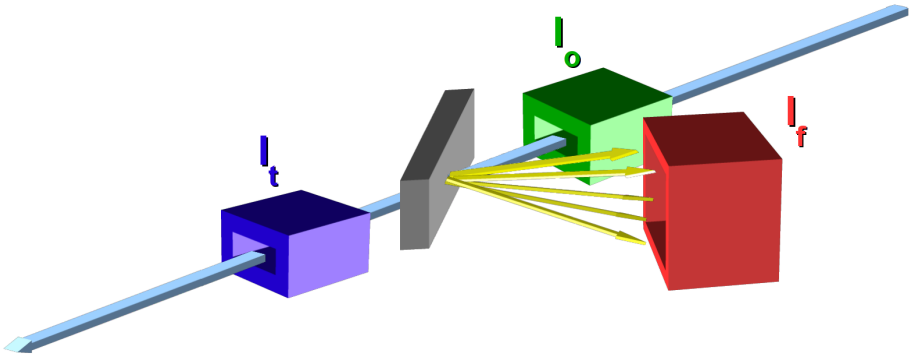

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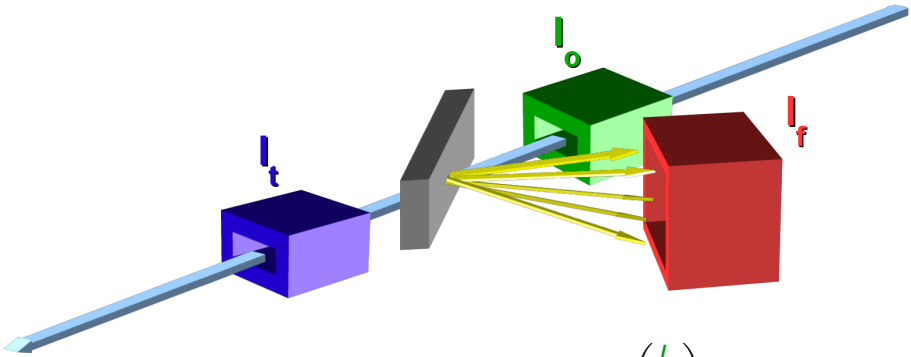

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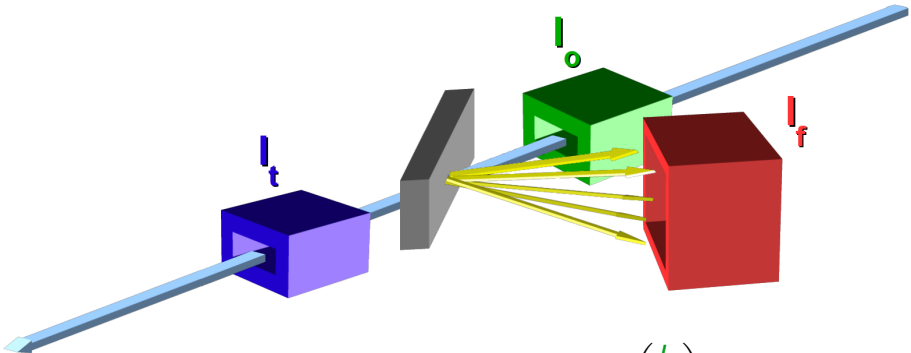

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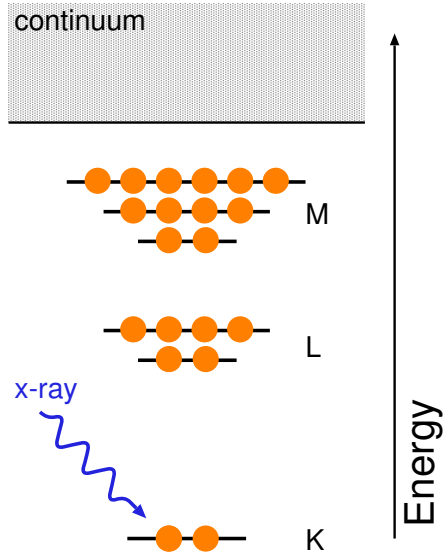
The x-ray absorption process

An x-ray is absorbed by an atom when the energy of the x-ray is transferred to a core-level electron (K, L, or M shell).



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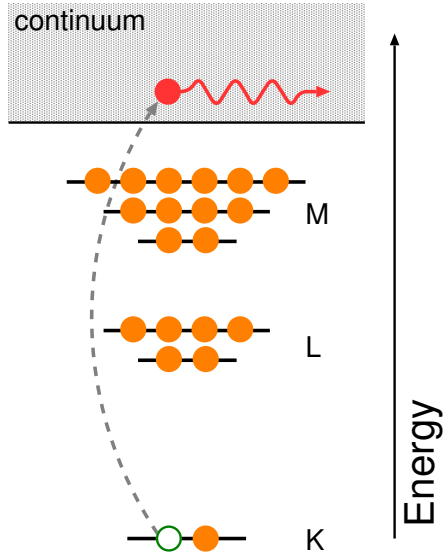

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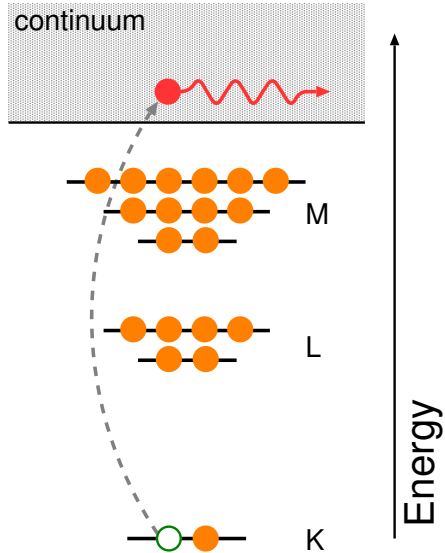

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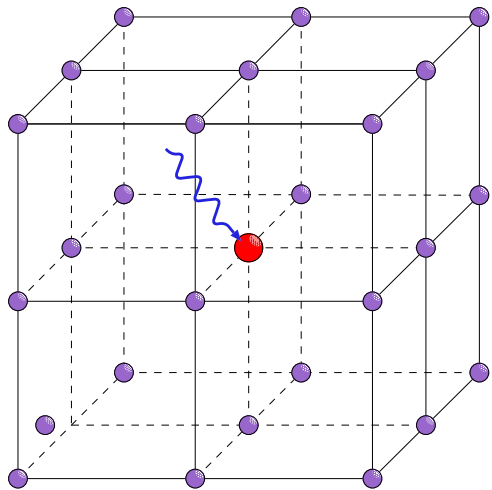

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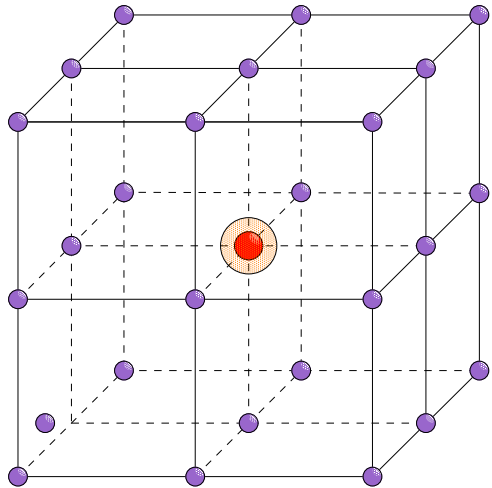

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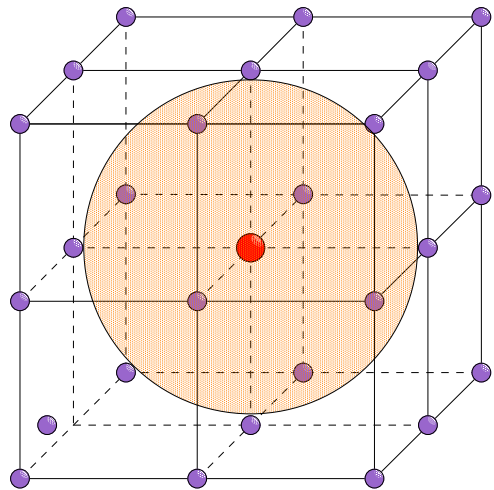

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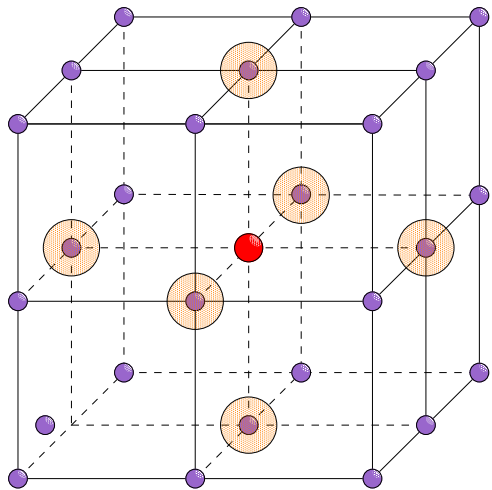

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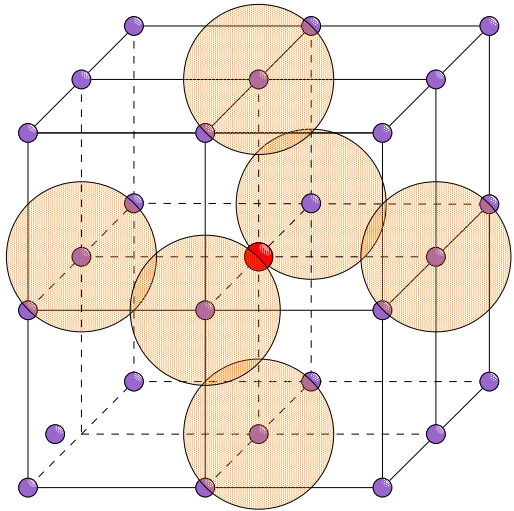

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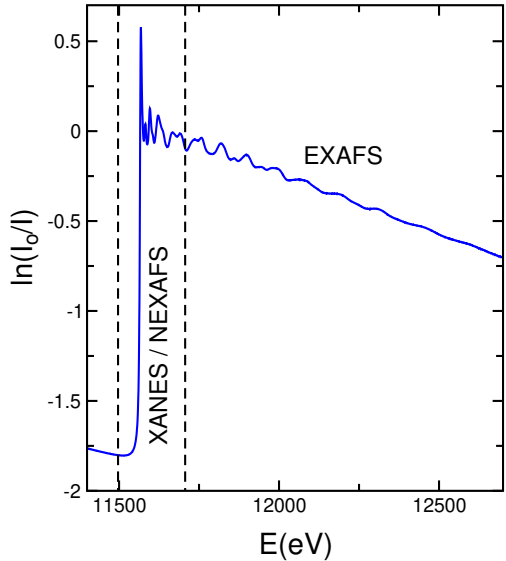
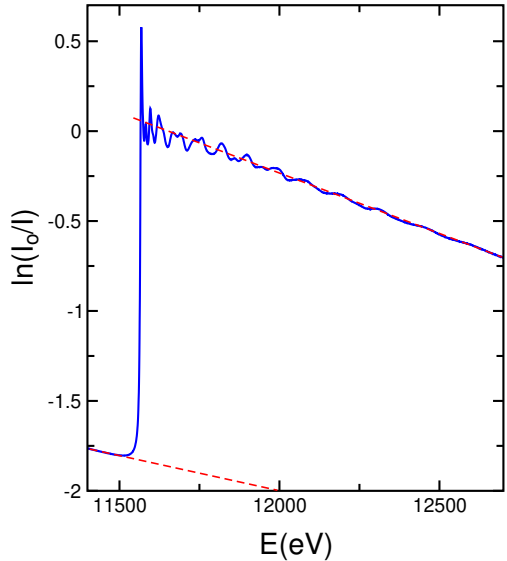


EXAFS data extraction

normalize by fitting pre-edge and post-edge trends



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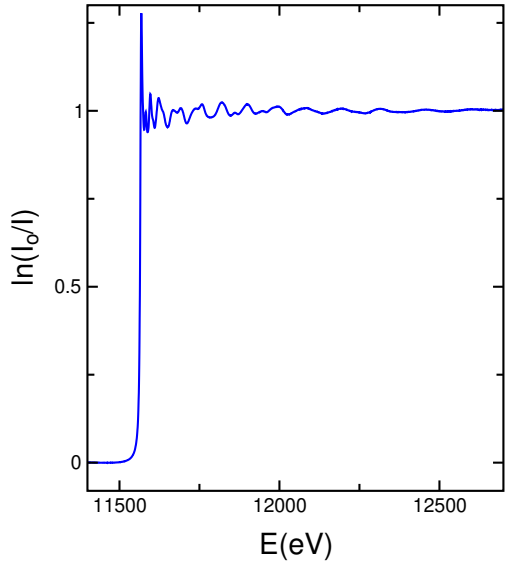

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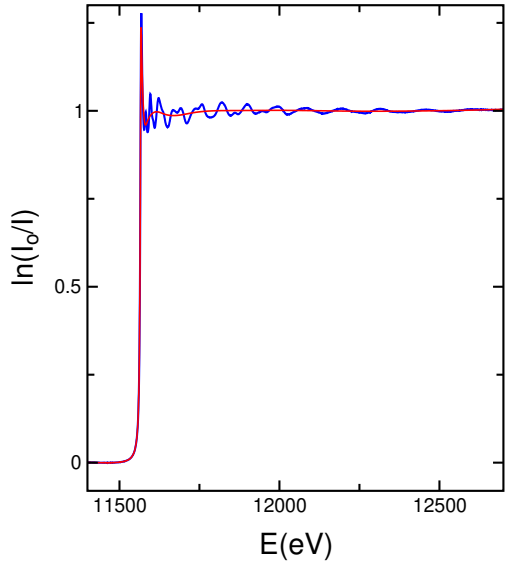

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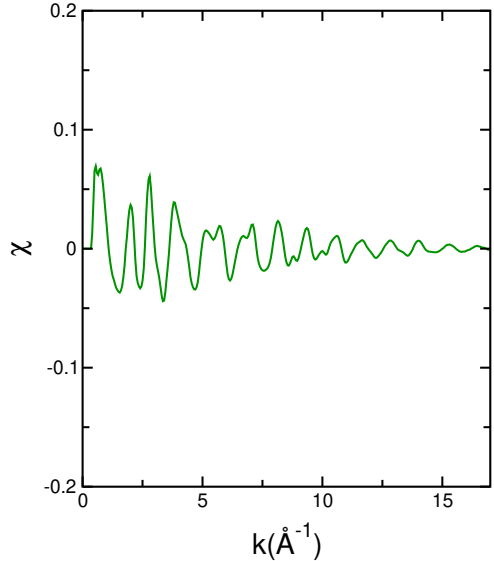

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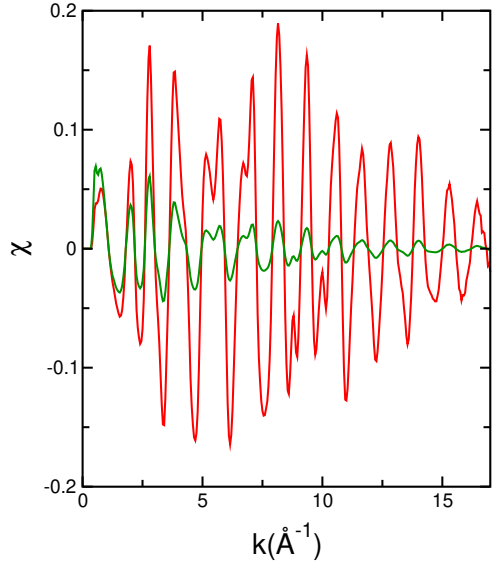

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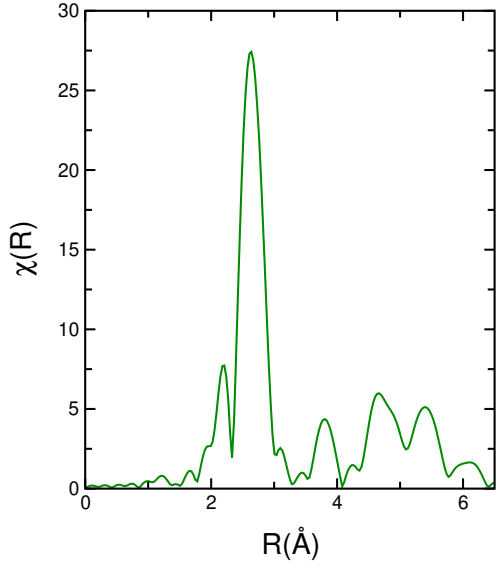
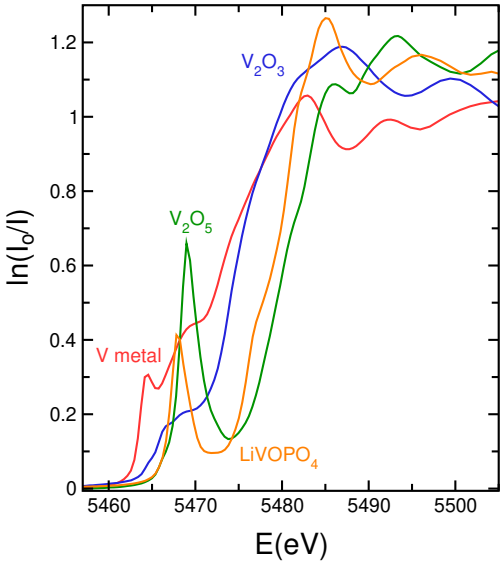
Fourier transform to get real space EXAFS



XANES edge shifts and pre-edge peaks



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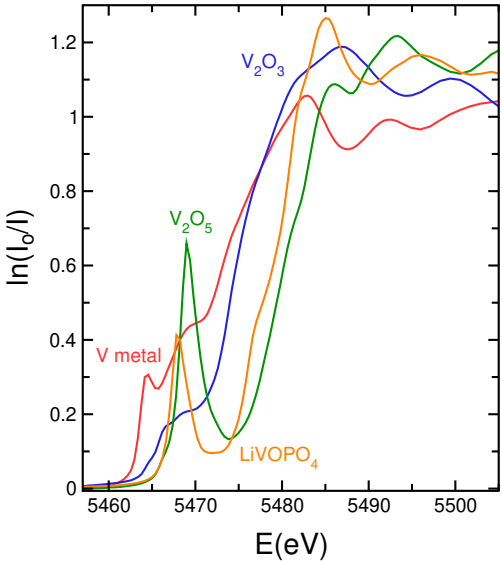

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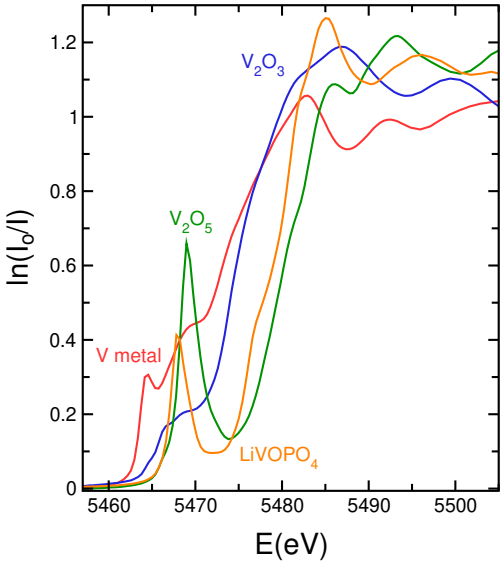

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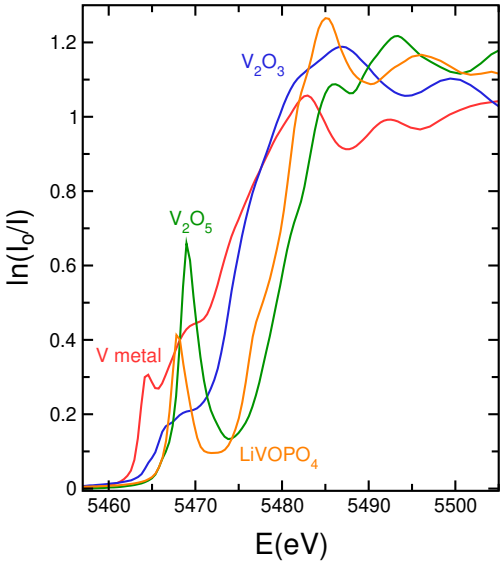

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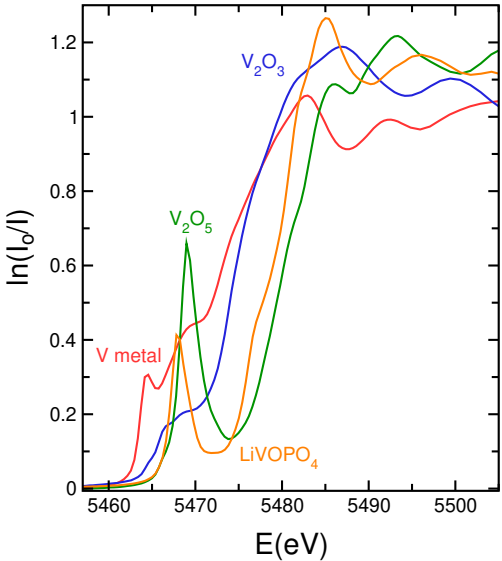

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Modern codes, such as FEFF9, are able to accurately compute XANES features.