Methoden moderner Röntgenphysik II: Streuung und Abbildung

Lecture 18	Vorlesung zum Haupt- oder Masterstudiengang Physik, SoSe 2018
	G. Grübel, A. Philippi-Kobs, O. Seeck, T. Schneider, L. Frenzel, M. Martins, W. Wurth
Location	Lecture hall AP, Physics, Jungiusstraße
Date	Tuesday 13:00 - 14:30 (starting 3.4.)
	Thursday 8:30 - 10:00 (until 12.7.)

Outline

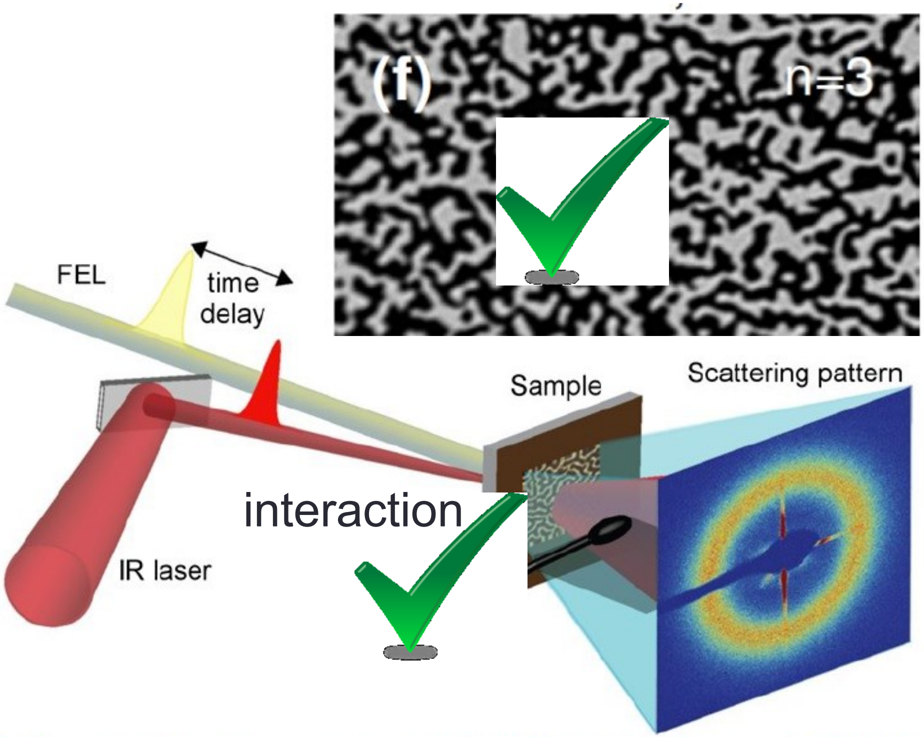
Part II/1:

Studies on Magnetic Nanostructures

by André Philippi-Kobs (AP)

[15.5.] **Ferromagnetism in a Nutshell**

- Introduction to Magnetic Materials
- Magnetic Phenomena
- Magnetic Free Energy
- Perpendicular Magnetic Anisotropy
- Magnetic Domains and Domain Walls



B. Pfau et al., Nature Communications, Vol. 3, 11; DOI:doi:10.1038/ncomms2108 (2012)
L.Müller et al., Rev. Sci. Instrum. 84, 013906 (2013)

[17.5.] **Interaction of Polarized Photons with Ferromagnetic Materials**

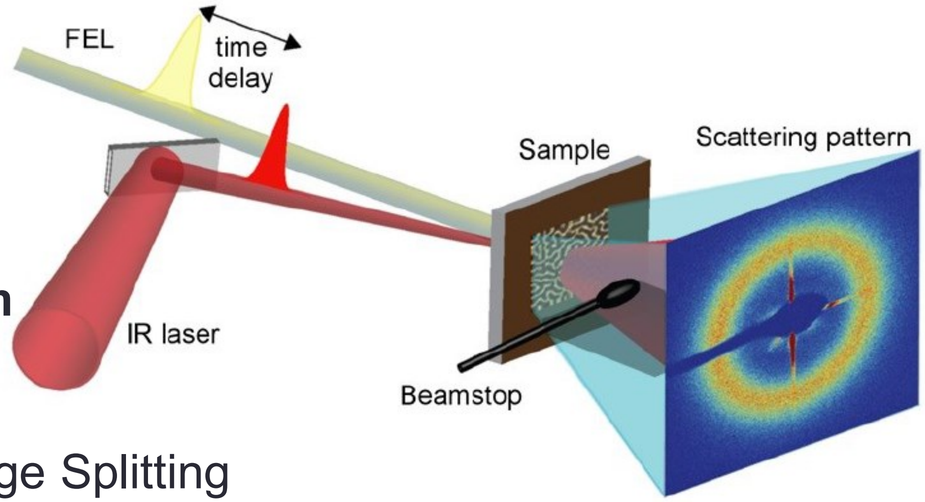
- Charge and Spin X-ray Scattering by a Single Electron
- Absorption and Resonant Scattering of Ferromagnets (Semi-Classical and Quantum-Mechanical Concepts)

Outline

Part II/2:

Studies on Magnetic Nanostructures

by André Philippi-Kobs (AP)



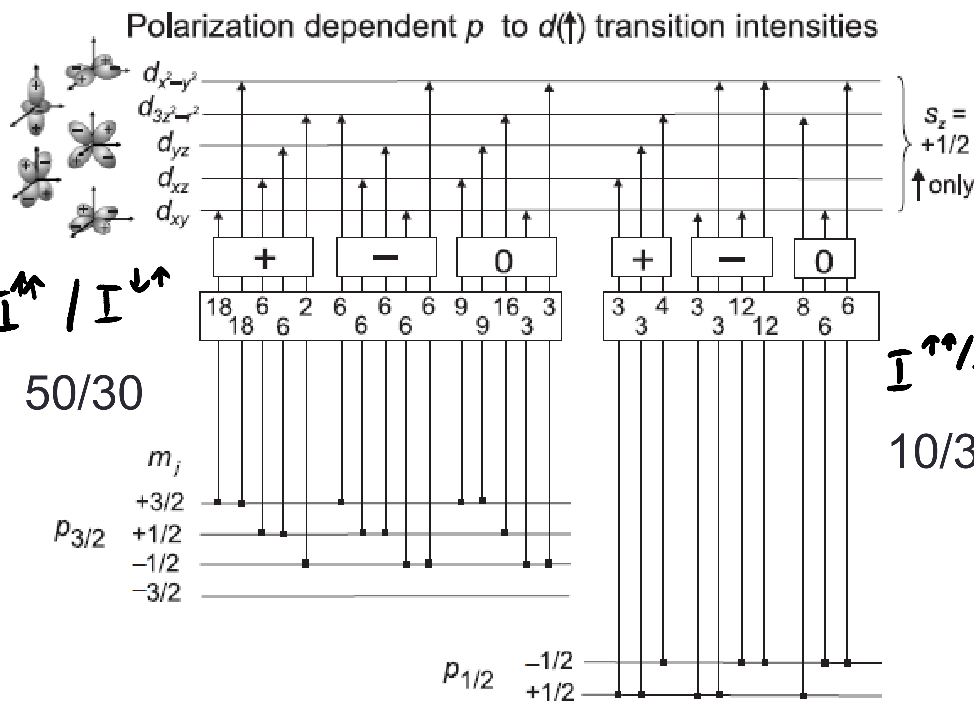
[19.6.] **X-ray Magnetic Circular Dichroism (XMCD) & Resonant Magnetic Small Angle X-ray Scattering (mSAXS)**

- Role of Spin-Orbit Coupling and Exchange Splitting
- Sum Rules
- XMLD and Natural Dicroisms
- mSAXS of Magnetic Domain Patterns

Interaction of **polarized** photons with matter

> X-ray magnetic circular dicroism (XMCD) effect

Crystal-field-split-d-states



$I^{\uparrow\uparrow} / I^{\downarrow\uparrow}$

50/30

$I^{\uparrow\uparrow} / I^{\downarrow\uparrow}$

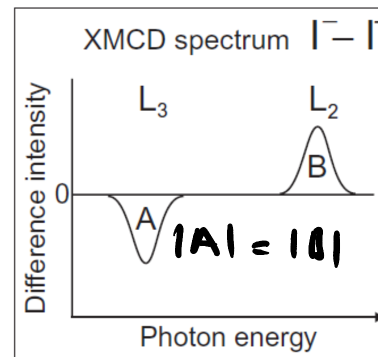
10/30

- Strong ferromagnet: one subband is completely filled
- Spin in conserved during transition

→ Calculate transition matrix elements for **Spin-Up** electrons & helicity q = ± 1 (RCP and LCP)

→ XMCD:

$\Delta I = I^{\uparrow\downarrow} - I^{\uparrow\uparrow} \neq 0$



|A| = |B|

$\frac{I_{total,L_3}}{I_{total,L_2}} = \frac{80}{40} = 2:1$

$$\Delta I_{L_3} = A\mathcal{R}^2 \sum_{n,m_j} |\langle d_n, \chi^+ | C^{(1)}_{-1} | p_{3/2}, m_j \rangle|^2 - |\langle d_n, \chi^+ | C^{(1)}_{+1} | p_{3/2}, m_j \rangle|^2 \propto \text{"}-20\text{"}$$

$$\Delta I_{L_2} = A\mathcal{R}^2 \sum_{n,m_j} |\langle d_n, \chi^+ | C^{(1)}_{-1} | p_{1/2}, m_j \rangle|^2 - |\langle d_n, \chi^+ | C^{(1)}_{+1} | p_{1/2}, m_j \rangle|^2 \propto \text{"}20\text{"}$$

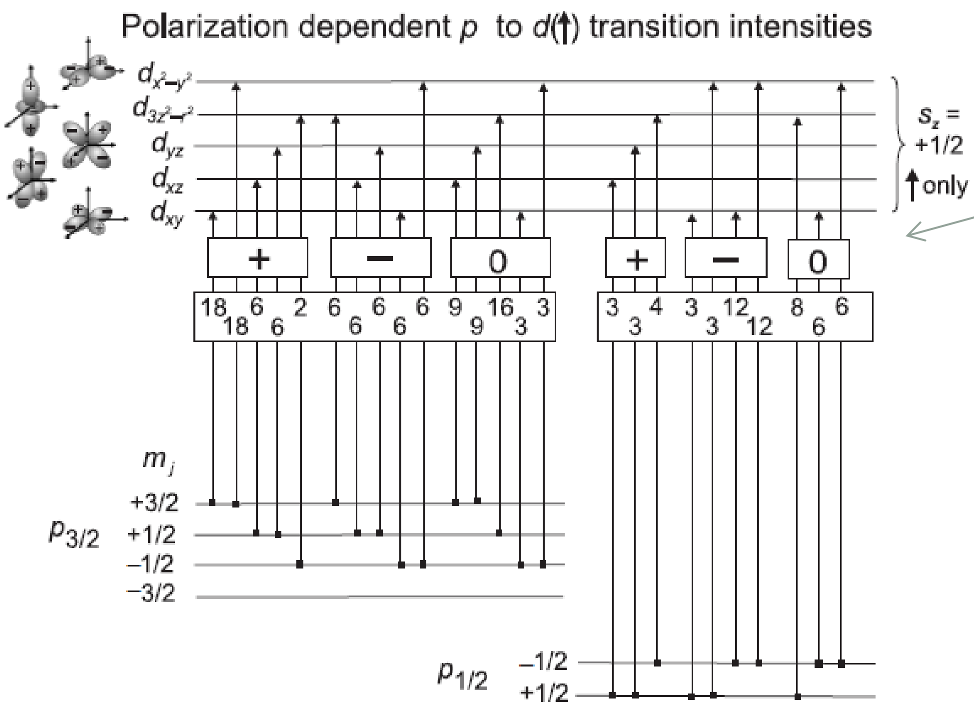
$\} \; \Delta I_{L_3} = -\Delta I_{L_2}$

DESY

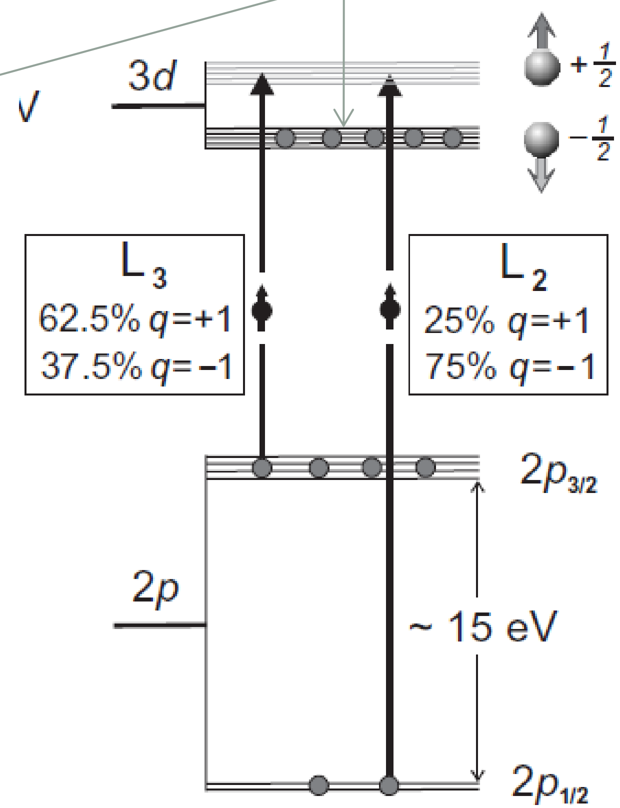
Interaction of **polarized** photons with matter

> X-ray magnetic circular dicroism (XMCD) effect

Strong ferromagnet:
One subband is
Completely filled



Crystal-field-split-d-states



Atomic-exchange-split d-states (w/o SOC)

Same results for $I_{L_{3,total}} : I_{L_{2,total}} = 2:1,$

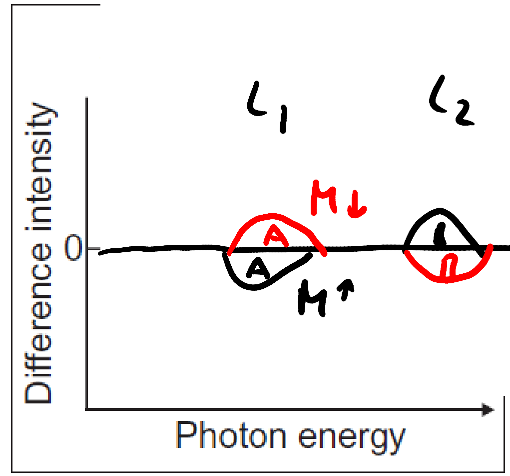
$$\Delta I_{L_{3,total}} : \Delta I_{L_{2,total}} = 1:-1$$

when using atomic d-states (w/o SOC); today‘s lecture

Interaction of **polarized** photons with matter

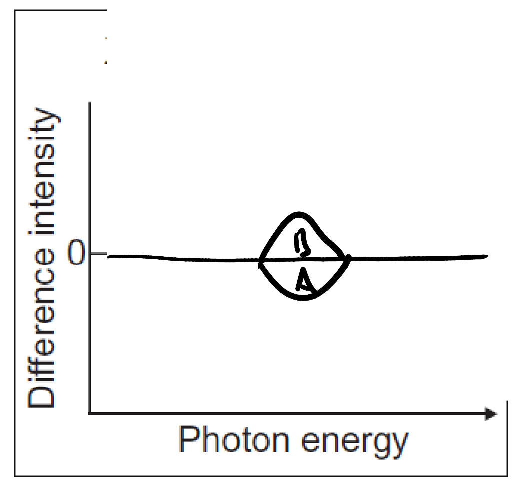
- X-ray magnetic circular dicroism (XMCD) effect

What is happening in a paramagnet?



➔ No XMCD

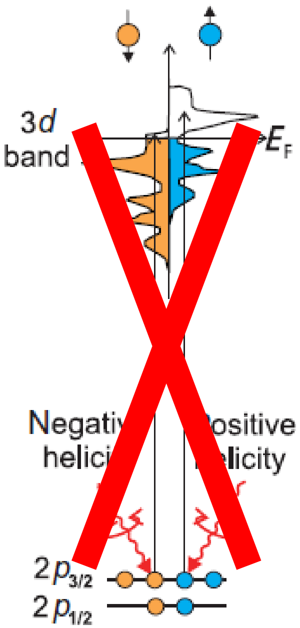
What is happening w/o Spin-Orbit-Coupling for the p-states?

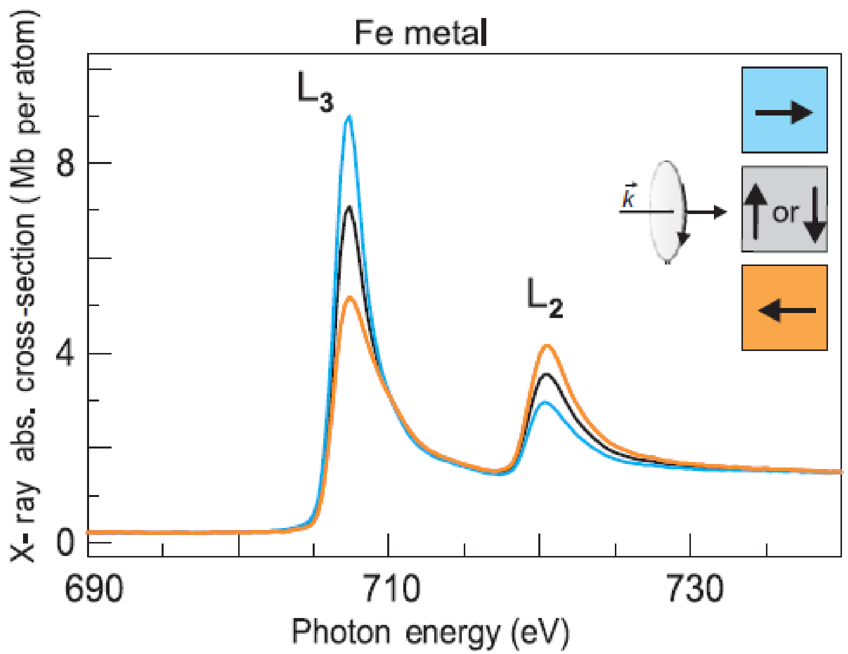


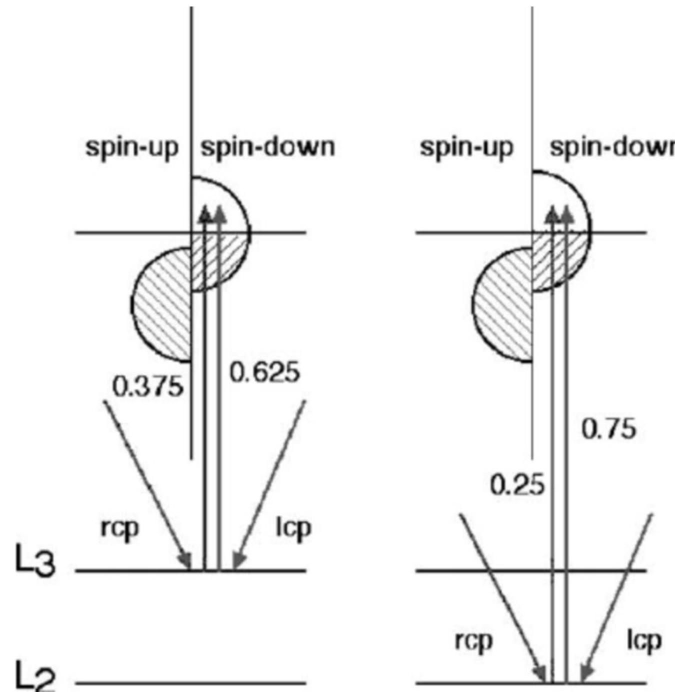
➔ No XMCD

Interaction of **polarized** photons with matter

- X-ray magnetic circular dicroism (XMCD) effect







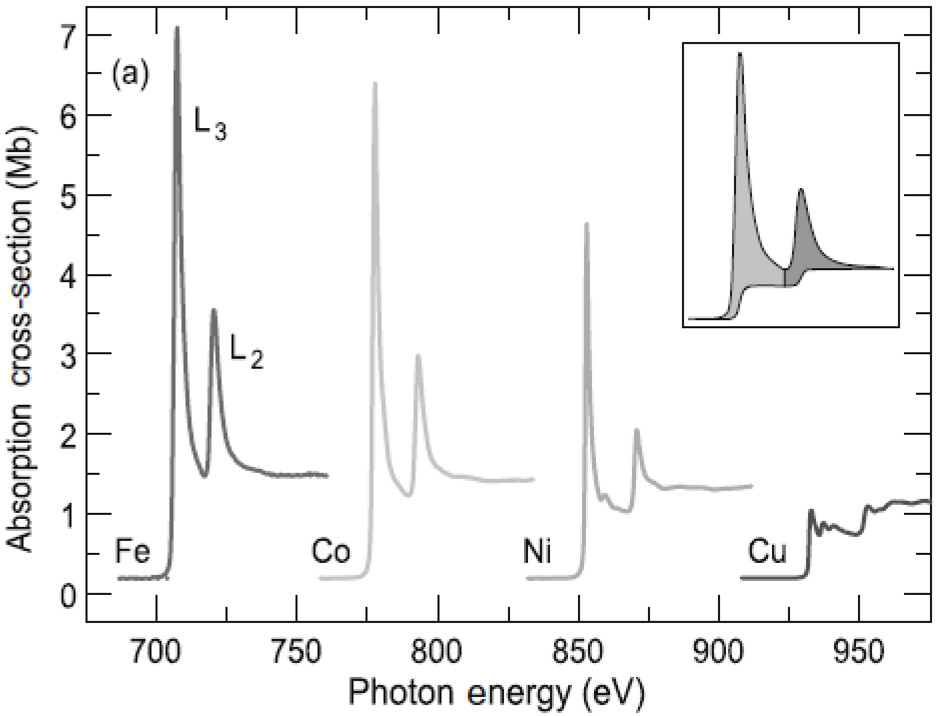
(sketches in textbooks can be misleading!)

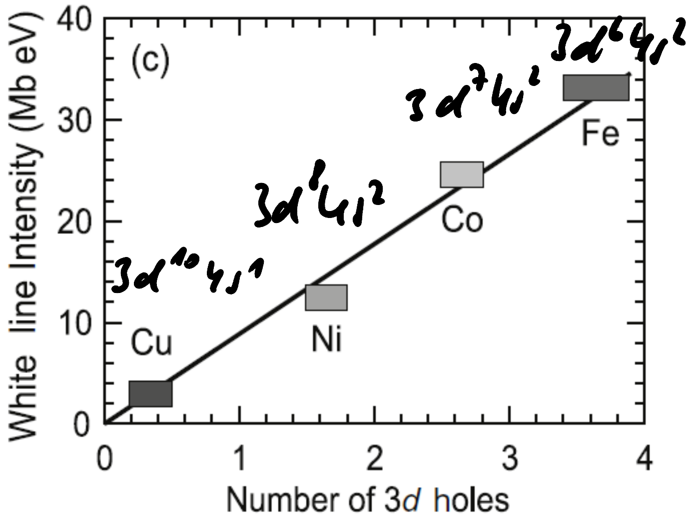
$\Delta I_{XMCD} \propto \vec{n} \cdot \vec{L}_{ph} = \cos\theta \qquad \theta \sphericalangle (\vec{n}, \vec{L}_{ph})$

Interaction of **polarized** photons with matter

> (Orientation averaged) Sum rules $\langle I \rangle = \frac{1}{3}\left(I_\alpha^{-1} + I_\alpha^{0} + I_\alpha^{+1}\right)$ ($\alpha = z$)

Density of d-states at E_F $\sigma^{\mathrm{abs}} = 4\pi^2 \frac{e^2}{4\pi\epsilon_0 \hbar c} \hbar\omega \, |\langle b|\, \epsilon \cdot r \,|a\rangle|^2 \, \delta[\hbar\omega - (E_b - E_a)] \, \rho(E_b)$





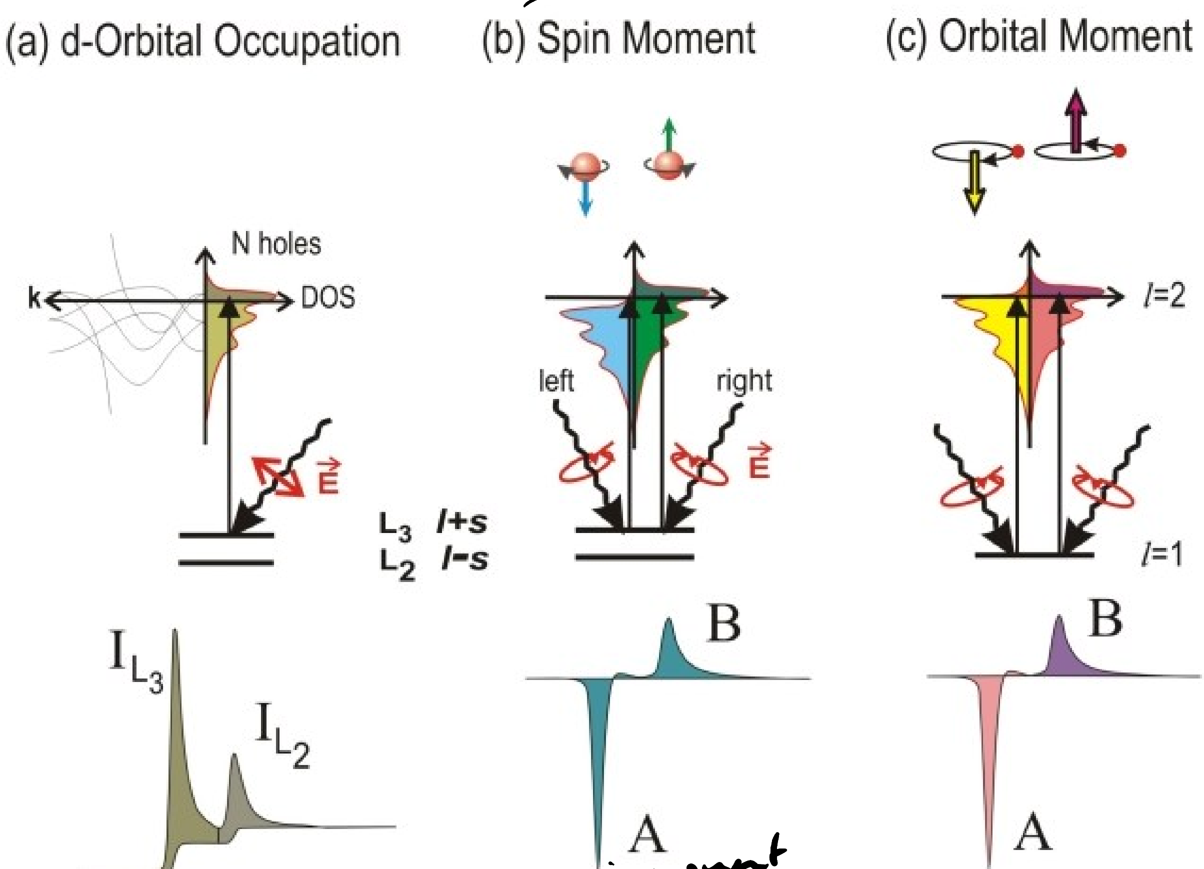
$D_d(E_F) = \frac{\langle I_{L_3} + I_{L_2} \rangle}{C}$

2p → 4s transitions have to be considered as well but as $D_s(E_F) \ll D_d(E_F)$ 2p → 3d channels dominate

Interaction of **polarized** photons with matter

> (Orientation averaged) Sum rules

XMCD



as $\vec{L}$ (and soc) exists, also for d-states
$\Rightarrow \langle -A \rangle \neq \langle B \rangle$
but difference is small as $m_L \ll m_S$

$$m_L = -2\mu_B \frac{\langle A+B \rangle}{c}$$
angular momentum

(see last slide)

spin moment
$$m_S = \mu_B \frac{\langle -A+2B \rangle}{c}$$

Interaction of **polarized** photons with matter

> Application of XMCD

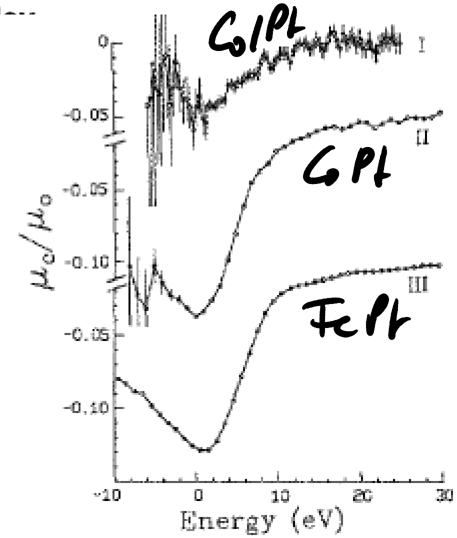
J. Appl. Phys. 67 (9), 1 May 1990

DORIS II at HASYLAB, DESY, Hamburg.

Spin-dependent x-ray absorption in Co/Pt multilayers and $Co_{50}Pt_{50}$ alloy

G. Schütz, R. Wienke, and W. Wilhelm
Fak. f. Physik, TU München, D-8046 Garching, Federal Republic of Germany
W. B. Zeper
Philips Research Laboratories, P.O. Box 80.000, 5600 JA Eindhoven, The Netherlands
H. Ebert
Siemens AG, ZFE ME TPH 11, Postfach 3220, D-8520 Erlangen, Federal Republic of Germany
K. Spörl
Institut für Angew. Physik, University of Regensburg, Federal Republic of Germany

The spin dependence of $L_{2,3}$ absorption in 5d atoms oriented in a ferromagnetic matrix contains information on the spin density of the empty d-projected states of the absorbing atom. Spin-dependent absorption spectroscopy using circularly polarized synchrotron radiation was applied to study the polarization of the Pt atoms in the binary alloy $Co_{50}Pt_{50}$ and Pt/Co layered structures, which are promising candidates for magneto-optical recording. The spin-dependent absorption signals for vapor-deposited 250(4 Å Co + 18 Å Pt) and 250(6 Å Co + 18 Å Pt) multilayers indicate a ferromagnetic coupling on Pt and Co atoms with a significant Pt polarization. This is reduced on average by about 60% with respect to the Pt polarization in the $Co_{50}Pt_{50}$ alloy. The experimental results are discussed on the basis of spin-polarized band-structure calculations.



$E_\gamma^{Pt\,L_2} = 11.5$ keV

$|m_j^{Pt}| = 0.25\ \mu_B$/atom for alloy

$|m_j^{Pt}| = 0.09\ \mu_B$/atom for ML

example: use element selectivity to study polarized Pt (due to proximity to Co) in CoPt alloys and Co/Pt multilayers

Interaction of **polarized** photons with matter

> From Absorption to Resonant Scattering (exp. approach):

$f'' = -(k/4\pi)\,\sigma_a\,(E)$

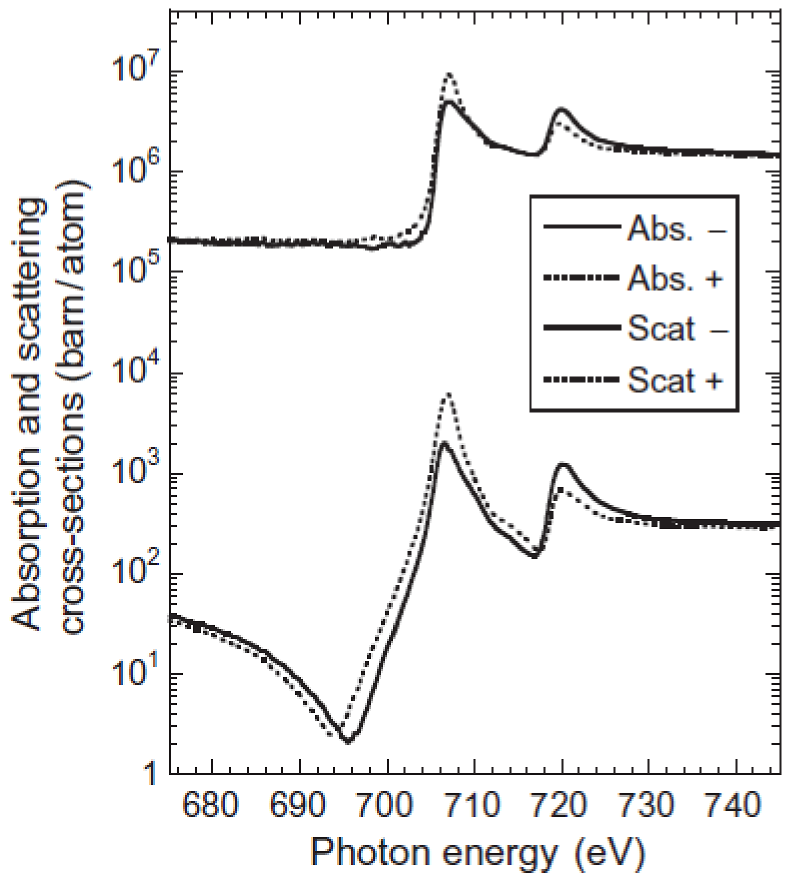
Measure absorption cross-section for both helicities

↓ Kramers-Kronig relation

f'

↓

$$\sigma_{\text{scattering}} = f^2$$
$$= [Z + f'(\omega, \boldsymbol{\varepsilon})]^2 + [f''(\omega, \boldsymbol{\varepsilon})]^2$$



Interaction of **polarized** photons with matter

- Resonant scattering (qm concept): 2. Term of Fermi's Golden rule in dipole approx.

$$T_{if} = \frac{2\pi}{\hbar} \left| \langle f|\mathcal{H}_{\text{int}}|i\rangle + \sum_n \frac{\langle f|\mathcal{H}_{\text{int}}|n\rangle\langle n|\mathcal{H}_{\text{int}}|i\rangle}{\varepsilon_i - \varepsilon_n} \right|^2 \delta(\varepsilon_i - \varepsilon_f)\rho(\varepsilon_f) \qquad \sigma = \frac{T_{if}}{\Phi_0}$$

Dipol approximation etc. (as done for absorption term)

$$\frac{\hbar^2\omega^4}{c^2}\,\alpha_f^2 \left| \sum_n \frac{\langle a|\boldsymbol{r}\cdot\boldsymbol{\epsilon}_2^*|n\rangle\langle n|\boldsymbol{r}\cdot\boldsymbol{\epsilon}_1|a\rangle}{(\hbar\omega - E_R^n) + \mathrm{i}(\Delta_n/2)} \right|^2$$

Δ_n: line width

J. P. Hannon et al., Phys. Rev. Lett **61**, 1245 (1988)

$$\langle a|\boldsymbol{r}\cdot\boldsymbol{\epsilon}_2^*|n\rangle\langle n|\boldsymbol{r}\cdot\boldsymbol{\epsilon}_1|a\rangle = \frac{\mathcal{R}^2}{2}\Big[(\boldsymbol{\epsilon}_2^*\cdot\boldsymbol{\epsilon}_1)\left\{|C_{+1}|^2 + |C_{-1}|^2\right\}$$
$$+\, \mathrm{i}(\boldsymbol{\epsilon}_2^*\times\boldsymbol{\epsilon}_1)\cdot\hat{\boldsymbol{m}}\left\{|C_{-1}|^2 - |C_{+1}|^2\right\}$$
$$+\, (\boldsymbol{\epsilon}_2^*\cdot\hat{\boldsymbol{m}})(\boldsymbol{\epsilon}_1\cdot\hat{\boldsymbol{m}})\left\{2|C_0|^2 - |C_{-1}|^2 - |C_{+1}|^2\right\}\Big]$$

Interaction of **polarized** photons with matter

- Resonant scattering: 2. Term of Fermi's Golden rule in dipole approximation

$$T_{if} = \frac{2\pi}{\hbar}\left| \langle f|\mathcal{H}_{\text{int}}|i\rangle + \sum_n \frac{\langle f|\mathcal{H}_{\text{int}}|n\rangle\langle n|\mathcal{H}_{\text{int}}|i\rangle}{\varepsilon_i - \varepsilon_n}\right|^2 \delta(\varepsilon_i - \varepsilon_f)\rho(\varepsilon_f)$$

with $\sigma = \frac{T_{if}}{\Phi_0}$ and $\sigma_{\text{scattering}} = f^2$

➔ The *elastic resonant magnetic scattering factor* in units [number of electrons] is given by

$$f(\omega,\boldsymbol{\varepsilon}_1) = \frac{\hbar\omega^2\alpha_f R^2}{2cr_0}\left[\underbrace{(\epsilon_2^*\cdot\epsilon_1)\,G_0}_{\text{charge}} + \underbrace{\mathrm{i}(\epsilon_2^*\times\epsilon_1)\cdot\hat{m}\,G_1}_{\text{XMCD}} + \underbrace{(\epsilon_2^*\cdot\hat{m})(\epsilon_1\cdot\hat{m})\,G_2}_{\text{XMLD}}\right]$$

$$G_1 = \sum_n \frac{|\langle a|C_{-1}^{(1)}|n\rangle|^2 - |\langle a|C_{+1}^{(1)}|n\rangle|^2}{(\hbar\omega - E_R^n) + \mathrm{i}(\Delta_n/2)}$$

For circularly polarized light

$$\mathrm{i}\left[(\boldsymbol{\epsilon}^{\pm})^* \times \boldsymbol{\epsilon}^{\pm}\right] = \mp\,\mathbf{e}_z$$

Charge: Natural dicroism

XMLD: X-ray magnetic linear dicroism

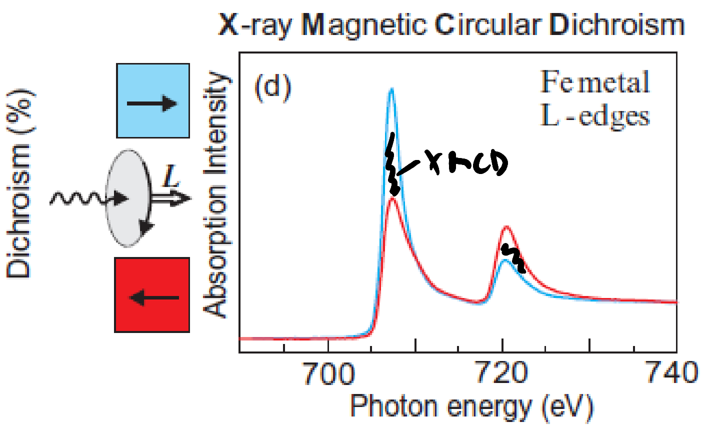
$$G_0 = \sum_n \frac{|\langle a|C_{+1}^{(1)}|n\rangle|^2 + |\langle a|C_{-1}^{(1)}|n\rangle|^2}{(\hbar\omega - E_R^n) + \mathrm{i}(\Delta_n/2)}$$

$$G_2 = \sum_n \frac{2|\langle a|C_0^{(1)}|n\rangle|^2 - |\langle a|C_{-1}^{(1)}|n\rangle|^2 - |\langle a|C_{+1}^{(1)}|n\rangle|^2}{(\hbar\omega - E_R^n) + \mathrm{i}(\Delta_n/2)}$$

Interaction of **polarized** photons with matter

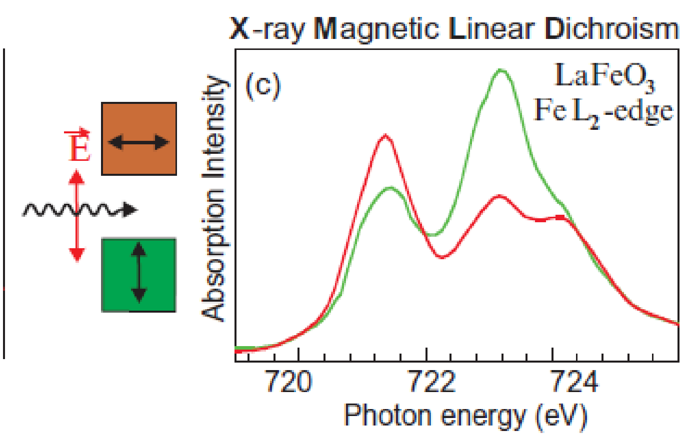
> XMCD and XMLD effect

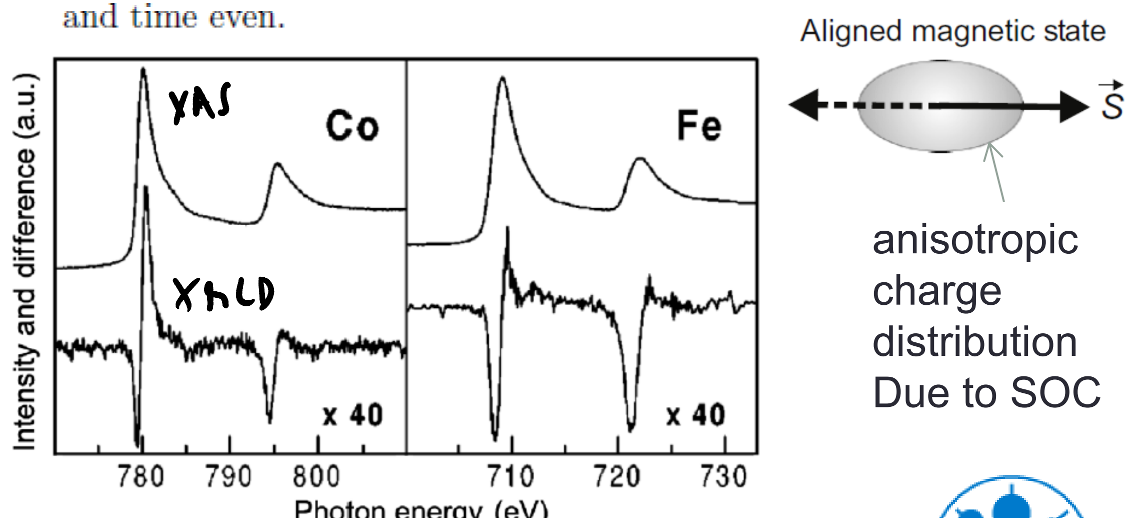
X-ray "magnetic" dichroism is due to spin alignment and the spin–orbit coupling.



- X-ray magnetic circular dichroism – XMCD – arises from *directional* spin alignment. The effect is parity even and time odd.

- X-ray magnetic linear dichroism – XMLD – arises from a charge anisotropy induced by *axial* spin alignment. The effect is parity even and time even.

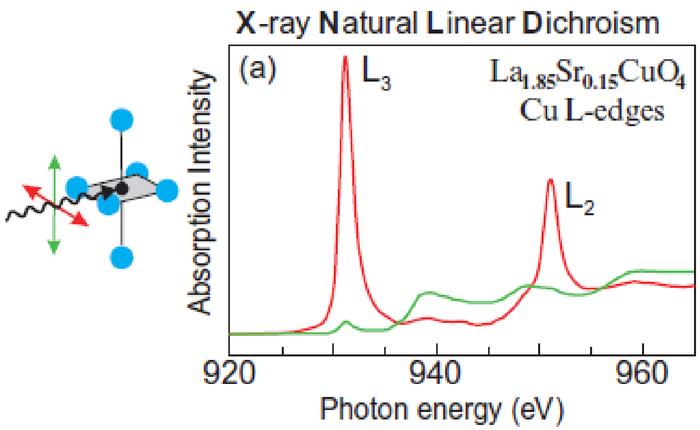


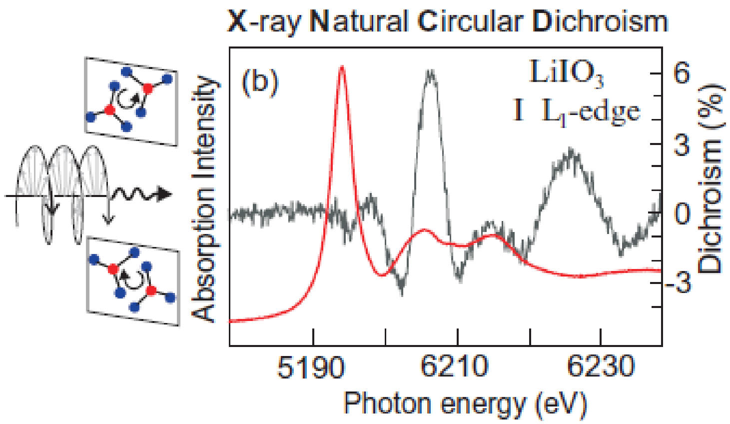


DESY

Interaction of **polarized** photons with matter

> XNLD and XNCD effect

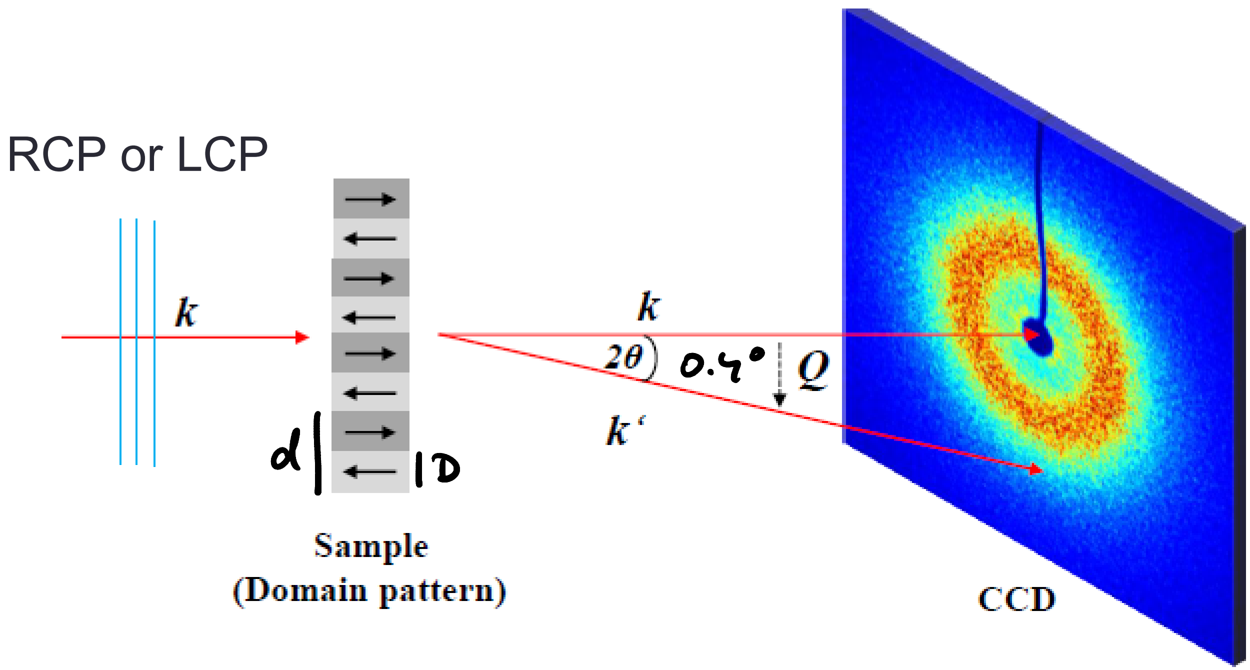




X-ray "natural" dichroism refers to the absence of spin alignment.

- X-ray natural linear dichroism – XNLD – is due to an anisotropic charge distribution. The effect is parity even and time even.
- X-ray natural circular dichroism – XNCD – may be present for anisotropic charge distributions that lack a center of inversion. The effect is parity odd and time even.

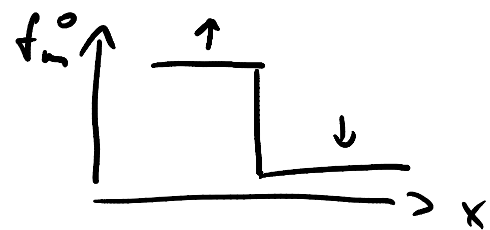
mSAXS of magnetic domain patterns



„magnetic grating/lattice“ = stripe domain pattern with equal domain size *D* (periodicity of *d* = 2*D*)

➔ Scattering factor $f_m = M_z F^m$ varies in x-direction due to XMCD effect & alternating M_z

$$f_m(x) = \underbrace{f_m^0(x)}_{\text{unit cell}} \otimes \sum_{n=-\infty}^{\infty} \delta(x - nd)$$



mSAXS of magnetic domain patterns

Scattering amplitude (Fourier transform of scattering factor):

$$A(Q) = FT(f_n(x)) = \underbrace{\tilde{f}_n^{0}(Q)}_{\text{unit cell}} \underbrace{\sum_{n=-\infty}^{\infty} e^{-iQnd}}_{\text{lattice sum}}$$

with scattering vector (momentum transfer): $Q = k - k' = \frac{4\pi}{\lambda} \sin\theta$

Scattering intensity:

1/2 number of domains

$$I(Q) = |A(Q)|^2 = \begin{cases} |f_n^{0}(Q)|^2 \cdot N_d^2 \\ \sim 0 \end{cases}$$

$e^{iQnd} = 1^{\otimes}$, i.e. condition for mSAXS

$\otimes$ for $Q \cdot d = 2\pi \Rightarrow Q = \frac{2\pi}{d}$

$d = 200\,nm$

$\lambda_{L\text{-edge}} = 1.5\,nm$

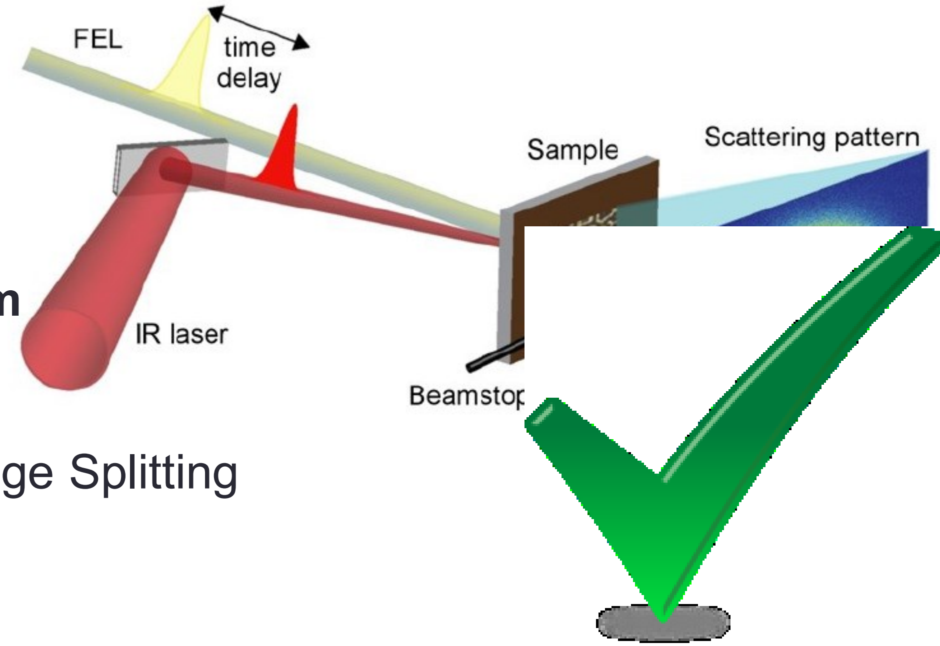
$$\theta = \arcsin\left(\frac{\lambda}{2d}\right) = 0.2^{\circ}$$

Outline

Part II/2:

Studies on Magnetic Nanostructures

by André Philippi-Kobs (AP)



[19.6.] **X-ray Magnetic Circular Dichroism (XMCD) & Resonant Magnetic Small Angle X-ray Scattering (mSAXS)**

- Role of Spin-Orbit Coupling and Exchange Splitting
- Sum Rules
- XMLD and Natural Dicroisms
- mSAXS of Magnetic Domain Patterns