Today's Outline - March 24, 2020 (part A)

Today's Outline - March 24, 2020 (part A)

- Standing wave experiments

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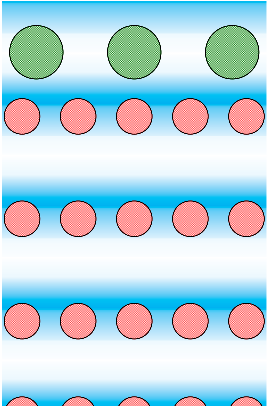
Homework Assignment #05:
Chapter 5: 1, 3, 7, 9, 10
due Thursday, April 02, 2020

Standing wave experiments



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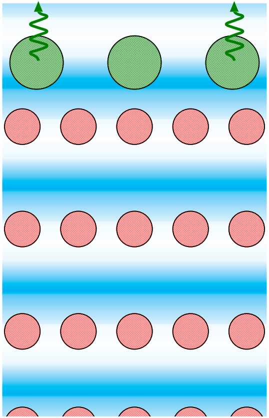

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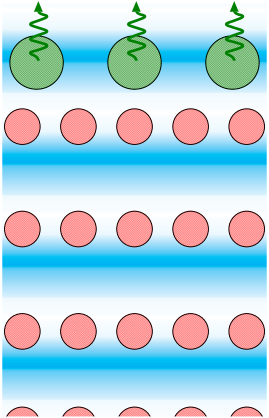

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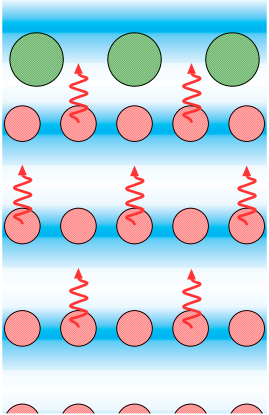

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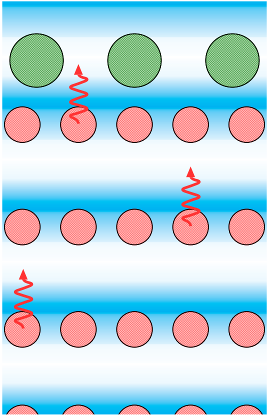

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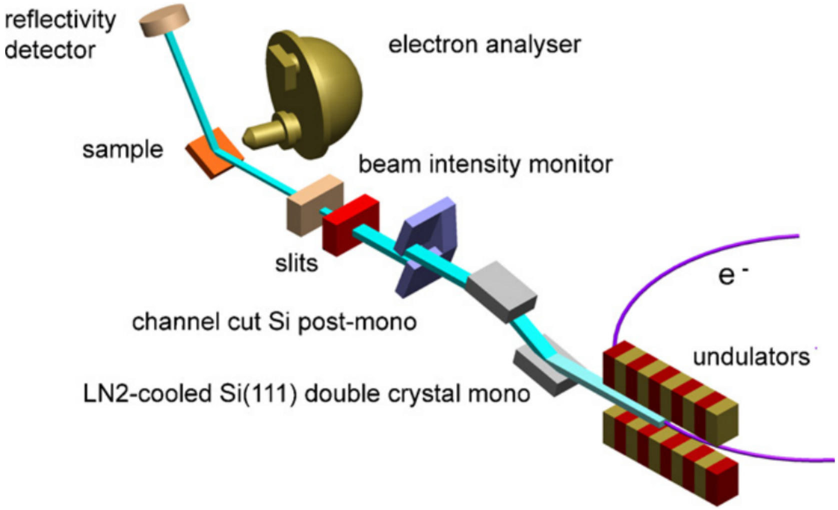
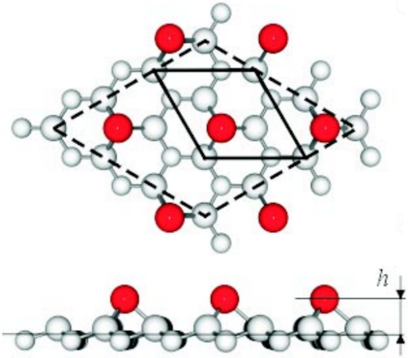
A high resolution monochromator is required for this kind of experiment

Beam line ID32 @ ESRF



Structure of Sn on Ge(111)

The low temperature 3×3 structure (dashed line) is well known but the room temperature $\sqrt{3}\times\sqrt{3}$ surface structure (solid line) is unresolved



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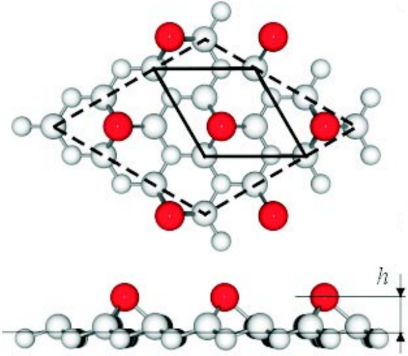

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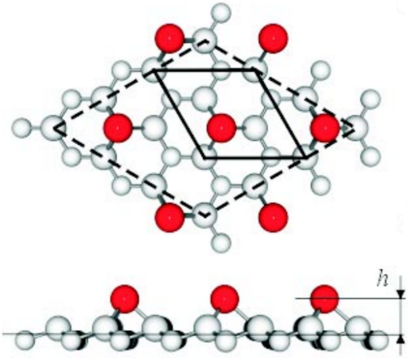

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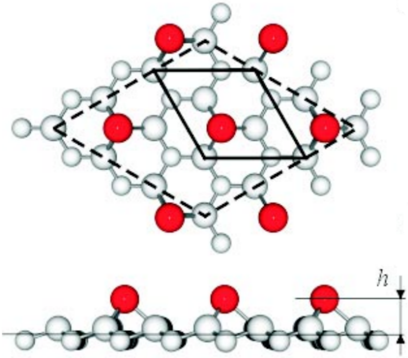
Above 0.2 ML, the $\sqrt{3}\times\sqrt{3}$ structure appears and then dominates



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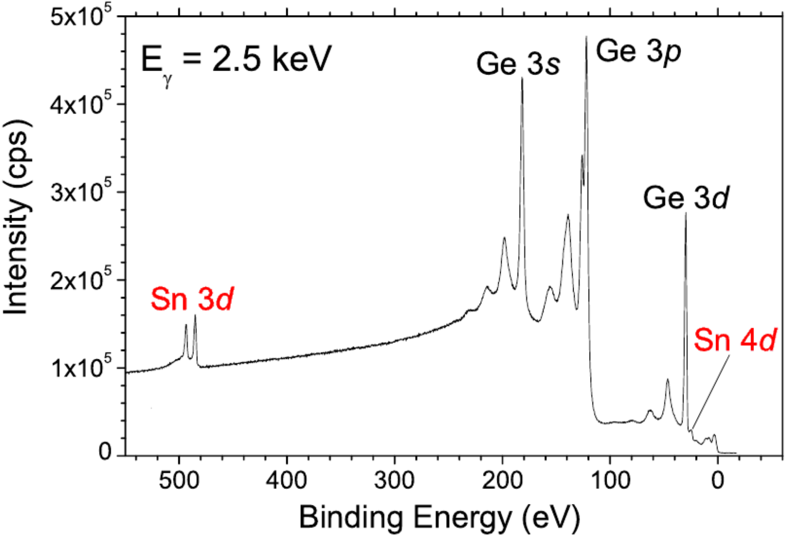

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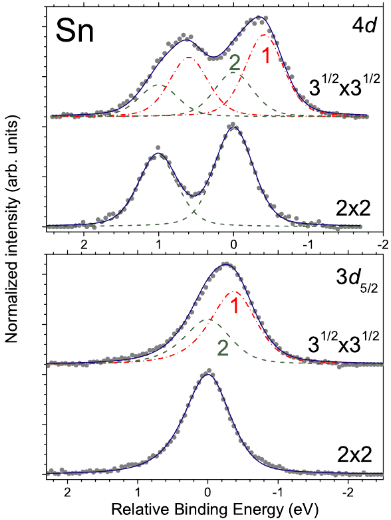

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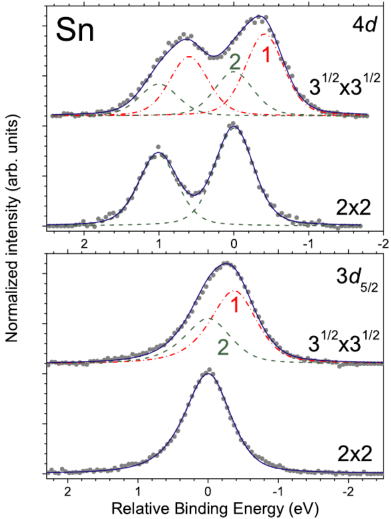

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The $\sqrt{3} \times \sqrt{3}$ structure shows two distinct chemical shifts, with the majority component, I_1, having a slightly lower binding energy than the minority component, I_2

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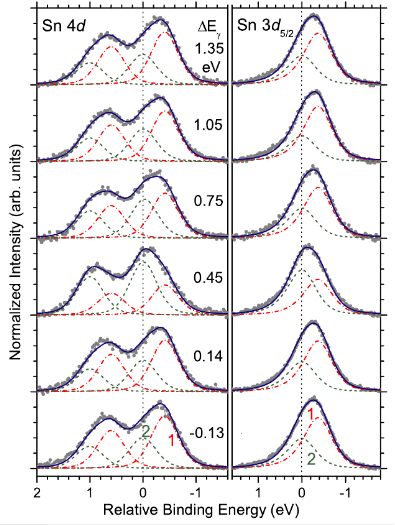

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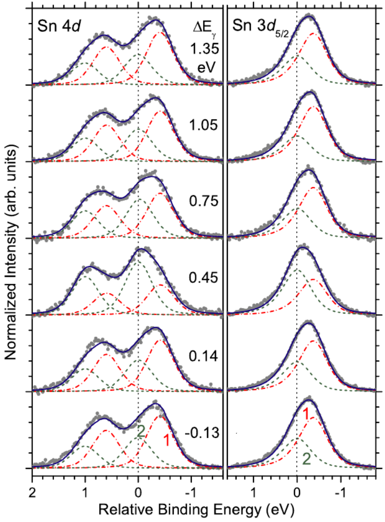

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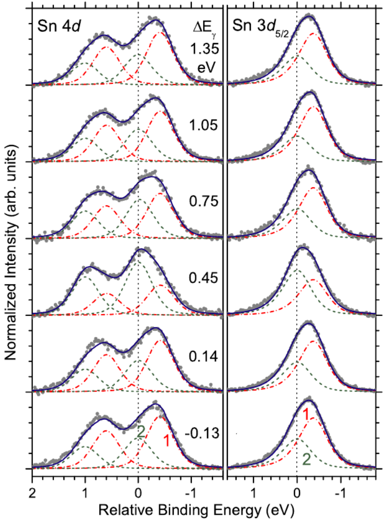
At $\Delta E_\gamma = 0.45$ eV, the I_1/I_2 ratio almost completely inverts, showing that the two atom populations are at different heights above the surface



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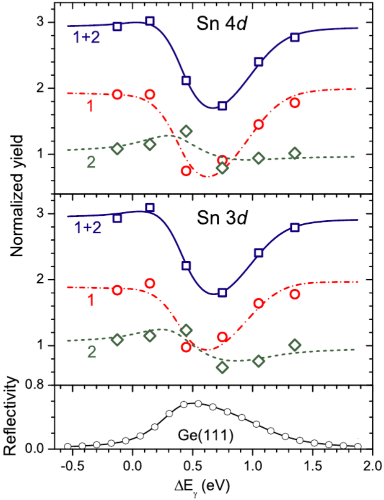

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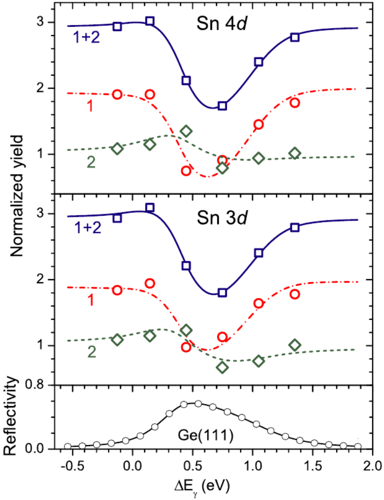
Population 1 is two times larger than population 2 and is located a height $\Delta h = 0.23$ Å further from the Ge(111) surface



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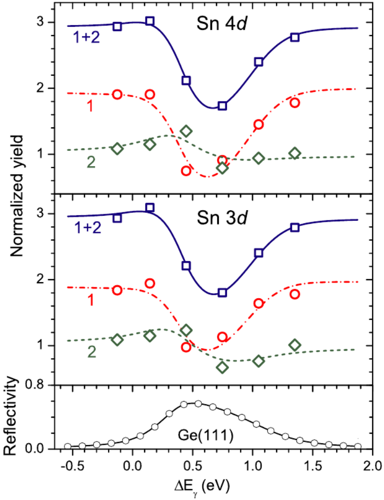
Population 1 also has a lower binding energy, demonstrating that the binding energy is directly correlated to the height from the surface



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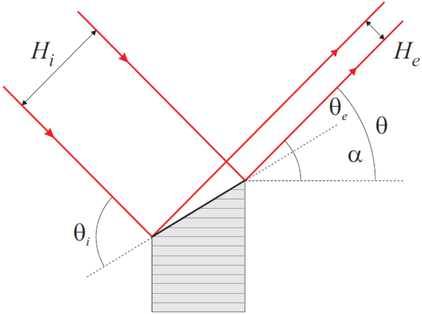
Practically, it is nearly impossible to obtain this perfect alignment, therefore it is important to understand the consequences of what is called asymmetric Bragg geometry

Recall that for a perfect crystal in symmetric Bragg geometry, the angular acceptance of the Darwin curve is

$$\omega_D = \delta\theta_D = \zeta_D \tan\theta_{Bragg}$$

Asymmetric geometry

When the diffracting planes are not precisely aligned with the surface of the crystal it is parametrized by the asymmetry angle, α, with



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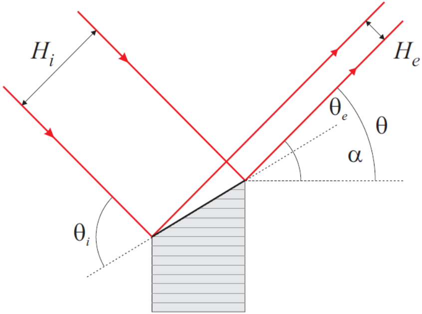

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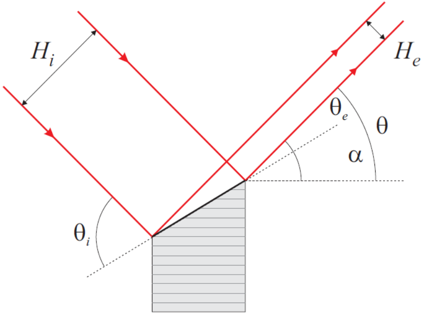

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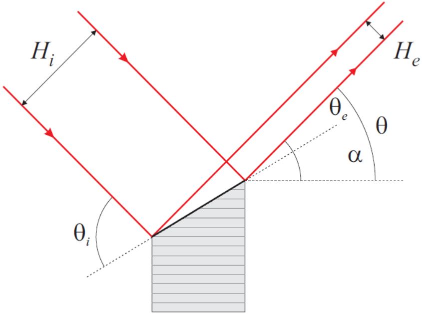

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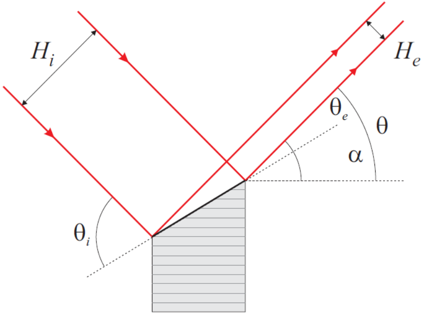

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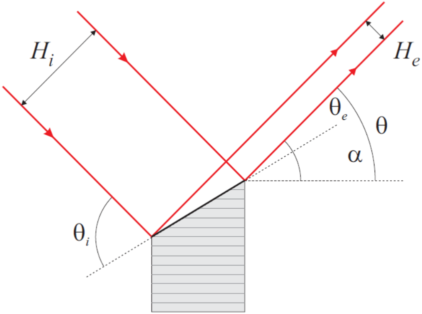

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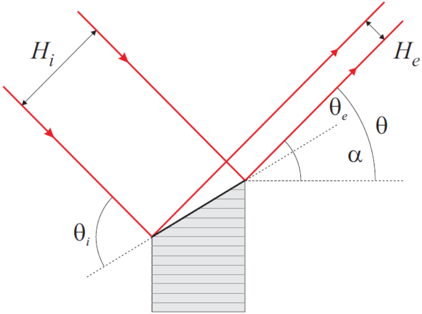

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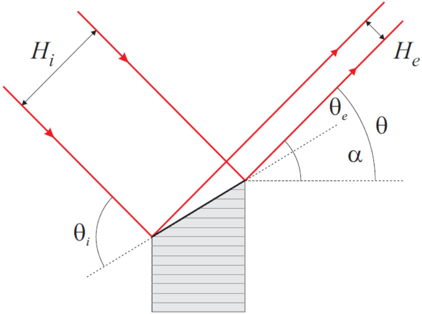

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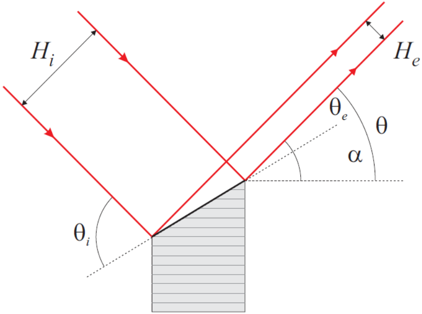

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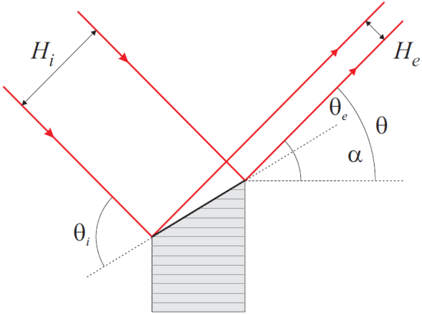

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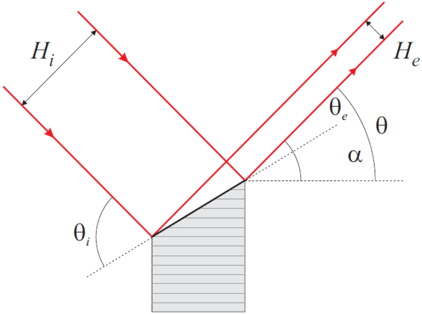

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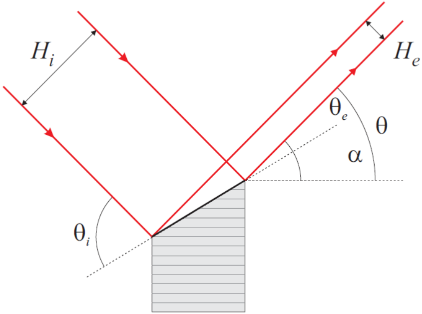

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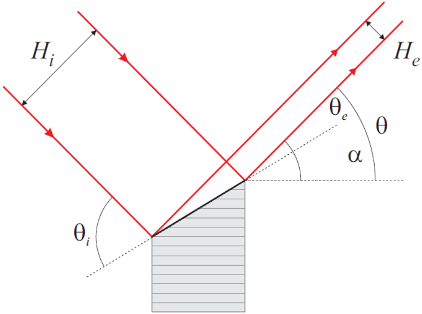

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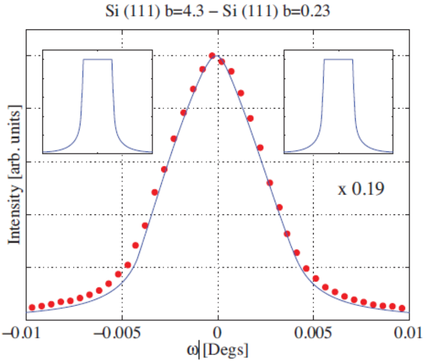

output divergence on left, input divergence on right

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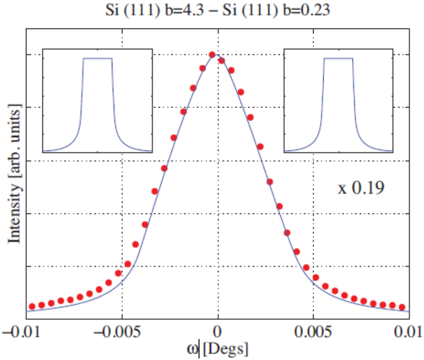

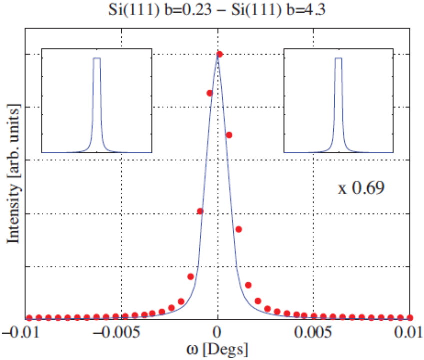

output divergence on left, input divergence on right

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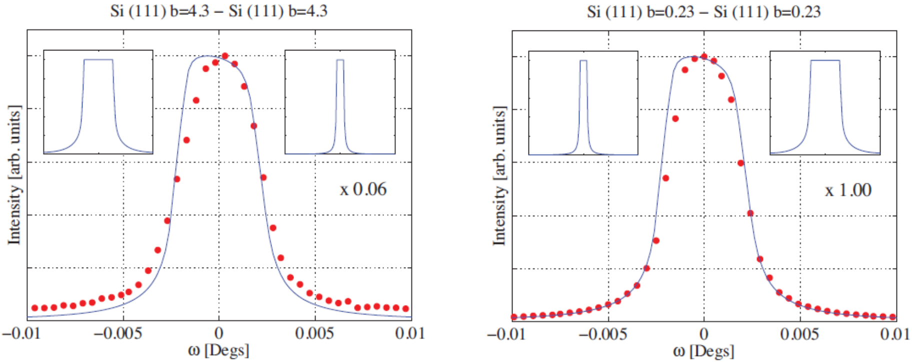

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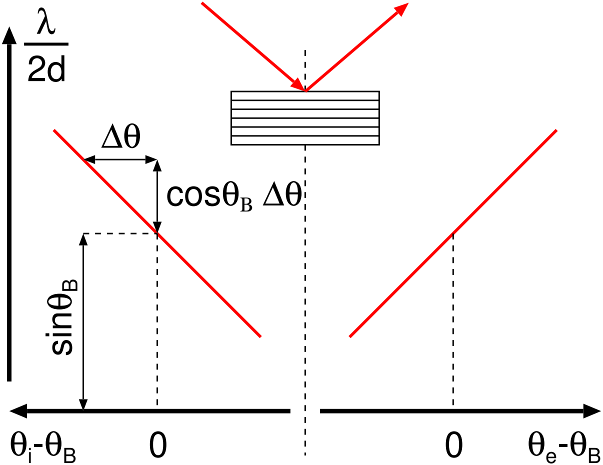
Dumond diagram: no Darwin width

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



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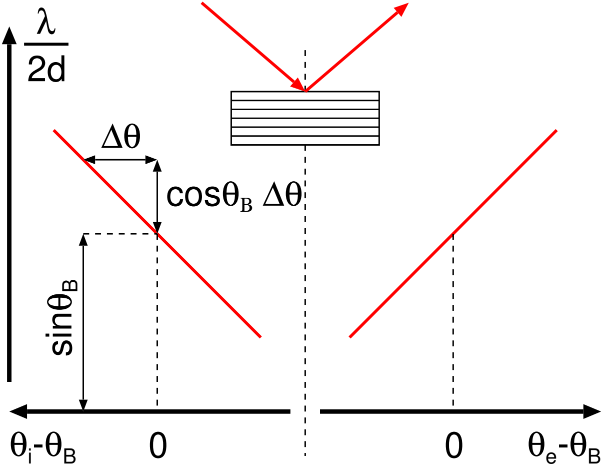

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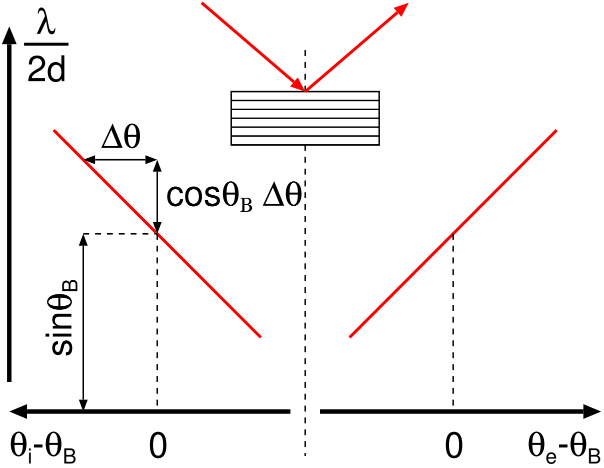

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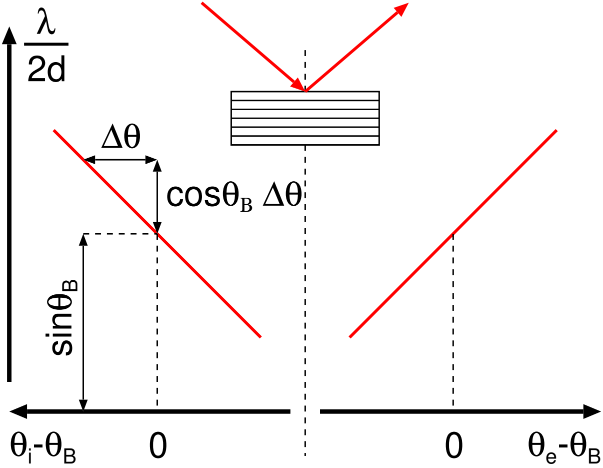

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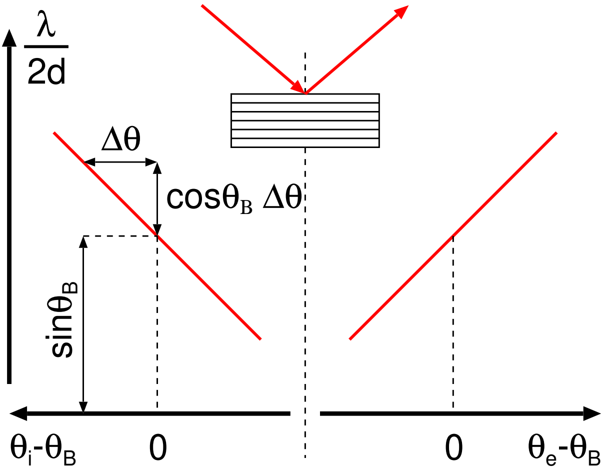

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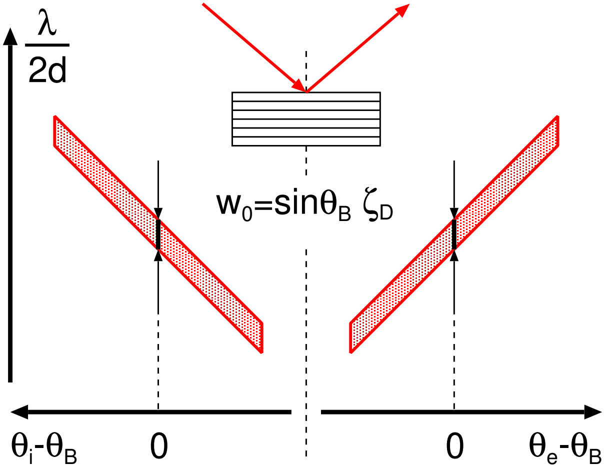
a horizontal line transfers input to output beam characteristics

Dumond diagram: symmetric Bragg

Including the Darwin width, we have a bandpass in wavelength.



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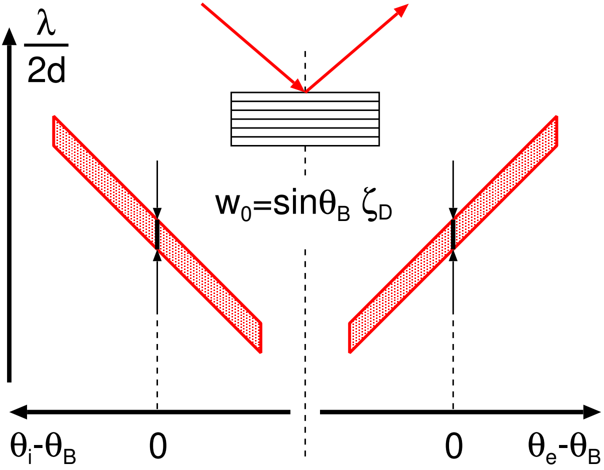

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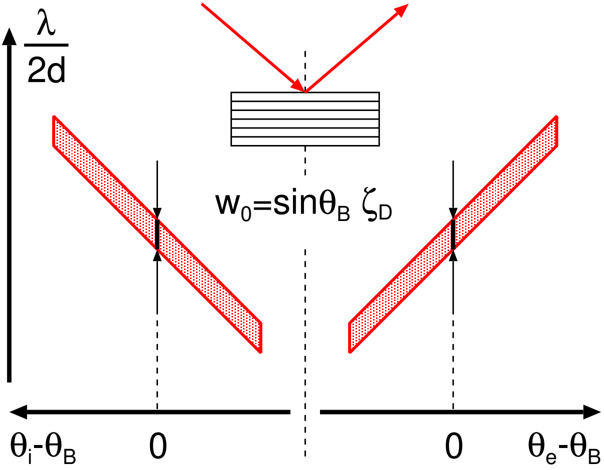

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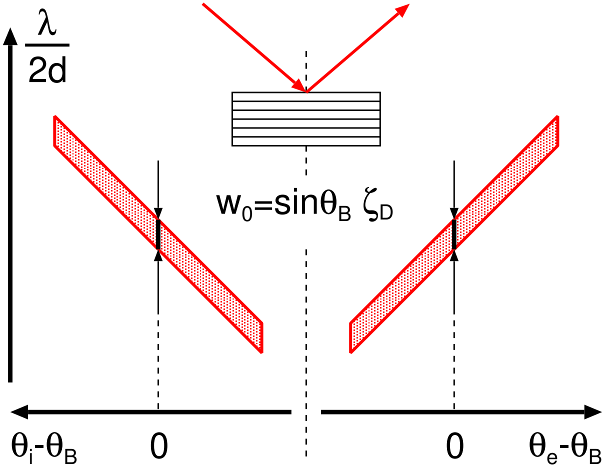

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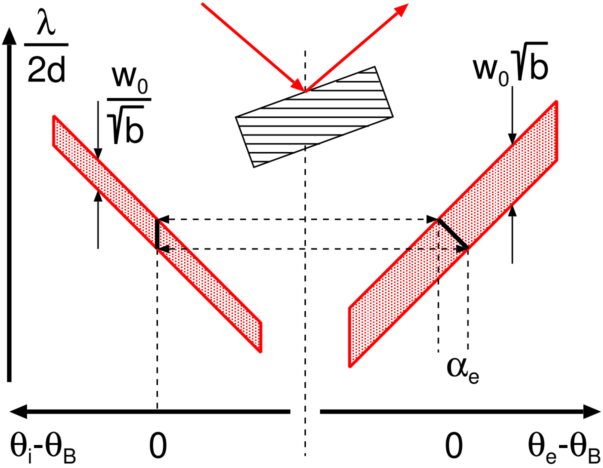
this input bandwidth is transferred to a similar output bandwidth which is also collimated

Dumond diagram: asymmetric Bragg

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



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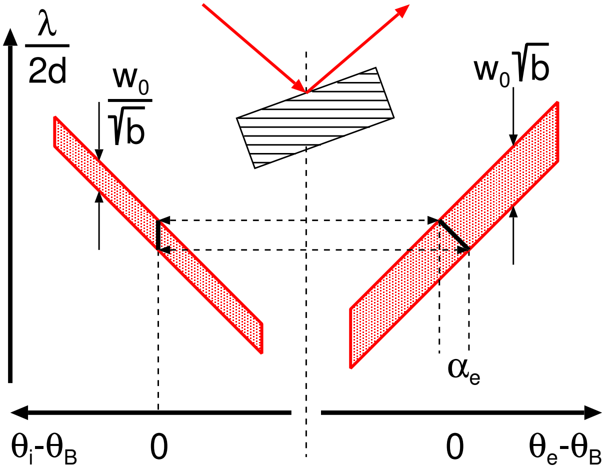

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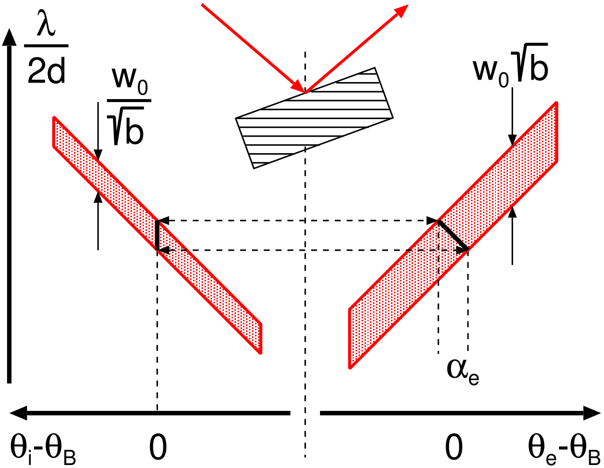

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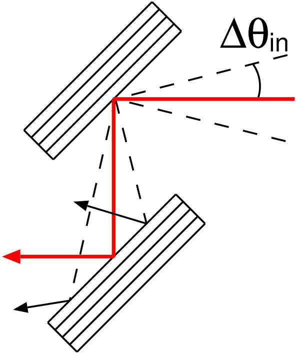
this is in addition to a compression (in this case) of the beam height (Liouville's theorem!)

Double crystal monochromator: Non-dispersive



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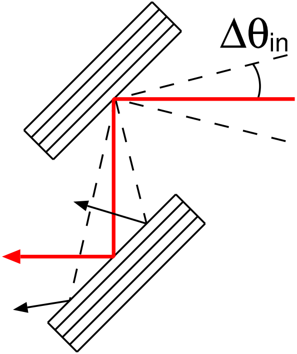

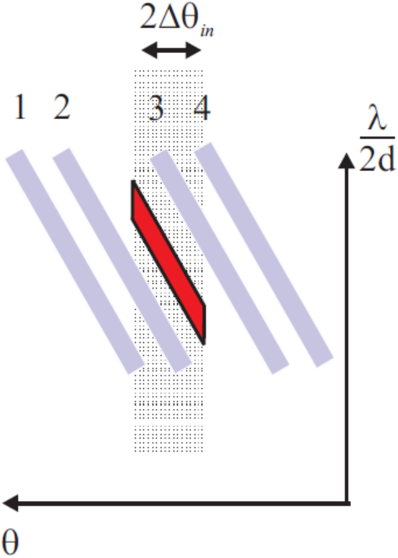

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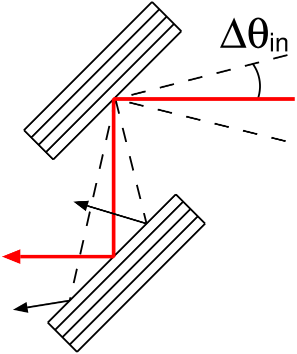
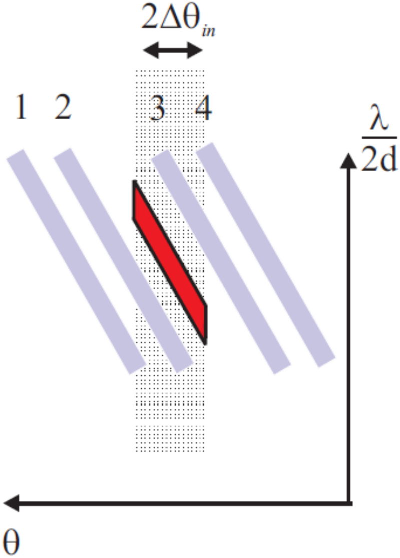


the transfer functions of the the two crystals match and full bandwith and divergence is preserved



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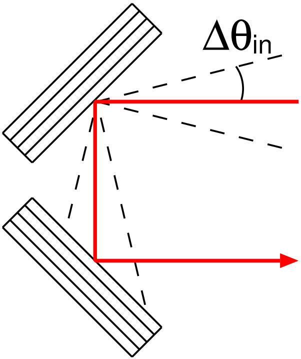

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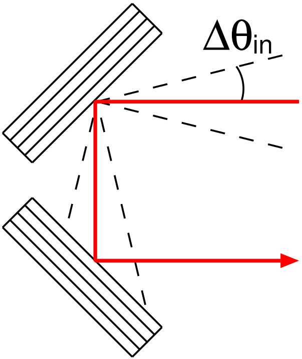

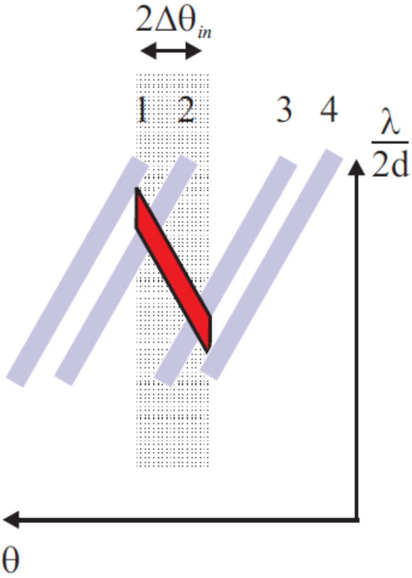

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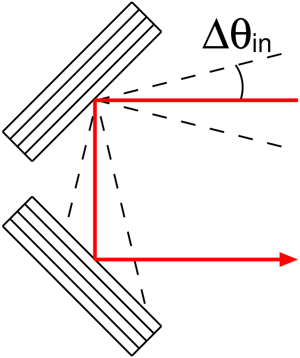
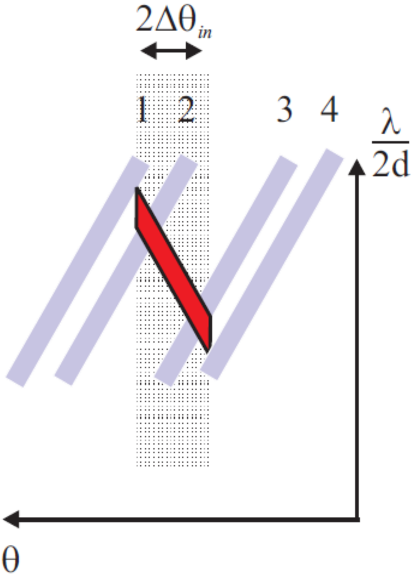
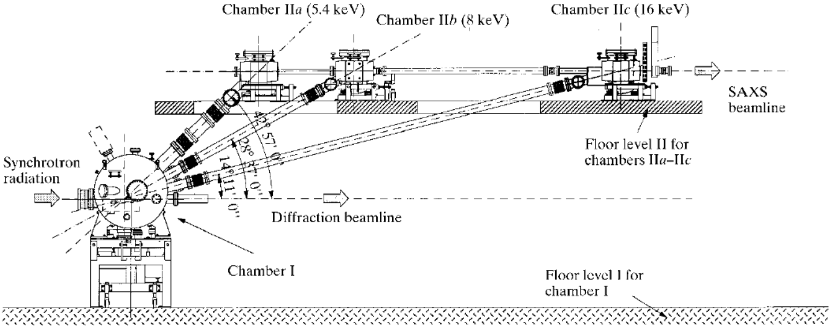


the transfer function matches only in small band that varies with angle of the second crystal



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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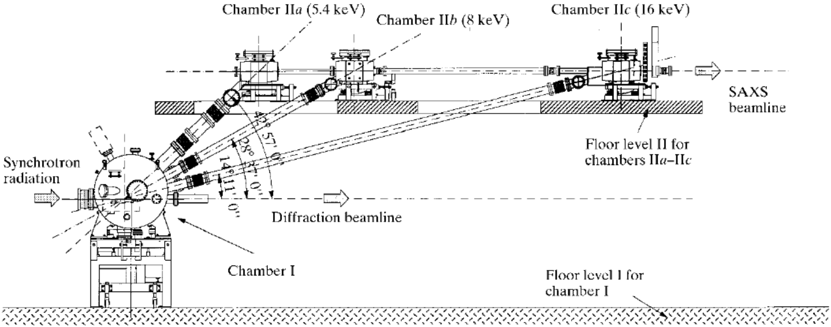

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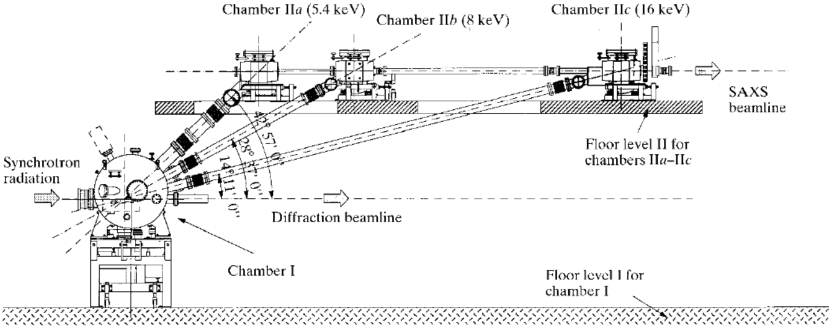

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The three crystals are set for single energies of 5.6, 8.0, and 16 keV with a vertical displacement of 1.5 m and asymmetry parameter, *b*, of 0.053, 0.078, and 0.17, respectively

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Today's Outline - March 24, 2020 (part C)

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Quantum mechanics uses some simplifying notation and has a one-to-one correspondence with linear algebra and matrix methods

Dirac bra-ket notation

Paul Dirac developed a formalism for quantum mechanics which is commonly used. We will see it in detail in Chapter 3, however one part of this formalism is a compact notation which simplifies writing expectation value integrals. We will start using this “bra-ket” notation immediately.

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

Similarity to linear algebra

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Today's Outline - March 24, 2020 (part D)

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- Absorption cross-sections

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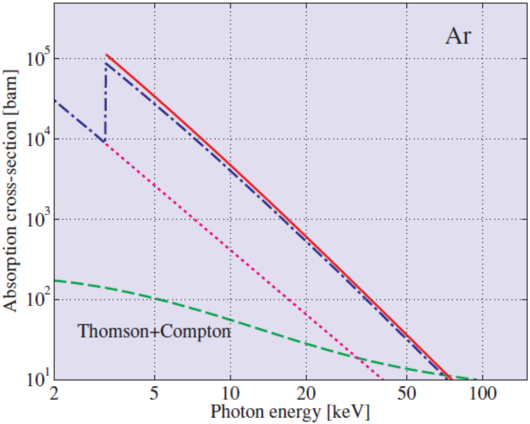
Now we will treat absorption and inelastic scattering of photons, which must be treated using quantum mechanics

Total cross section



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

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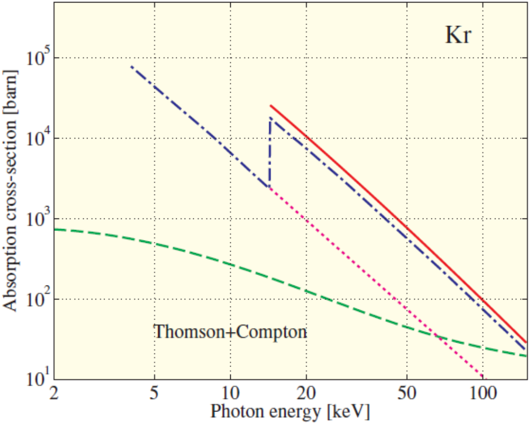

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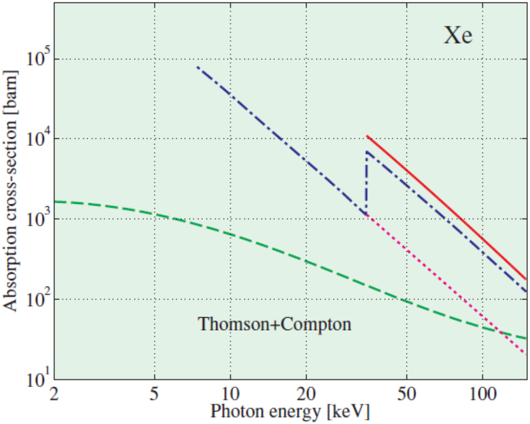

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These quantities vary significantly over many decades but can easily put on an equal footing.

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

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scale σ_a for different elements by E^3/Z^4 and plot together

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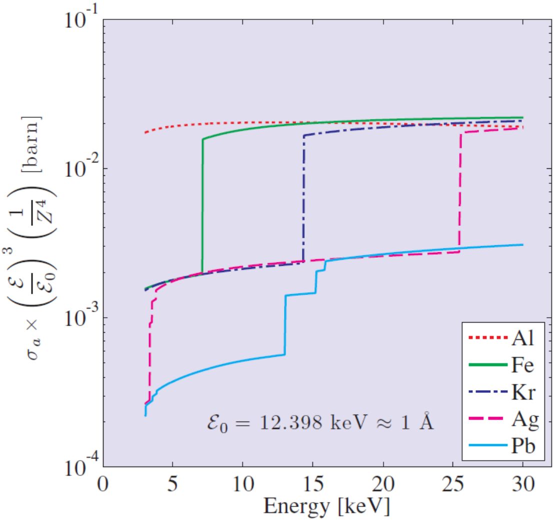
$$\mu = \frac{\rho_m N_A}{M} \sigma_a$$

$$\sigma_a \sim \frac{Z^4}{E^3}$$

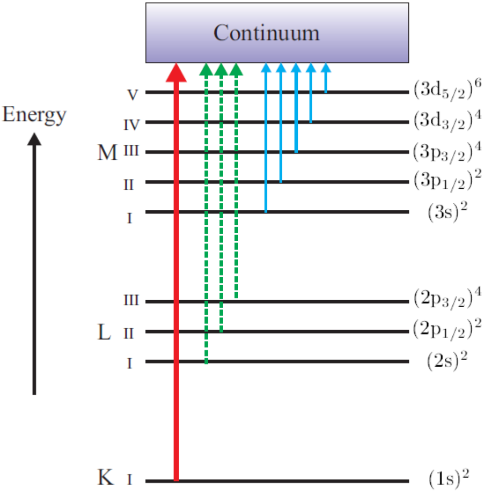
scale σ_a for different elements by E^3/Z^4 and plot together



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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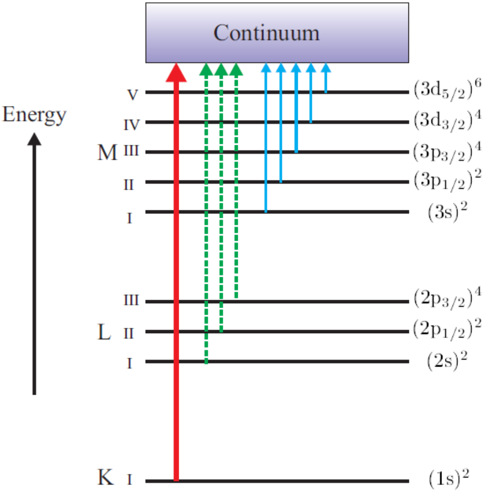

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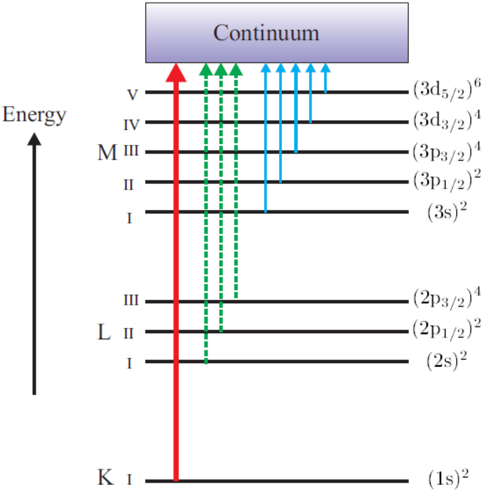

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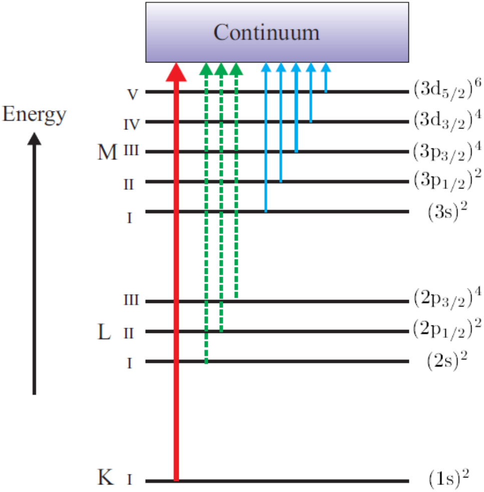

Roman numerals increase from low to high values of *l* and *j*

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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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Photoelectron integral

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

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Photoelectron cross-section

the overall matrix element squared for a particular photoelectron final direction (φ, θ) is

$$|M_{if}|^2 = \left(\frac{e\hbar}{m}\right)^2 \frac{\hbar}{2\epsilon_0 V^2 \omega}(q^2 \sin^2\theta \cos^2\varphi)\phi^2(\vec{Q})$$

and the final cross-section per K electron can now be computed as

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

where the integral I_3 is given by

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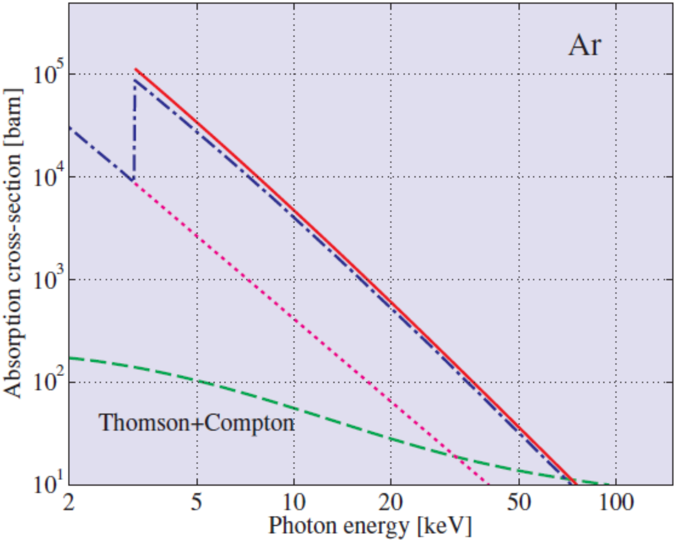
where the integral I_3 is given by

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

Calculated cross section



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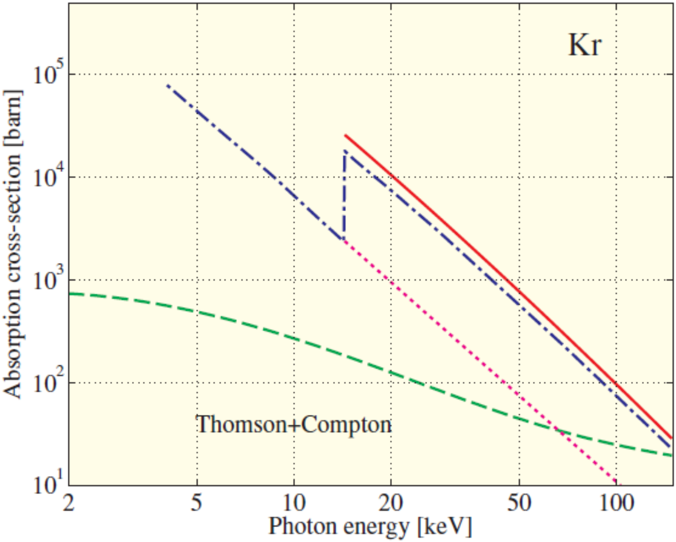

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