XMCD ....

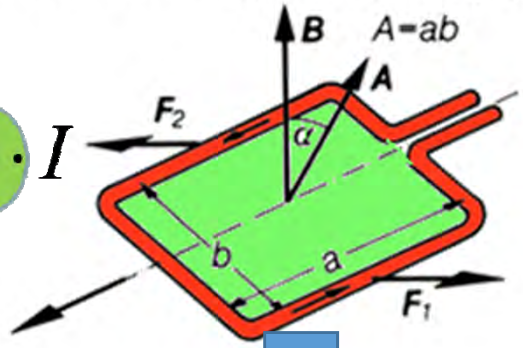
Outlook of the lecture

- Magnetism in nutshell
- X-ray absorption spectroscopy XAS
- Magnetic XAS = XMCD (X-ray Magnetic Circular Dichroism)

Magnetism in a nutshell

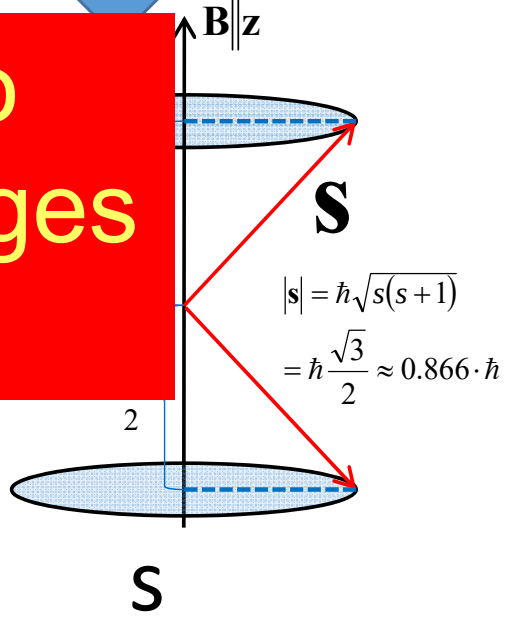
- „Rotating“ charges produce magnetic field (angular momentum)
- There are two types spin (S) and orbital (L) magnetic moments

$$|\vec{m}| = A \cdot I$$



macroscopic

Magnetism is related to angular momenta of charges L and S



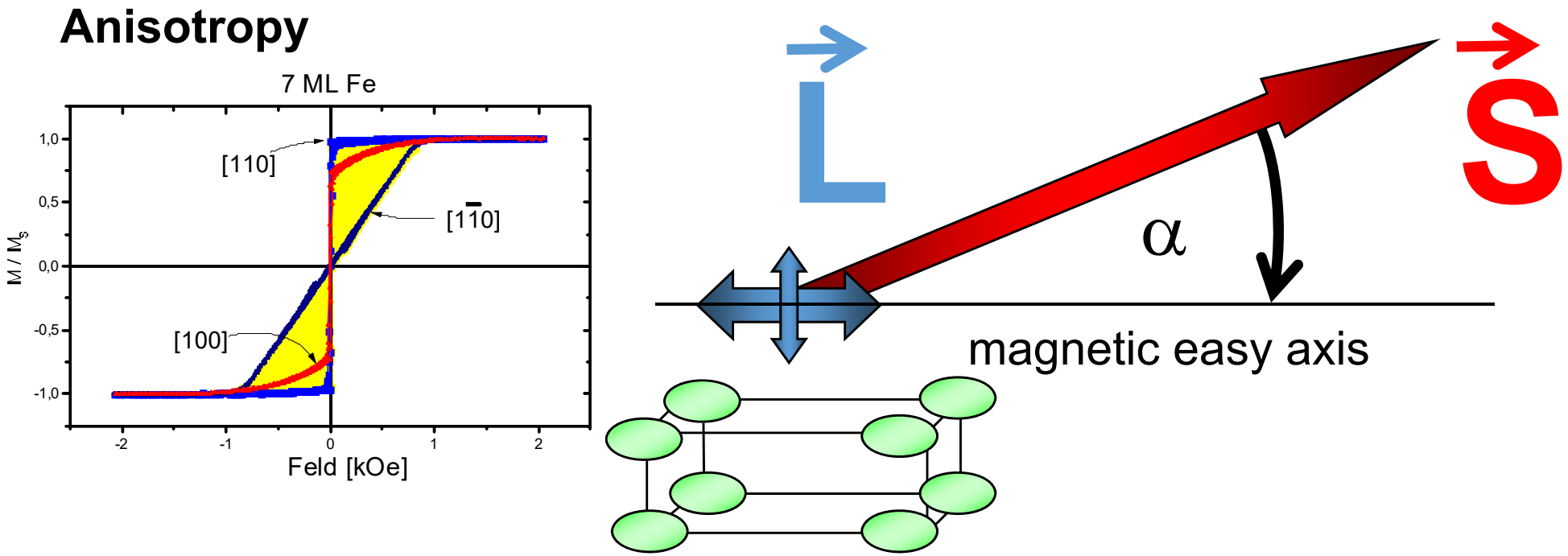
L interacts with the lattice

L is often quenched (3d) = close to zero ➔ super important, but hard to quantify!

$$\langle m_L \rangle_z = \langle L_z \rangle \cdot \mu_B \qquad \langle m_S \rangle_z = g \cdot \langle S_z \rangle \cdot \mu_B \approx 2 \cdot \langle S_z \rangle \cdot \mu_B \qquad \mu_B = 9.274 \cdot 10^{-24}\ \text{J/T}$$

$$\text{g} = \text{G} - \text{factor} \qquad \mu_B = \text{Bohr's Magneton}$$

orbital moment

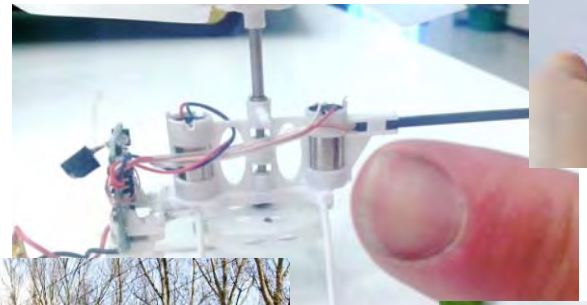


- orbital moment has preferred axis in anisotropic crystal field
  - LS-coupling in 3d-shell orients the spin
- The small L is important for almost all properties, especially for technology
  - remnant field, easy and hard axis, coercivity ….

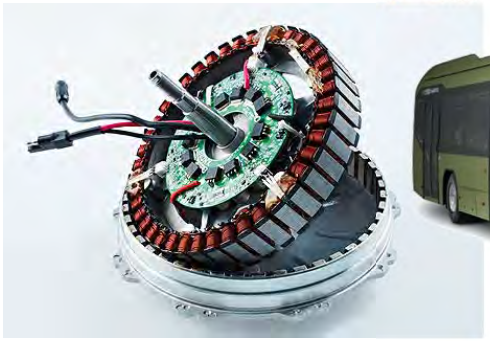
P. Bruno, Physical Review B **39** (1989) 865

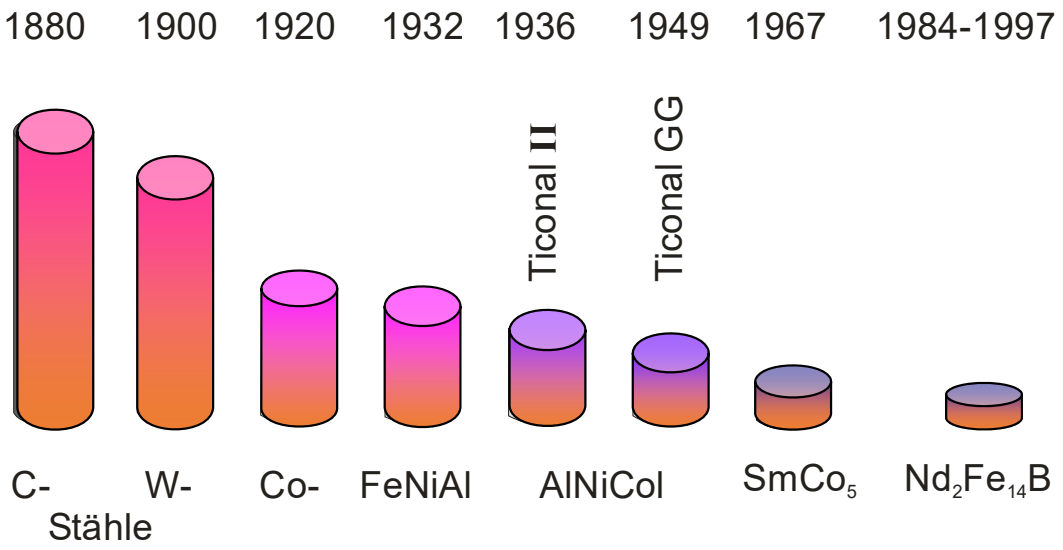
Some examples for “modern” magnetism applications!

- Supermagnets



www.helbling.ch



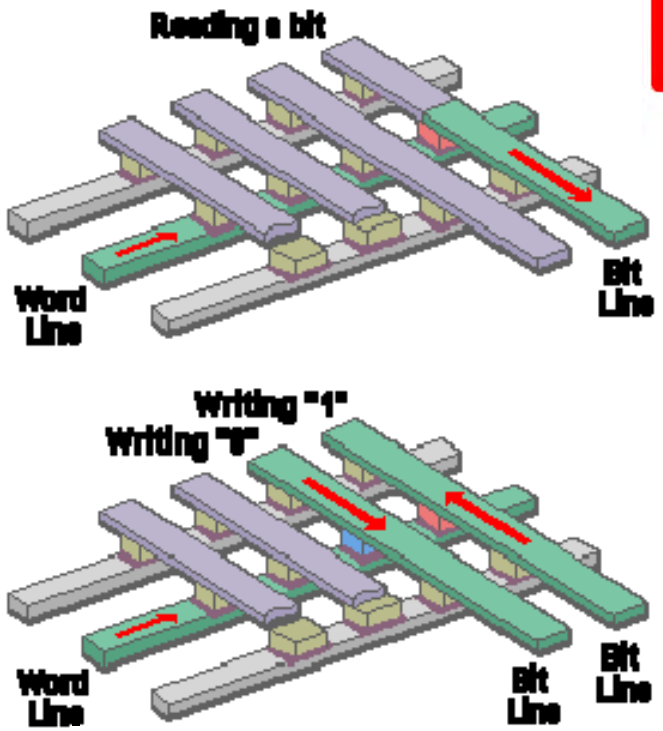


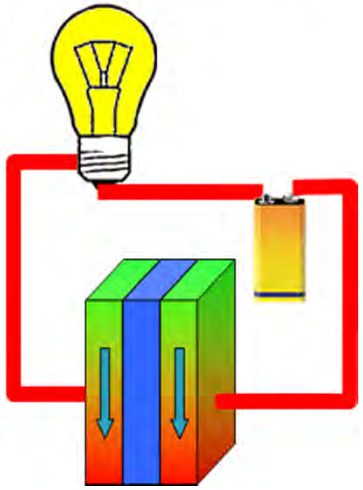
Low weight and high field = forces
Optimizing interaction strength between lattice and magnetic moments ➔ orbital moments

Important to know:
What is the magnetism of each element?
Nd? Fe? Co? Sm?....

Some examples for “modern” magnetism applications!

- Data storage





„Perpendicular Recording“

NdFeB-Servo-Motor

Optimizing interaction strength between lattice and magnetic moments
➔ orbital moments
permanent magnets, magnetostriction, spin wave damping, etc. etc.

Why X-rays and magnetism?

- It is important to know spin and orbital moments
- for each element in the system separately
- contact areas are important ➔ probing single atomic layers and separating them from others

- We know: X-rays provide significant spatial resolution on the atomic scale

- Your will see here how this is transferred to magnetism using X-ray Magnetic Circular Dichroism (XMCD)
- Or in other words: XMCD is able to transfer **ANY** X-ray technique in it's magnetic counterpart!

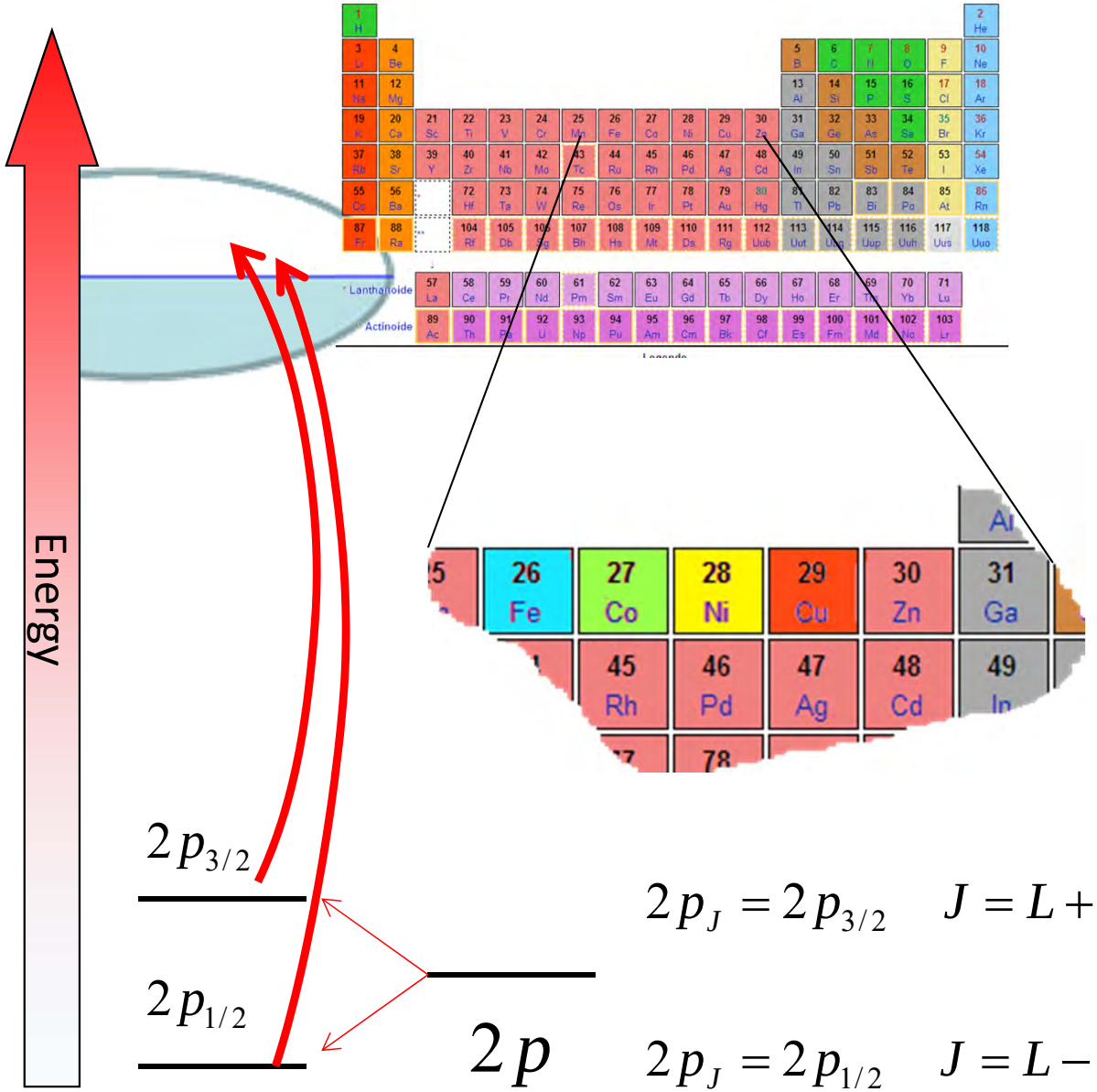
Now XAS

- X-ray absorption spectroscopy XAS
  - Dipole selection rules provide “wanted projections”
    - symmetry selective
  - Electric field vector can provide orbital occupation and orientation

- Further Examples:
  - Gas on a surface ➔ Chemistry and binding orientation
  - Valence and Band structure determination (unoccupied of cause)

Why XAS!

One famous example (also for magnetism): 2p ➔ 3d



- X-ray absorption spectroscopy (XAS)
  - dipole selection rules

$$m' = m + q$$

$$l' = l \pm 1$$

  - probing 3d magnetism 2p ➔ 3d
  - probing 4f magnetism 3d ➔ 4f

$$2p_J = 2p_{3/2} \quad J = L + S = 1 + 1/2$$

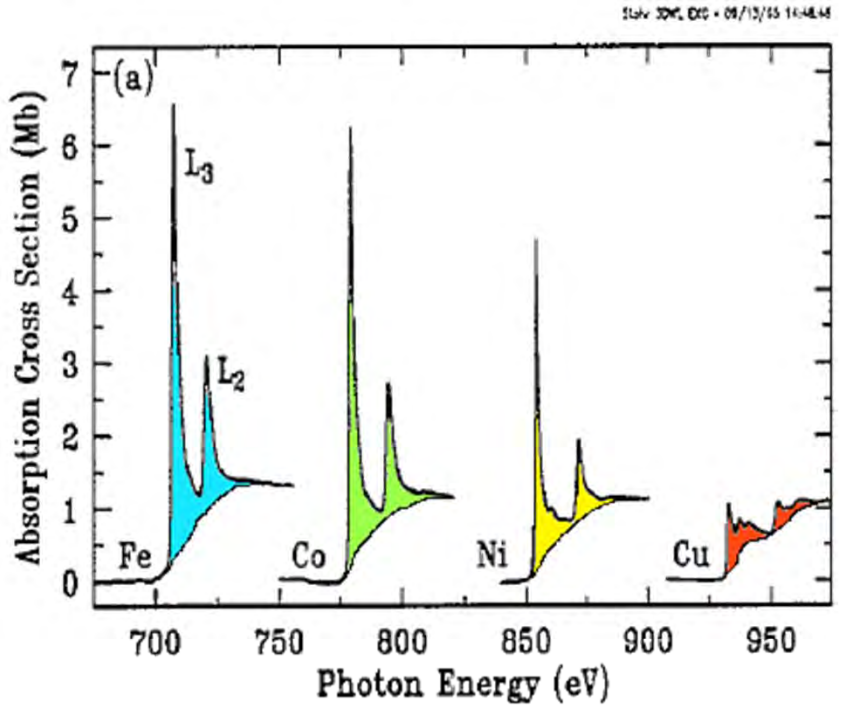
$$2p_J = 2p_{1/2} \quad J = L - S = 1 - 1/2$$

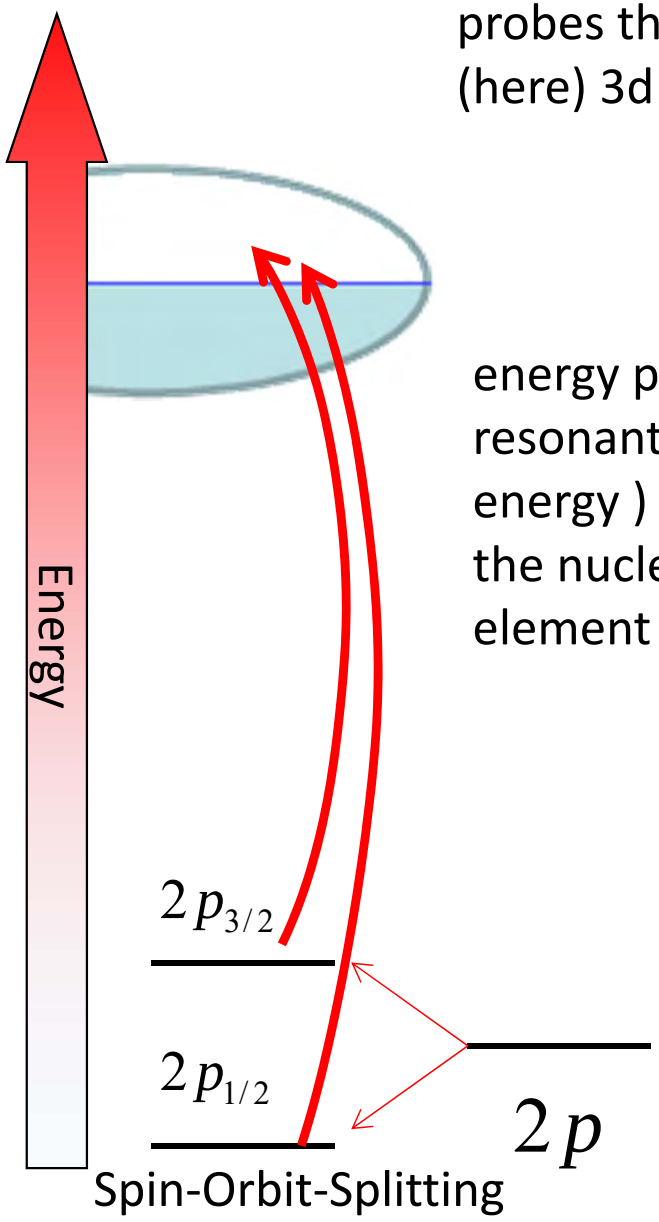
XAS: In resonance very strong effects

One famous example (also for magnetism): 2p ➔ 3d

probes the **unoccupied** (here) 3d electrons ➔ holes

energy position of the resonant spectra (binding energy) depends strongly on the nuclear charge➔ element specific!





All is based on Fermi's Golden Rule!

- It provides the probability $W_{ba} = \frac{\mathrm{d}}{\mathrm{dt}}\left|c_b^{(1)}(t)\right|^2$ to excite an electron from the initial state $|\psi_i\rangle$ to the final state $|\psi_f\rangle$

$$\text{Fermi's Golden Rule:} \quad W_{fi} = \frac{2\pi}{\hbar}\left|\langle\psi_f|H_{phot}|\psi_i\rangle\right|^2 \cdot \delta(E_f - E_i - \hbar\omega)$$

$$\text{The total Hamiltonian is:} \quad \mathrm{H}_{\mathrm{tot}} = H_0 + H_{phot}(t)$$

Based on time dependent pertbation theory

Time integral ➔ "Energy-Conserving- Deltafunction"

What have we learned so far?
XAS because ..

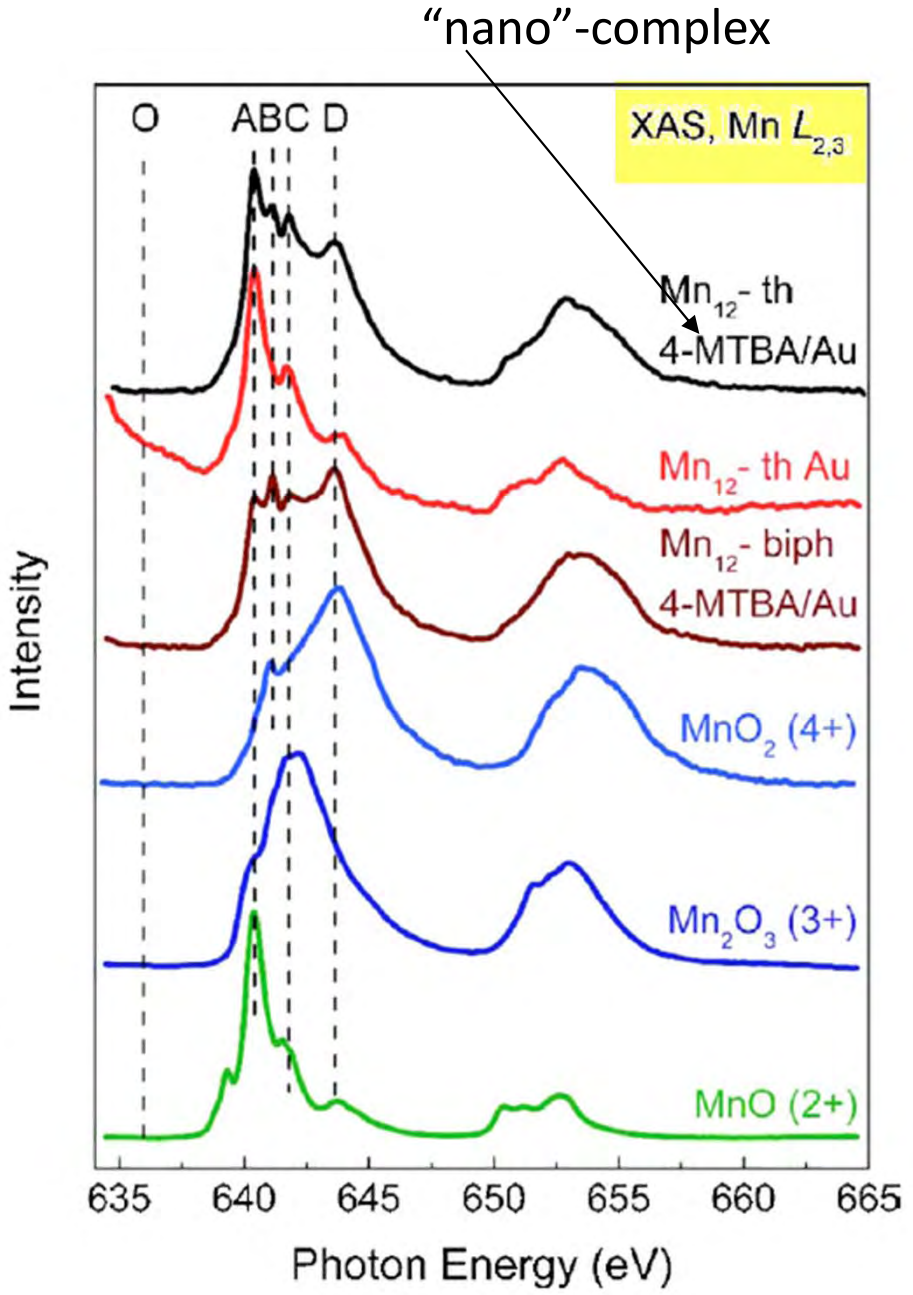
- it probes unoccupied states
- element specific due to energy position
- symmetry selective due to selection rules p → d

What else?

Good for chemistry and band structure determination

- Example: Mn $L_{2,3}$ 2p➔3d
  - different oxidization states
  - shape provides important information about the unoccupied density of states
  - some less clear chemical shift observable
    - reason: also the initial (here 2p) **and** the final states (here 3d) are shifted
  - details often complicated, due to electron-electron-interaction and so called *"multiplet effects"*

    (not discussed here)

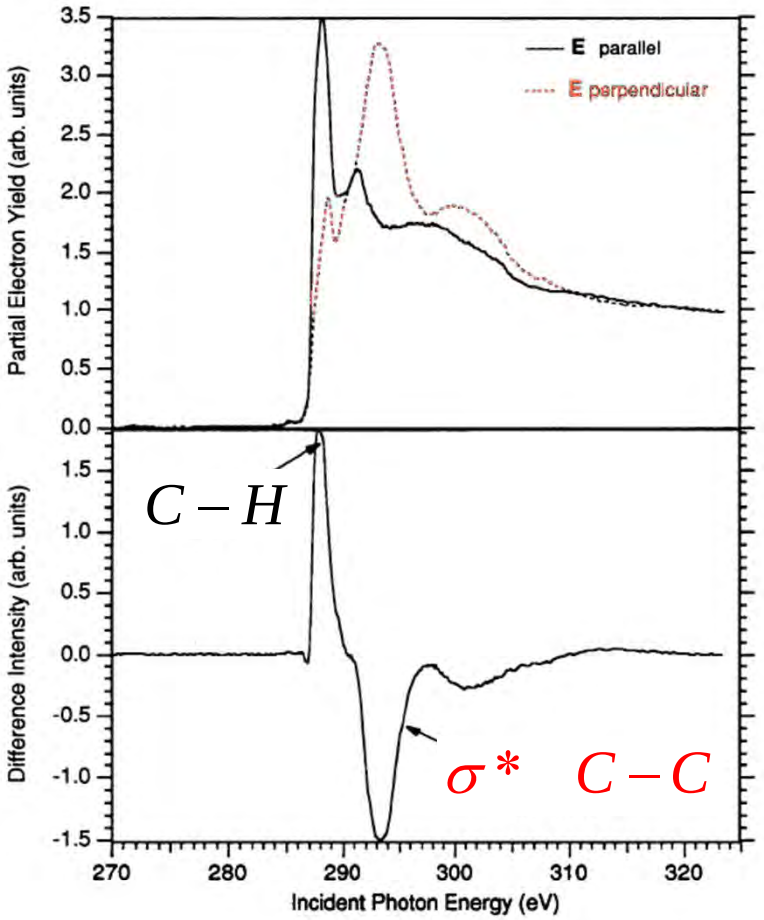


source: **PHYSICAL REVIEW B** Volume: **75** Issue: **4** Article Number: **045102**

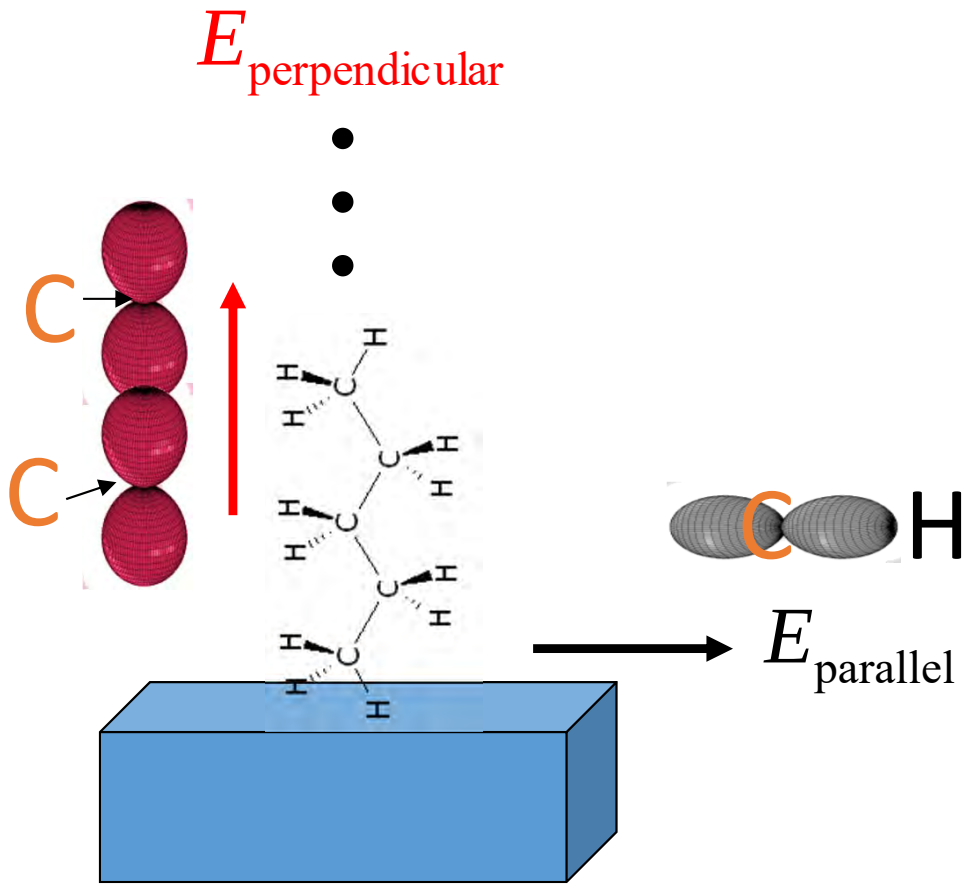
Hexadecane $C_{16}H_{34}$ on a Cu surface

- Molecular orientation on the surface

This also works nicely in anisotropic single crystals



C 1s ➔ 2p



Tilt angle determined by the angular dependency of the XAS spectra

Source: D.A.Fischer Tribology Letter 3 (1997) 41

XAS: How to measure X-ray Absorption Spectroscopy

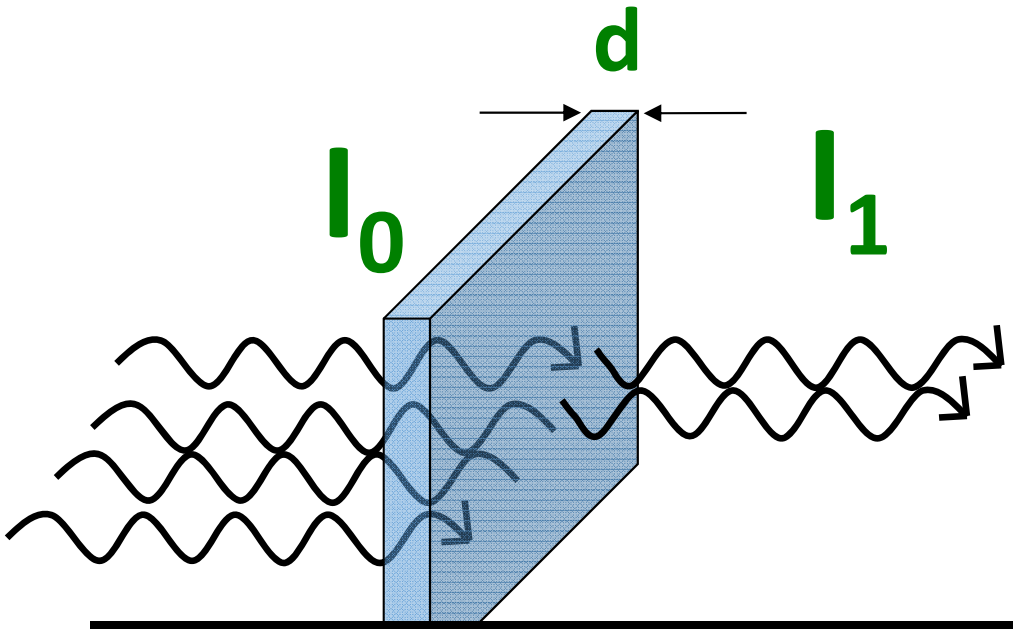
Lambert-Beer-Law:

$$I(E_{phot}) = I_0 \cdot e^{-\mu(E)\cdot d}$$

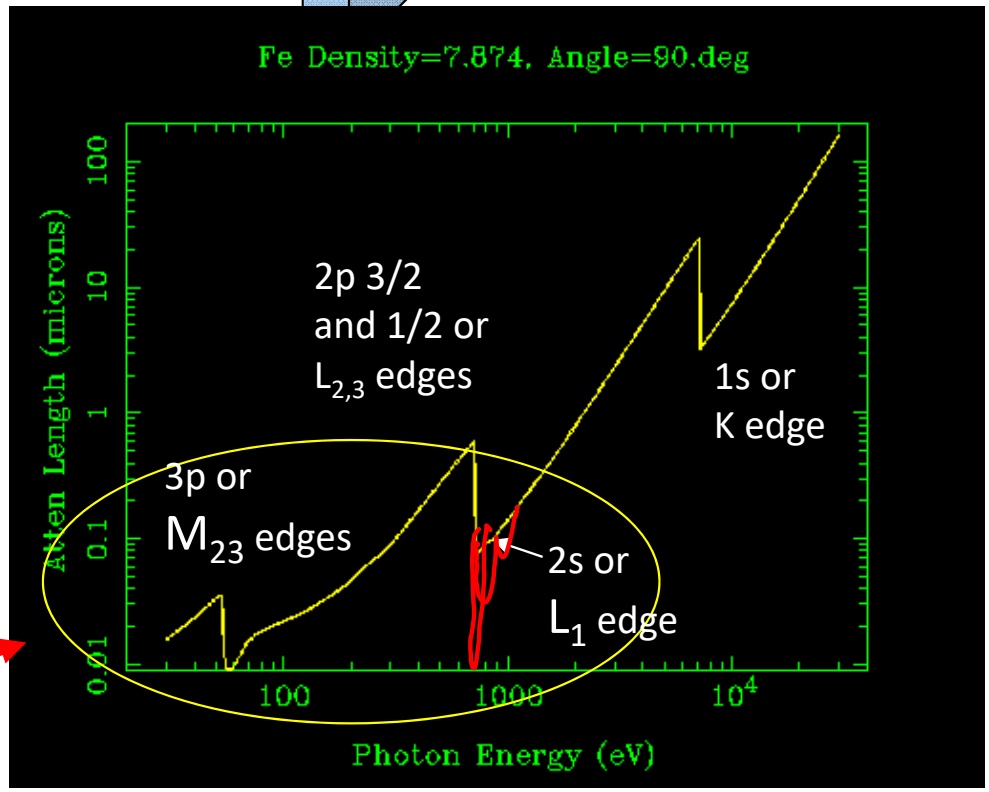
$$\Leftrightarrow \mu(E) = \frac{1}{d} \cdot \ln \frac{I_0}{I(E_{phot})}$$

$$\xi = \frac{1}{\mu(E)} = \text{attenuation length,}$$

i.e. the length for 1/e intensity



Example: Fe metal
(calculation without resonances and spin –orbit-splitting)



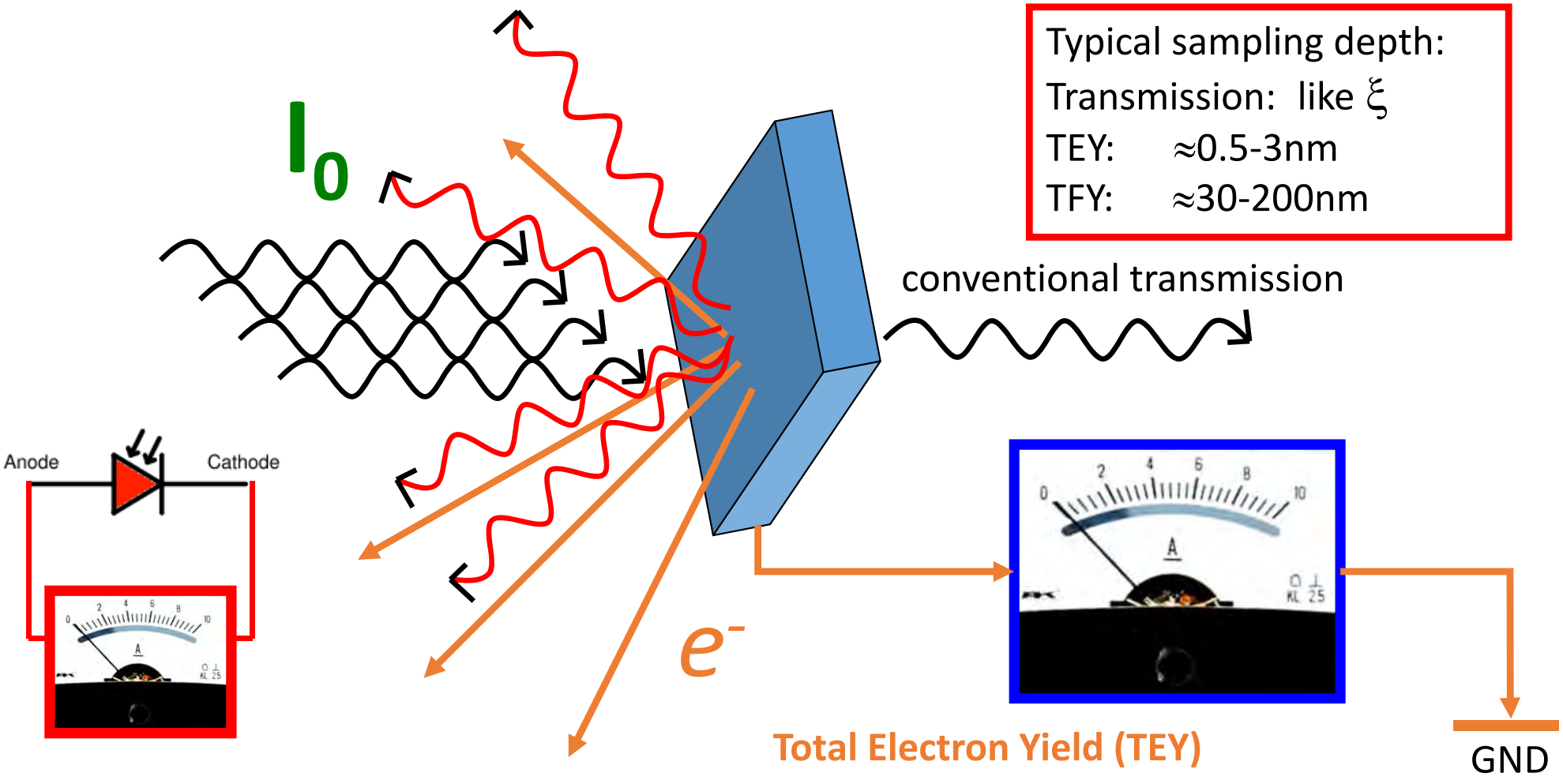
Hard to measure below 3-5keV,
due to the very short attenuation length
➔ Other techniques to measure the absorption

source: http://henke.lbl.gov/optical_constants/

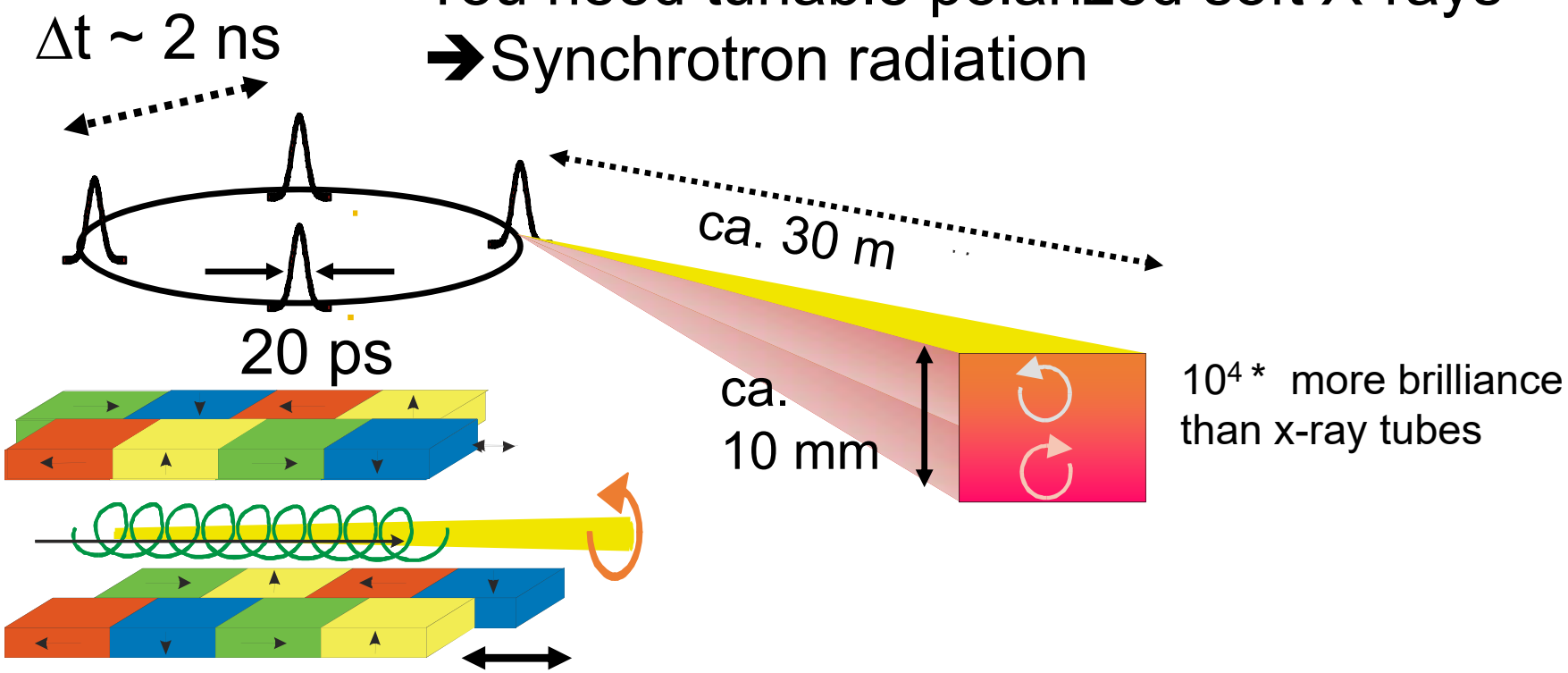
The absorption coefficient is often measured indirectly

- Example: Soft X-rays ~ 50-2000eV

Idea: Every additionally absorbed photon, for example due to the 2p➔3d transition, produce additional electrons (Photo el., AUGER and **secondaries**) and **fluorescence photons**
higher absorption ➔ more electrons (fluorescence photons)



You need tunable polarized soft X-rays
➔Synchrotron radiation

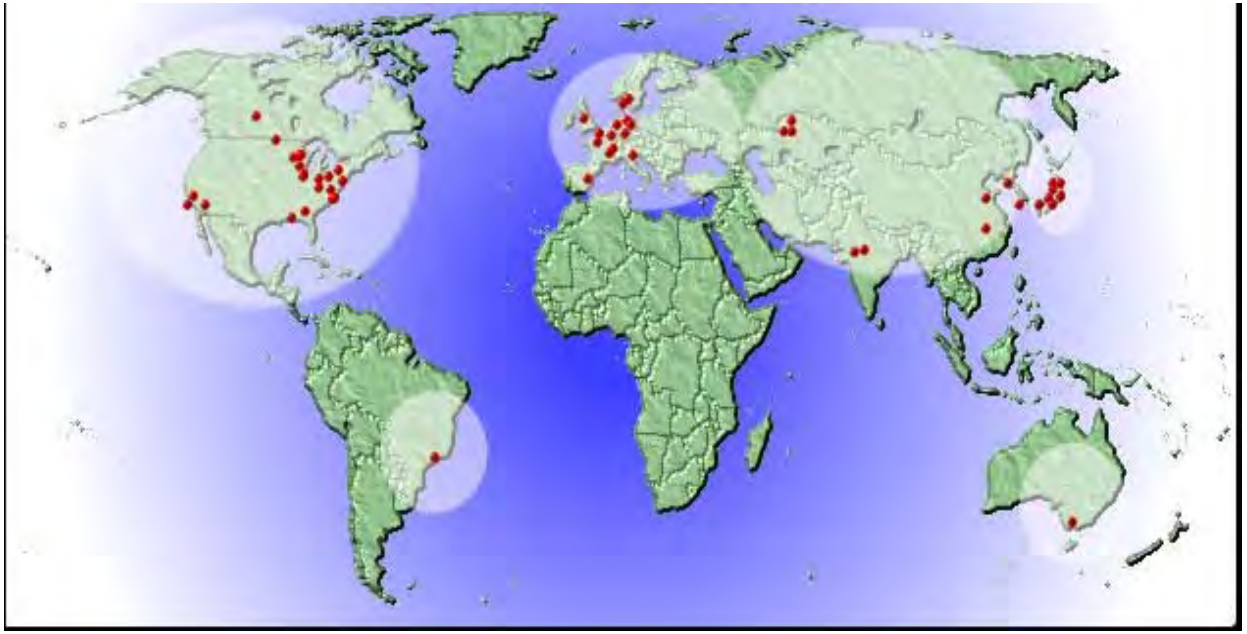


10^4 * more brilliance than x-ray tubes

Helical Undulator

10^8 x more brilliance than x-ray tubes

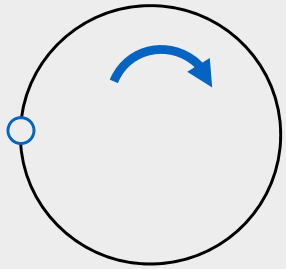
Global Synchrotron Density



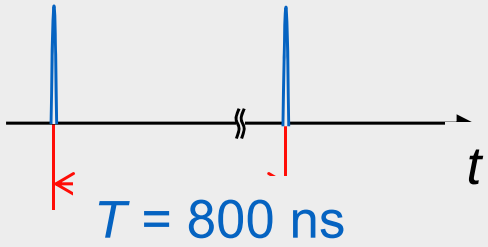
For dynamic investigations ➔ time structure of synchrotron radiation

Pulse width down to 10 psec

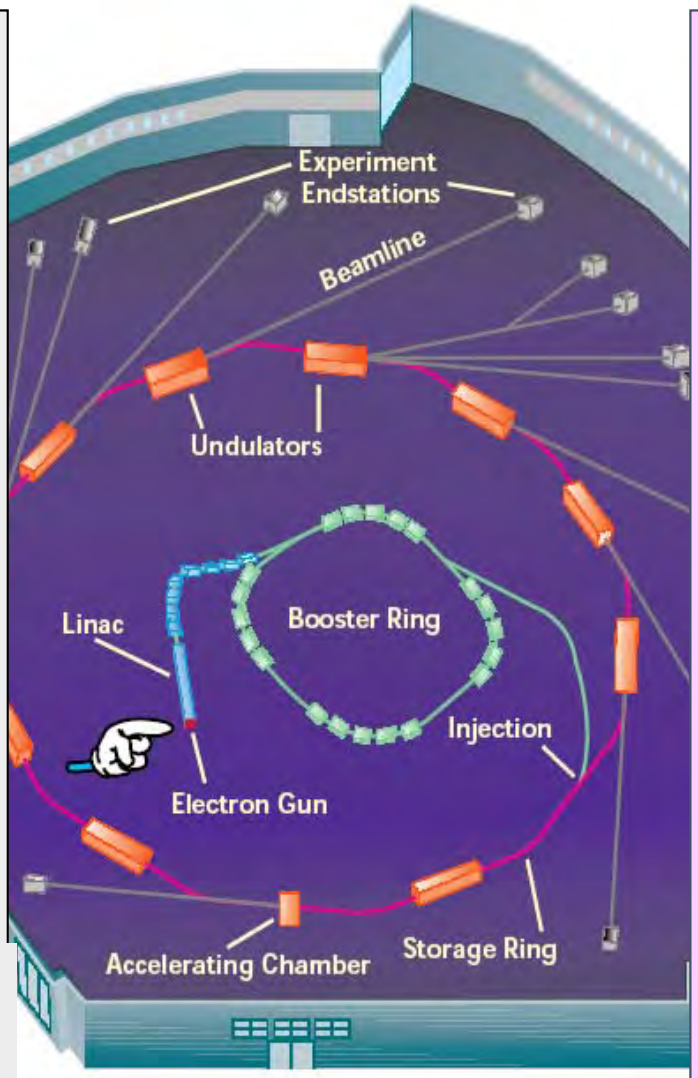
Single Bunch Mode



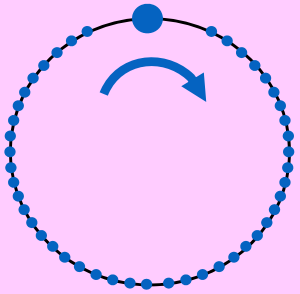
I = <25 mA



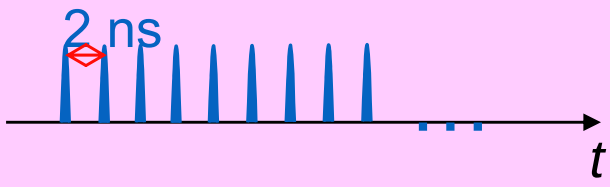
available only for 2 x 2 weeks/a



multi-bunch mode:
348 buckets (~ 0.75 mA)
+ “camshaft” (~ 10 mA)



I = 200-300 mA



standard operation mode

Now we go for Magnetism

- As magnetism is related to angular motion, why not using an “angular” probe?
- We will use circular polarized X-rays!

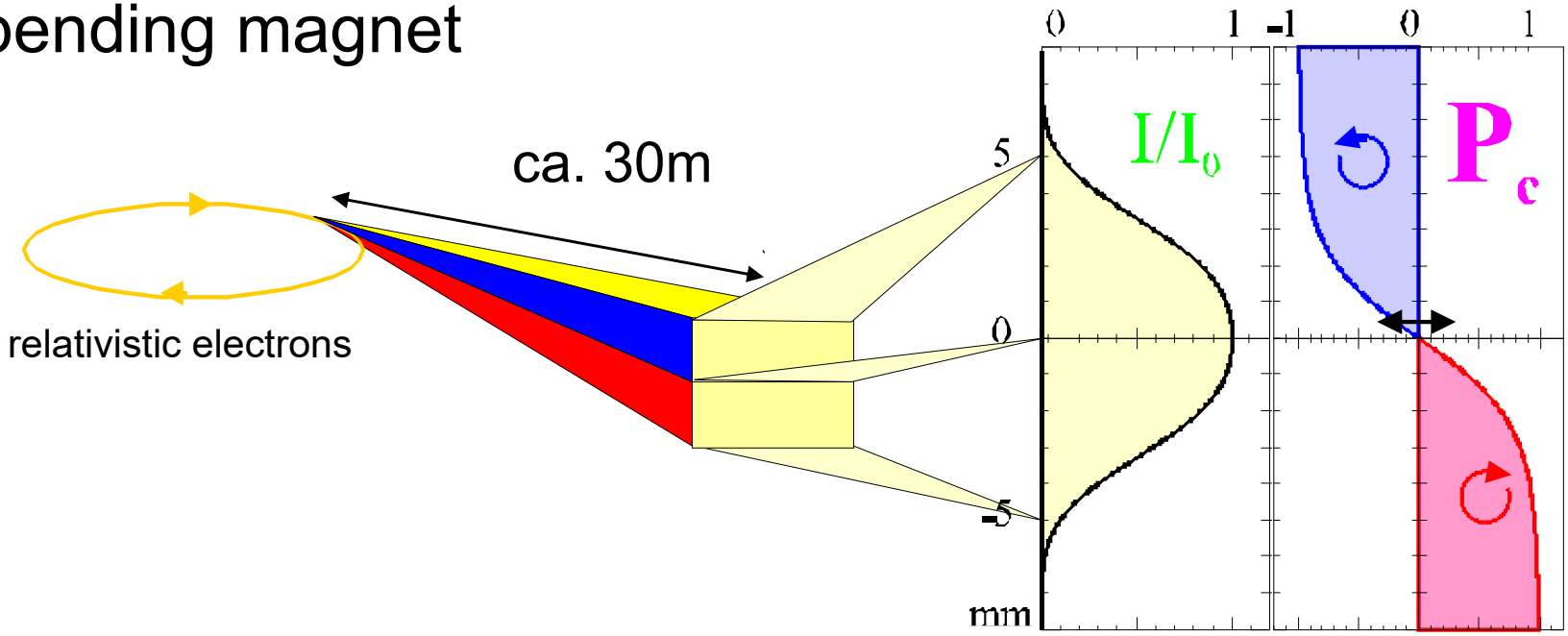
XMCD: X-ray Magnetic Circular Dichroism

- In other words: Sample magnetization changes the absorption of X-rays
  - Sometimes a rather dramatic effect
- Pathway
  - What is XMCD?
  - How does it look like? Example: Fe Metal
  - How is it used? Quantitative! ➔ sum rules
  - Can we understand this? Somehow!

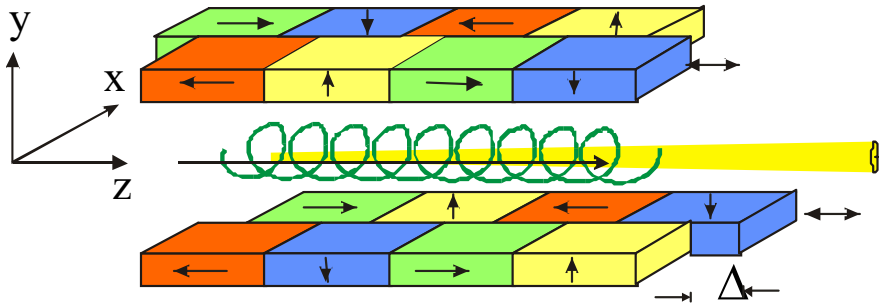
Actually: First observed by Gisela Schütz in 1987
Director MPI for Intelligent Systems

Again: How to get polarized X-rays?

1. bending magnet



2. Undulator

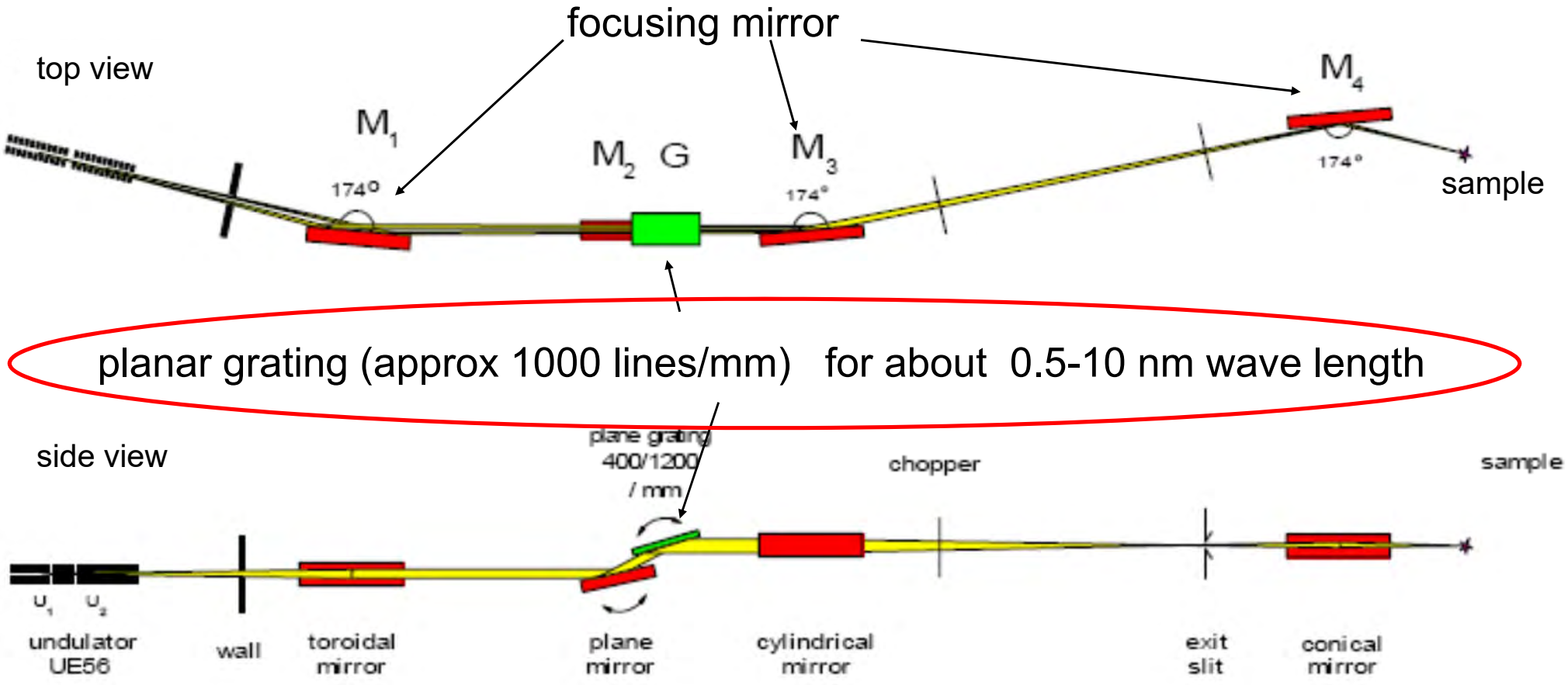


approx. 1000 times higher brilliance

We also need „optical“ components

How does it look exactly for soft x-rays

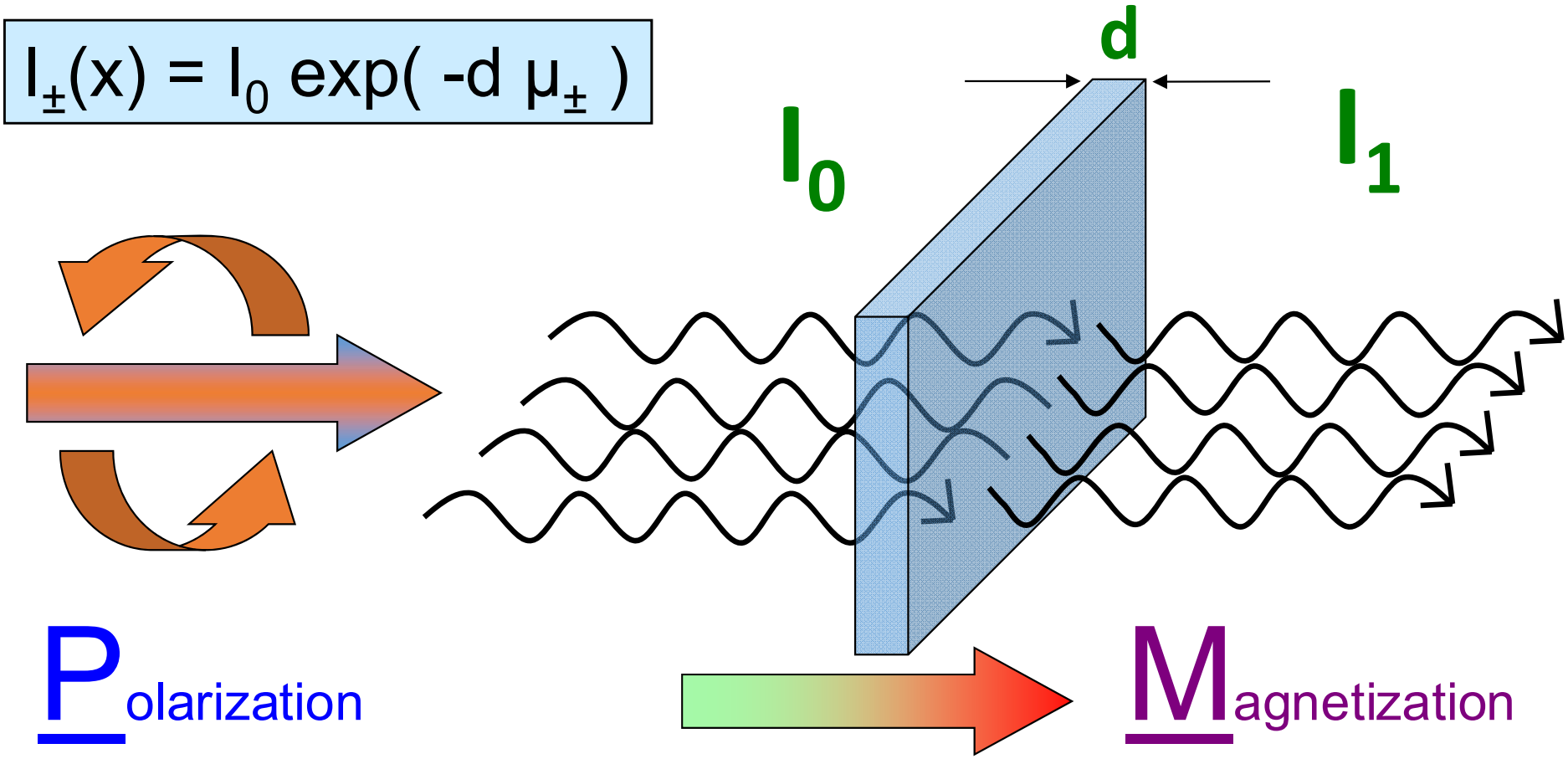
- typical setup for soft x-rays (100-2000eV)



Ultra-High-Vacuum! $\approx 10^{-10}$ mBar

Measurement of the absorption coefficient μ ➔ now depending on the sample magnetization

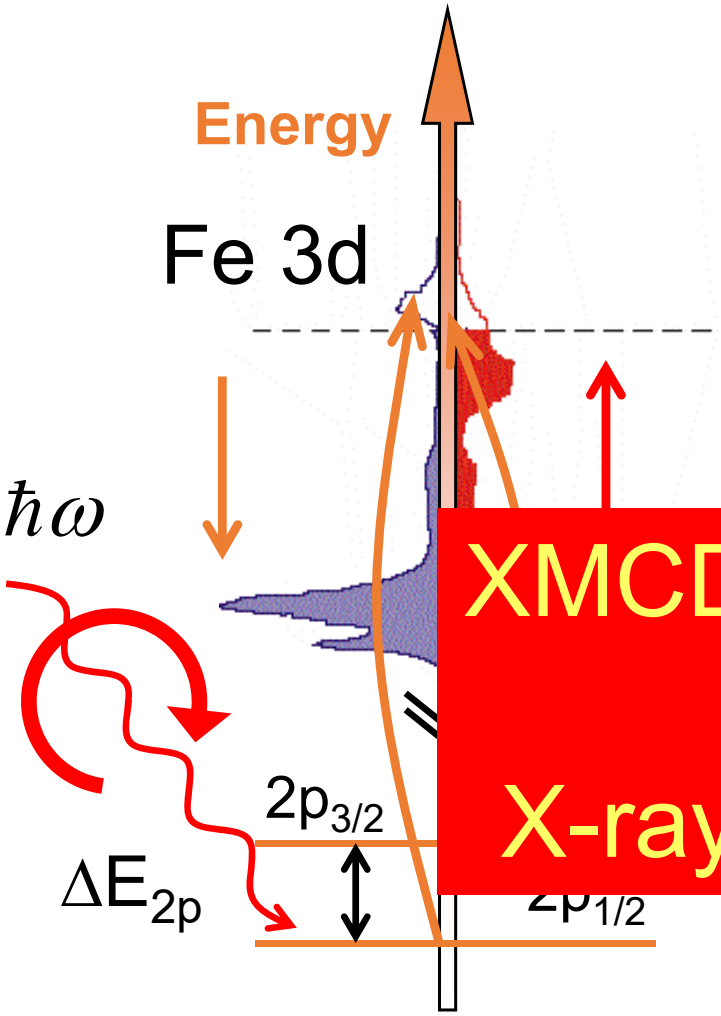
$I_{\pm}(x) = I_0 \exp(-d \mu_{\pm})$



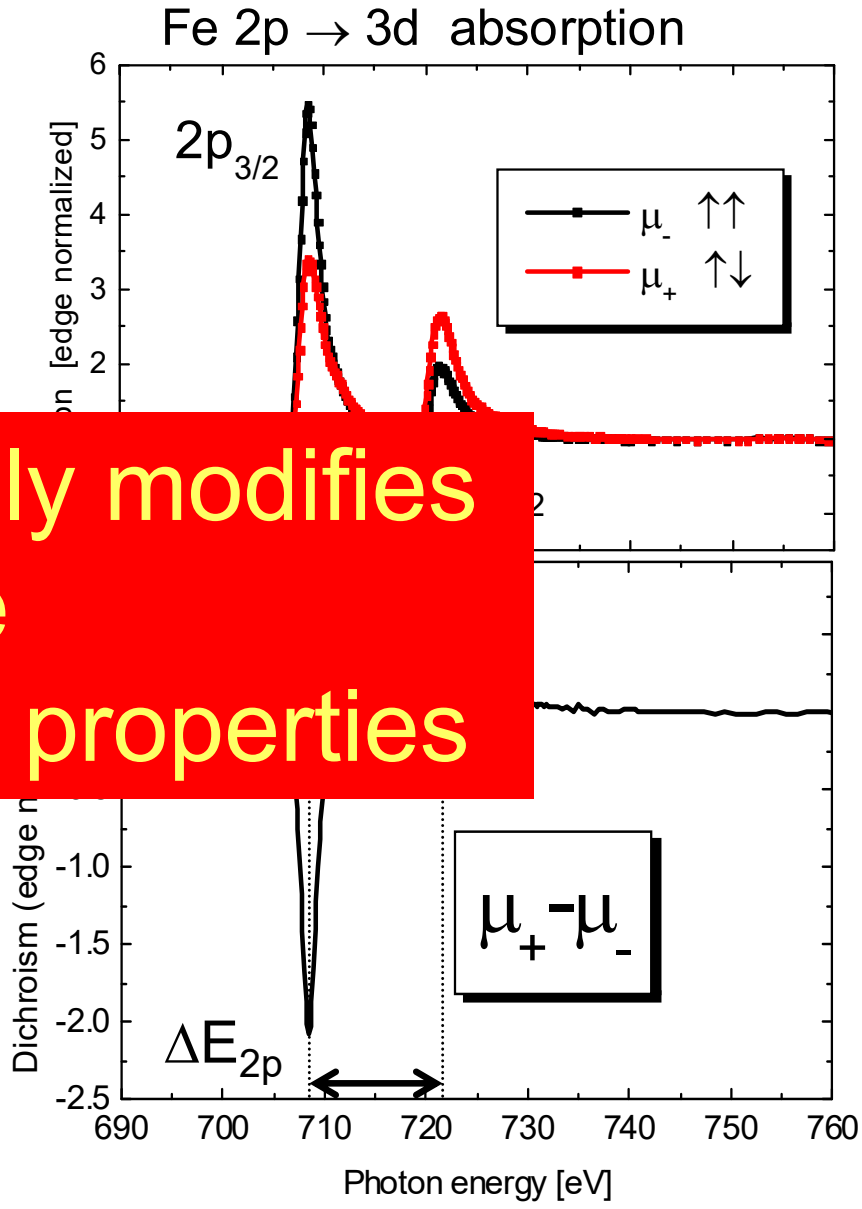
Measured quantity: $\Delta\mu = \mu^+ - \mu^- \sim \Delta(P \cdot M)$

X-ray magnetic circular dichroism: XMCD

XMCD: element specific, as XAS is!



XMCD strongly modifies the X-ray optical properties



- Element specific, due to the defined energy of the absorption edges!
- Magnetism has a strong impact on the absorption coefficient!

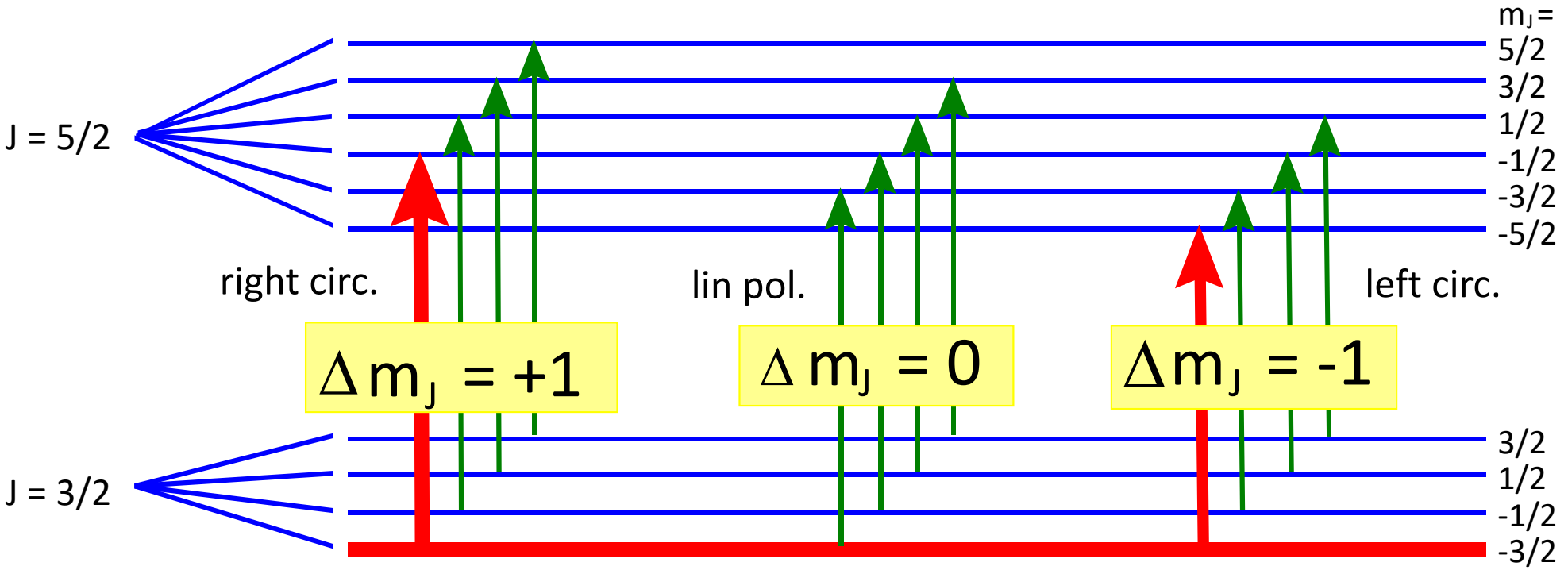
Magneto-Optic-Effects: Origin (also for XMCD :=)

Start: Hunds rules Groundstate: Simplest example $3d^1$

L = 2 ; S = ½ and J = L - S = 3/2

For **T➔ 0 and B ➔** ∞ only $m_J = -2 + 1/2 = -3/2$ is occupied (saturated)

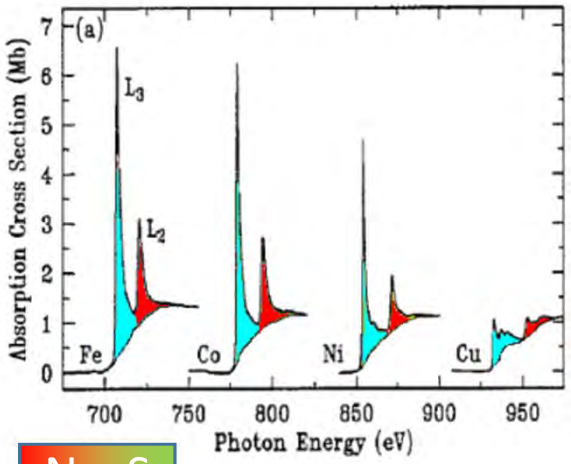
Dipole-Selection-Rules: $\Delta l = \pm 1$ ➔ circular Pol.: $\Delta m_J = \pm 1$



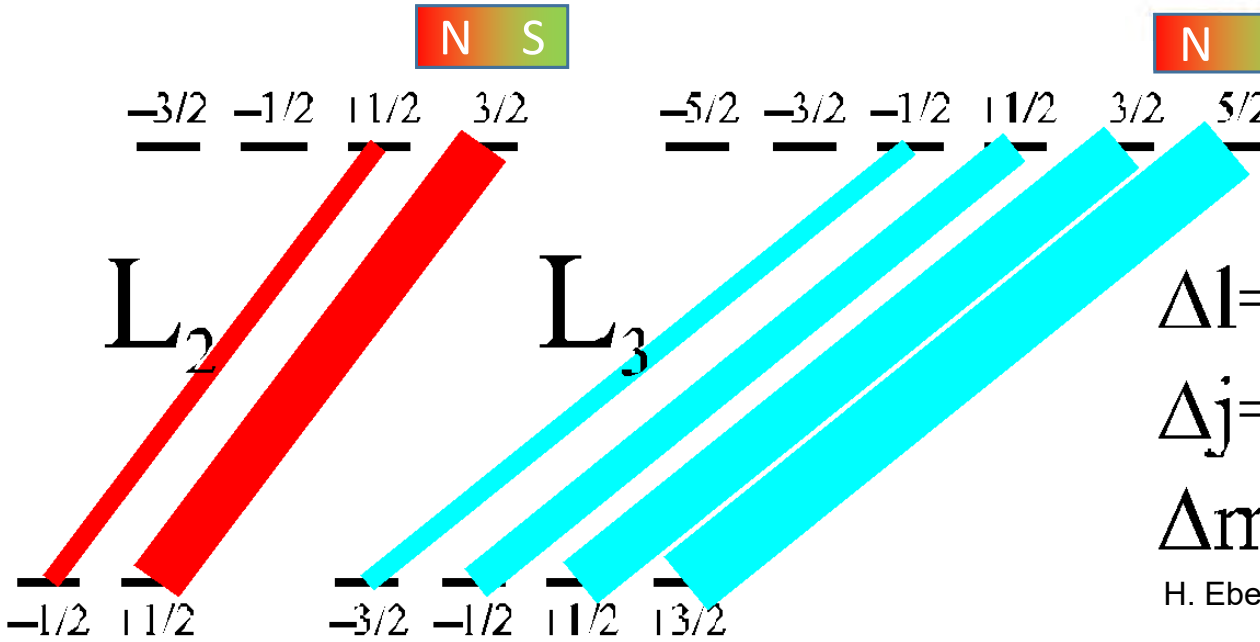
- This is a very general approach!
- Could be done in resonance or off resonance

Take home message:
For circular polarization absorption is modified by magnetism!

This is how the L2 and L3 edge excitations are using **right** circular polarized light!



- Schematics of the excitation:S



$\Delta l = +1$

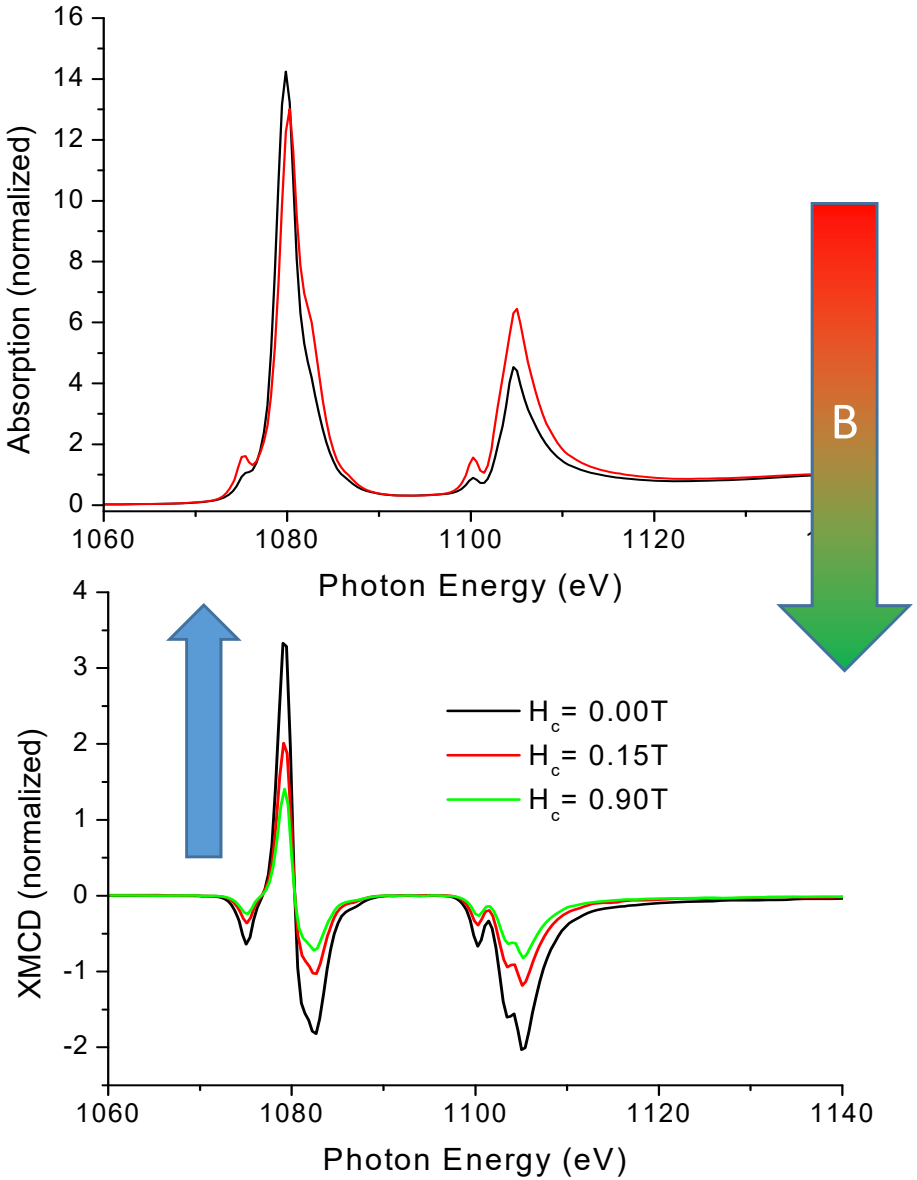
$\Delta j = 0, \pm 1$

$\Delta m = +1$

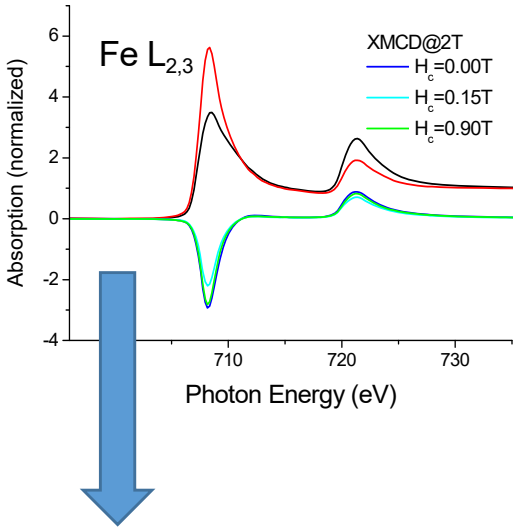
H. Ebert, Rep. Prog. Phys. **59**, 1996

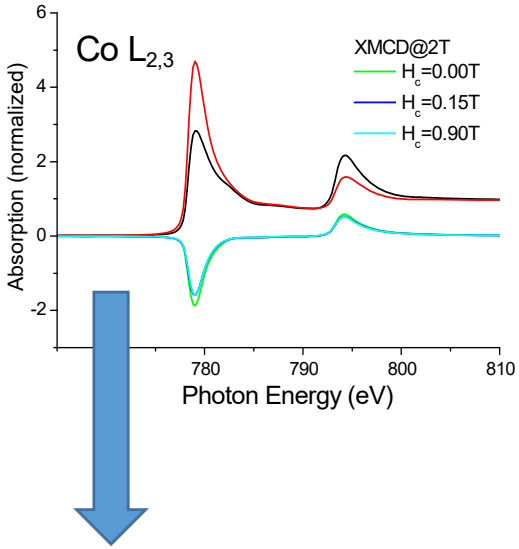
Flipping the magnetization gives different excitation probabilities

One example: $SmCo_5$ doped with some Fe



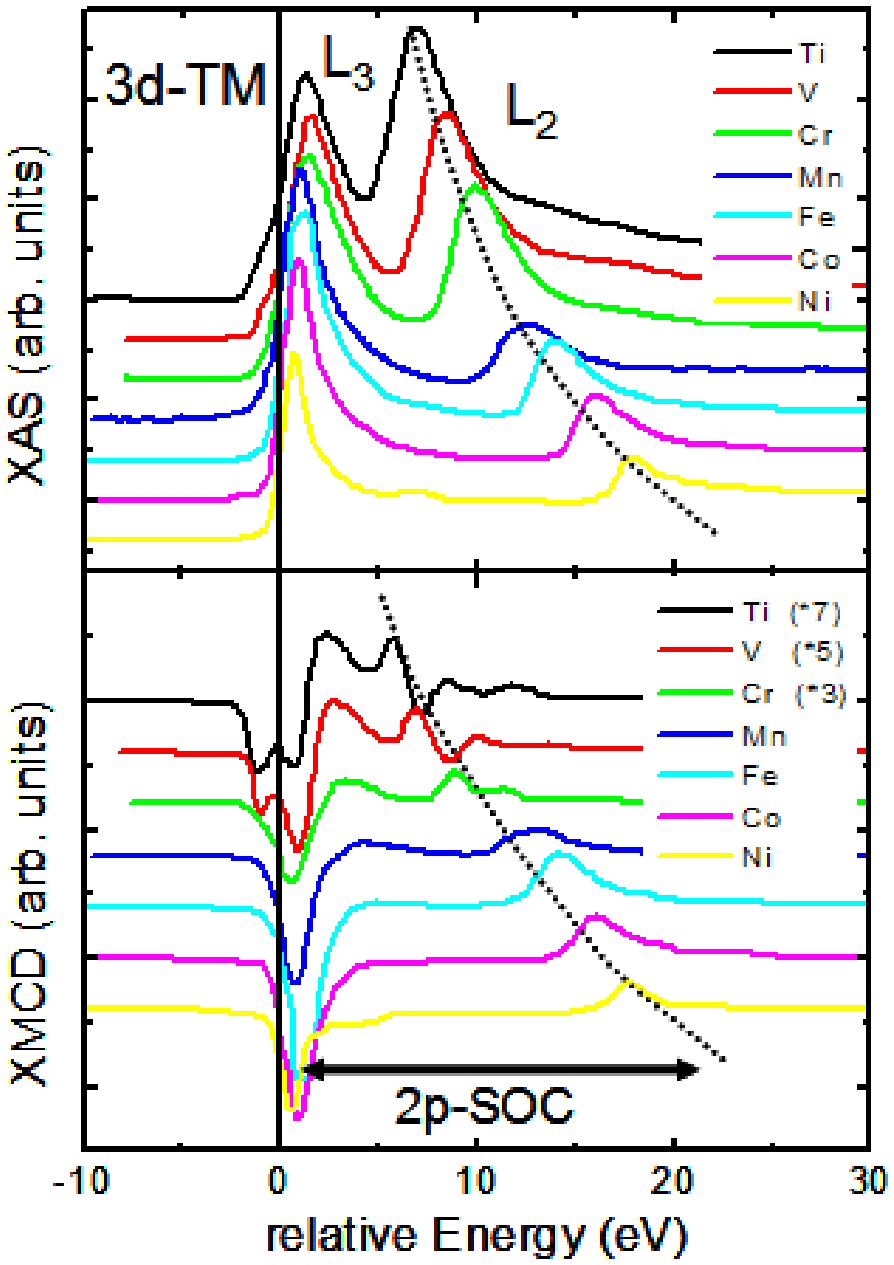
- The magnetic moment of each element could be extracted separately
- Good for the understanding of magnetism in complex systems
- Sample has been modified to change the coercive behavior ➔ Sm is responsible for that!





Schütz, Goering, Stoll, Int. J. Mat. Sci. **102** (2011) 773

XMCD in 3d Transition Elements



Spin orbit splitting of 2p shell decreases from Cu to Ti
Width increase ➔ more unoccupied electrons

Now it happens: Sum rules

X-Ray Circular Dichroism and Local Magnetic Fields

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[2]*Department of Chemical Physics, Materials Science Center, University of Groningen, Nijenborgh 16, 9747 AG Groningen, The Netherlands*
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(Received 13 July 1992)

Sum rules are derived for the circular dichroic response of a core line (CMXD). They relate the intensity of the CMXD signal to the ground-state expectation value of the magnetic field operators (orbital, spin, and magnetic dipole) of the valence electrons. The results obtained are discussed and tested for transition metals and rare earths.

PACS numbers: 78.70.Dm, 78.20.Ls

For circular dichroism in the x-ray region (CMXD), Thole *et al.* [1] have recently derived a new magneto-optical sum rule. It shows that, to a good approximation, the intensity of the CMXD signal, integrated over a complete core-level edge of a ferromagnet (or ferrimagnet), is proportional to the ground-state expectation value of the orbital angular momentum operator L_z. The derivation was carried out for electric dipole transitions in a localized model, considering a single ion in a crystal-field symmetry and including effects.

In this Letter we show that, within the work, another sum rule can be obtained. CMXD signal, integrated over a single partner orbit-split core-level edge, to the ground-state value of the operators (L_z, total spin S_z, and pole $[\sum_l \mathbf{s}_l - 3\hat{\mathbf{r}}_l(\hat{\mathbf{r}}_l\cdot\mathbf{s}_l)]_z$) that describe the magnetic field generated by the valence electrons. Our results indicate that, besides $\langle L_z\rangle$, as described in Ref. [1], CMXD spectroscopy can provide an independent determination of the ground-state expectation value of S_z [2]; this has been tested using CMXD data, taken at the $L_{2,3}$ edges of the ferromagnetic metals Fe, Co, and Ni [3]. Furthermore, valuable site-specific information on the magnetic anisot-

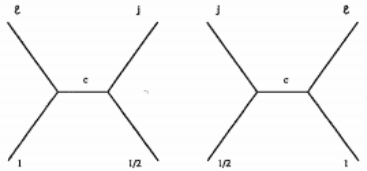
$$\langle\Psi|rC_q^{(1)}|\Psi' jm\rangle = \sum_{\lambda\sigma}\langle\Psi|c^\dagger_{jm}l_{\lambda\sigma}|\Psi' jm\rangle\langle cjm$$
$$= \sum_{\lambda\sigma}\langle\Psi|c^\dagger_{jm}l_{\lambda\sigma}c_{jm}|\Psi'\rangle$$
$$\times\sum_\gamma(-)^{m-\gamma-1/2}\begin{pmatrix}1/2 & & \\ \sigma & & \end{pmatrix}$$

The notation is as follows: $c^\dagger_{jm}$ and $l^\dagger_{\lambda\sigma}$ repr denotes a normalized spherical harmonic; $[j]$ tion; and $P_{cl}=\langle c||C^{(1)}||l\rangle R_{cl}$. The total inte

$$I^j = \sum_{\Psi' m\lambda\sigma\lambda'\sigma'}\langle\Psi|c^\dagger_{jm}l_{\lambda\sigma}|\Psi'\rangle\langle\Psi'|c^\dagger_{jm}l^\dagger_{\lambda'\sigma'}c_{jm}|\Psi\rangle[j]\sum_{\gamma\gamma'}\begin{pmatrix}1/2 & c & j\\ \sigma & \gamma & m\end{pmatrix}\begin{pmatrix}c & 1 & l\\ \gamma & q & \lambda\end{pmatrix}\begin{pmatrix}c & 1 & l\\ \gamma' & q & \lambda'\end{pmatrix}\begin{pmatrix}1/2 & c & j\\ \sigma' & \gamma' & m\end{pmatrix}P_{cl}^2 . \quad (2)$$

In this expression, the final states can be removed by extending the set $|\Psi'\rangle$ to the whole Hilbert space and using the closure relation. The added states give no contribution to I^j. Then, using a standard graphical notation for the angular factor [4], we have

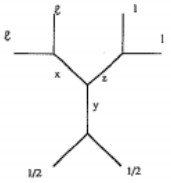
$$I^j = \sum_{m\lambda\sigma\lambda'\sigma'}\langle\Psi|c^\dagger_{jm}l_{\lambda\sigma}c_{jm}c^\dagger_{jm}l^\dagger_{\lambda'\sigma'}c_{jm}|\Psi\rangle[j]$$

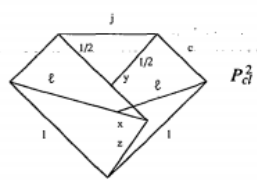


$$P_{cl}^2 . \quad (3)$$

Transforming the diagonal matrix element by means of $\{c^\dagger_{jm},c_{jm}\}=1$ and recoupling the angular part to obtain coupled tensor operators, one has the following:

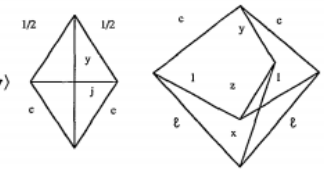
$$I^j = \sum_{\lambda\sigma\lambda'\sigma'}\langle\Psi|1-l^\dagger_{\lambda\sigma}l_{\lambda'\sigma'}|\Psi\rangle[j]\sum_{xyz}[xyz]$$





P_{cl}^2

$$= \left\{\frac{[j]}{[1c]} + [j]\sum_{xyz}[xyz]^{1/2}\langle\Psi|W_0^{(xy)z}|\Psi\rangle\right\}$$



$$P_{cl}^2 , \quad (4)$$

with $[a\cdots b]=(2a+1)\cdots(2b+1)$. On the basis of expression (4) one can see that the total intensity I^j of the j edge is given by the ground-state expectation value of a linear combination of double tensors $W^{(xy)z}$, as defined by Judd [5]. of the triads $(l\times l)$, $(1/2\ y\ 1/2)$, and

circular dichroism and the CMXD

$$\frac{(c+1)-2}{+1)}\langle\Psi|S_z|\Psi\rangle$$

$$-\langle\Psi|T_z|\Psi\rangle\Big\}(P_{cl}^{\pm})^2 , \quad (5)$$

ion coefficient.

artly filled spectator shell [1]; it can

In both cases only the l shell contributes to $\langle L_z\rangle$, $\langle S_z\rangle$, and $\langle T_z\rangle$ (shell selectivity).

On the basis of our findings, one can view CMXD spectroscopy as a probe of the magnetic field of the valence electrons. The probe is *shell specific*; furthermore, the orbital and spin contributions can be separated: (i) Adding the two partners of a spin-orbit-split edge and normalizing to the unpolarized x-ray-absorption spectroscopy spectrum, one has

$$\rho = \int_{j_+ + j_-} d\omega(\mu^+ - \mu^-)\Big/\int_{j_+ + j_-} d\omega(\mu^+ + \mu^- + \mu^0) = \frac{1}{2}\frac{l(l+1)+2-c(c+1)}{l(l+1)(4l+2-n)}\langle L_z\rangle , \quad (6)$$

yielding the ground-state expectation value of the orbital angular momentum per hole [1,6]. (ii) The ground-state expectation value of the spin-dependent part of the local magnetic field per hole is given by

$$\delta = \frac{\int_{j_+} d\omega(\mu^+ - \mu^-) - [(c+1)/c]\int_{j_-} d\omega(\mu^+ - \mu^-)}{\int_{j_+ + j_-} d\omega(\mu^+ + \mu^- + \mu^0)}$$
$$= \frac{l(l+1)-2-c(c+1)}{3c(4l+2-n)}\langle S_z\rangle + \frac{l(l+1)[l(l+1)+2c(c+1)+4]-3(c-1)^2(c+2)^2}{6lc(l+1)(4l+2-n)}\langle T_z\rangle . \quad (7)$$

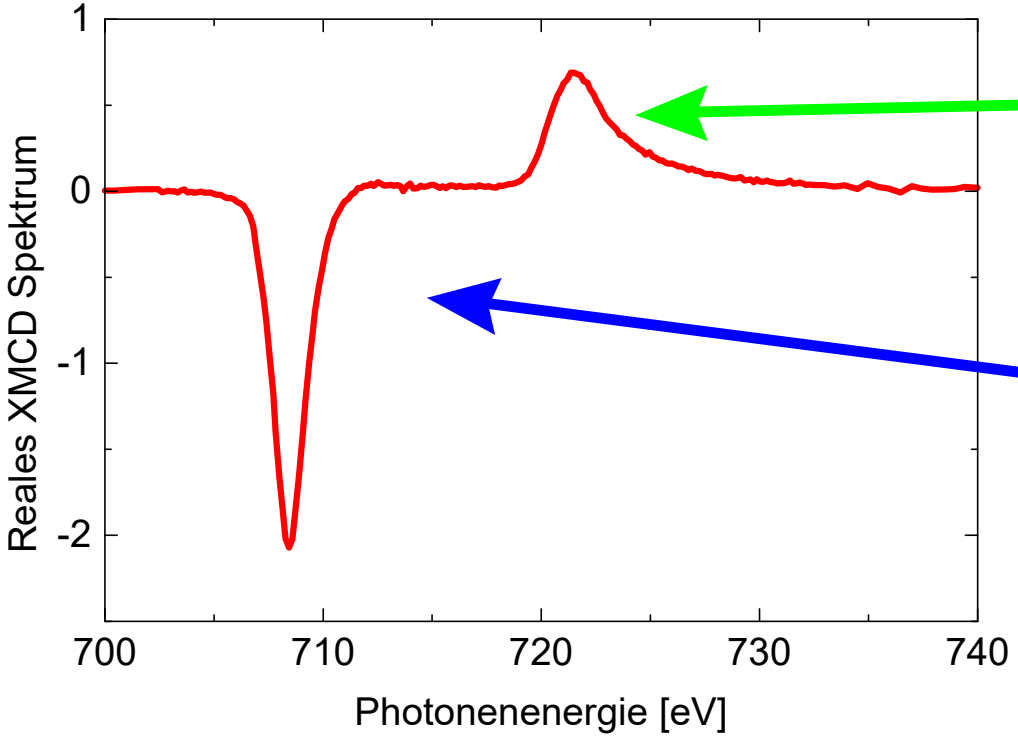
To obtain expressions (6) and (7) we neglected relativistic corrections to the radial part and set $P_{cl}^+ = P_{cl}^-$; this approxi-

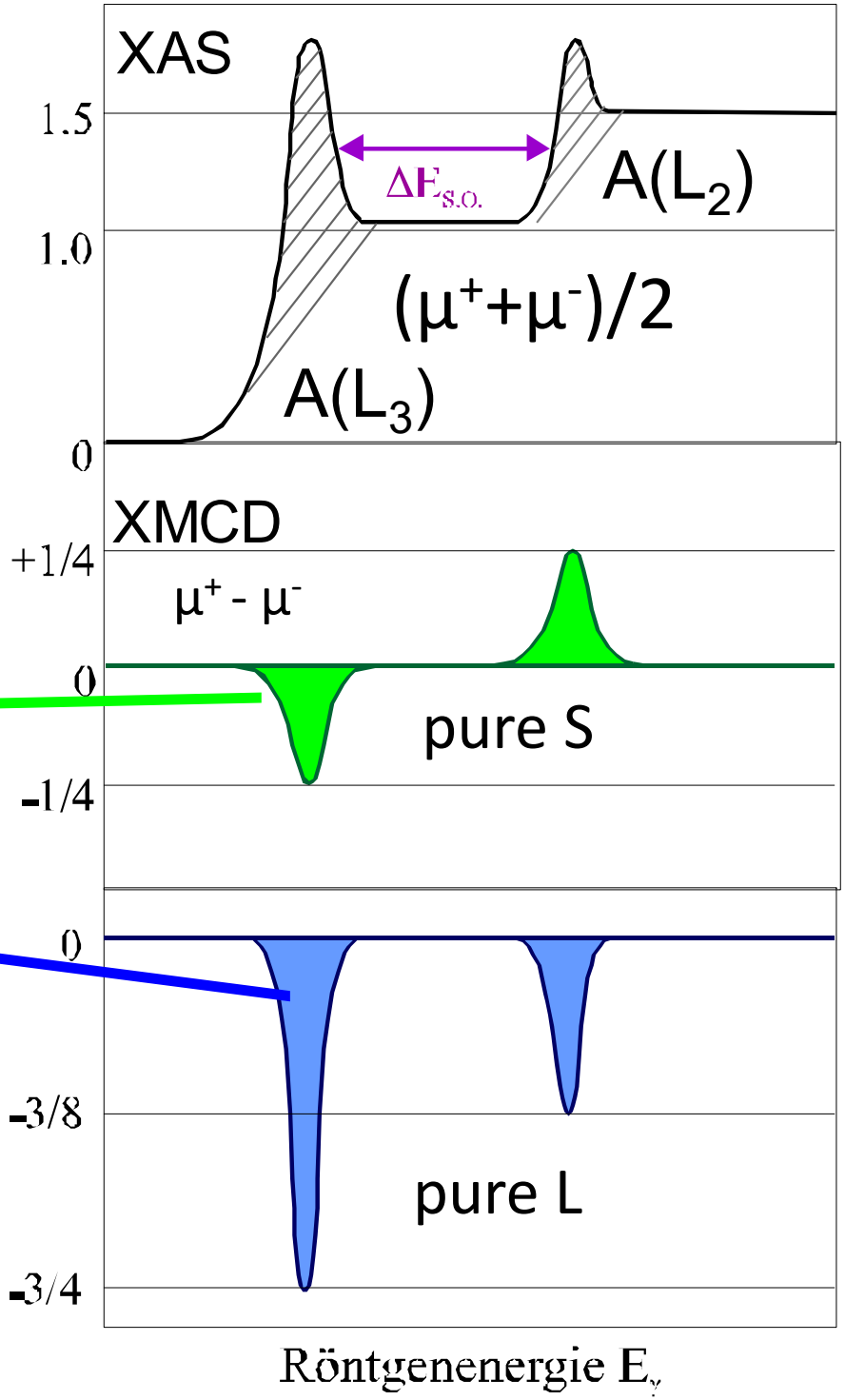
We cant do this here in detail!
This would take at least
3-4 times a 1.5h lecture!

T. Thole, P. Carra *et al.* : PRL **86** (1992) 1943 ; PRL **70** (1993) 694

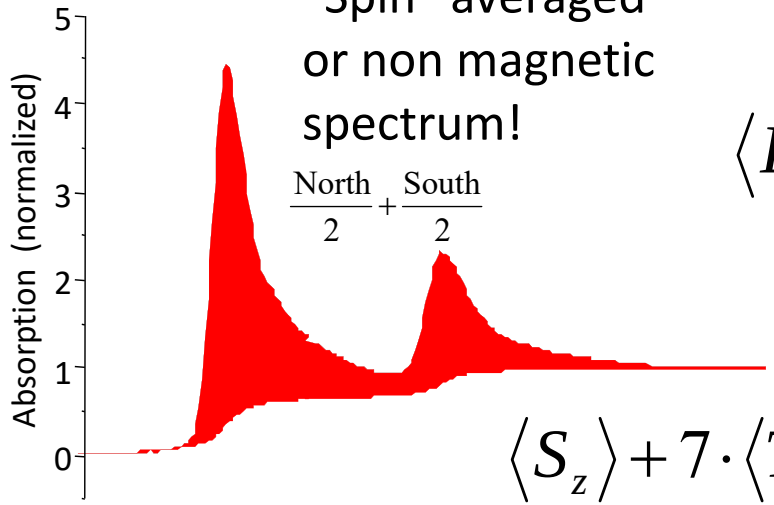
Orbital L and Spin S XMCD

„Real“ Spectra (Fe)



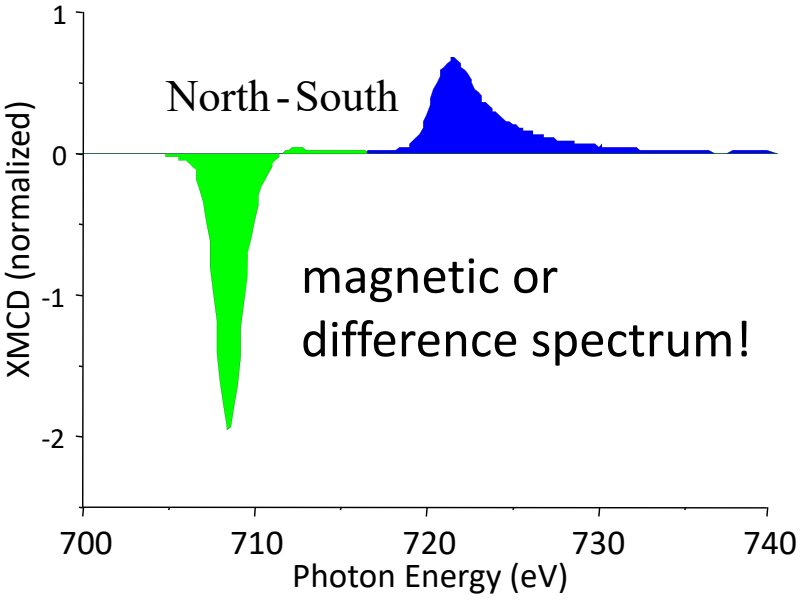


XMCD is famous because its quantitative: Sum-Rules



$$\langle L_z \rangle = -\frac{4}{3} \cdot \frac{\text{+} \quad \text{+}}{2 \cdot \quad \text{+}} \cdot \overbrace{(10 - n_{3d})}^{n_h}$$

$$\langle S_z \rangle + 7 \cdot \langle T_z \rangle = - \frac{\text{+} \quad -2 \cdot \text{+}}{2 \cdot \quad \text{+}} \cdot (10 - n_{3d})$$



- quantitative determination of projected magnetic moments
  - S, L and T_z separable
  - in projected Bohr-magnetons!
- one needs the "areas" and the number of holes
  - $(10\text{-}n_{3d})$

We will see T_z later more!

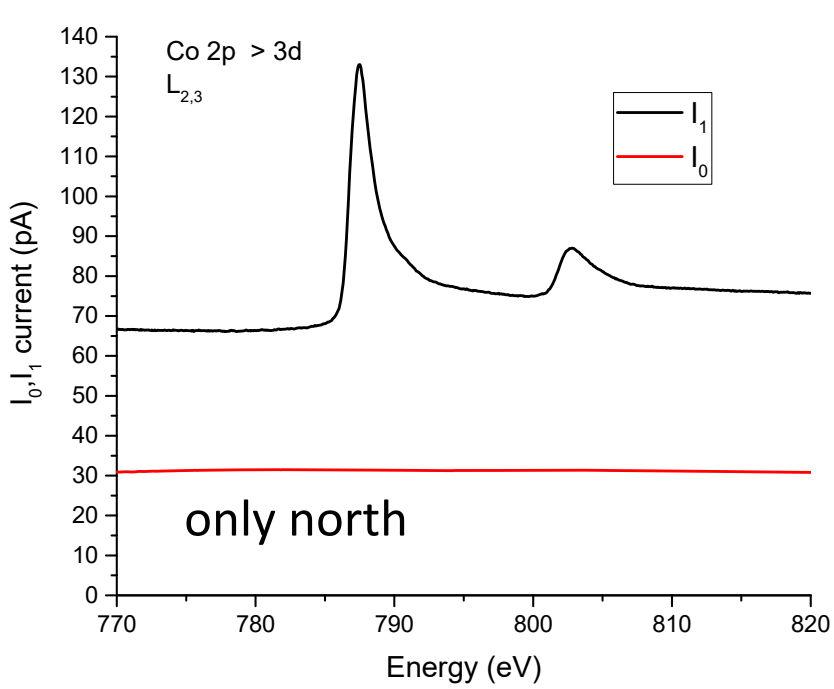
Theoretical prediction: T. Thole, P. Carra *et al.* : PRL **86** (1992) 1943 ; PRL **70** (1993) 694

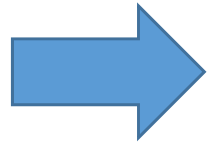
Exp. verification and rough procedure: C.T. Chen et al, PRL **75** (1995) 152

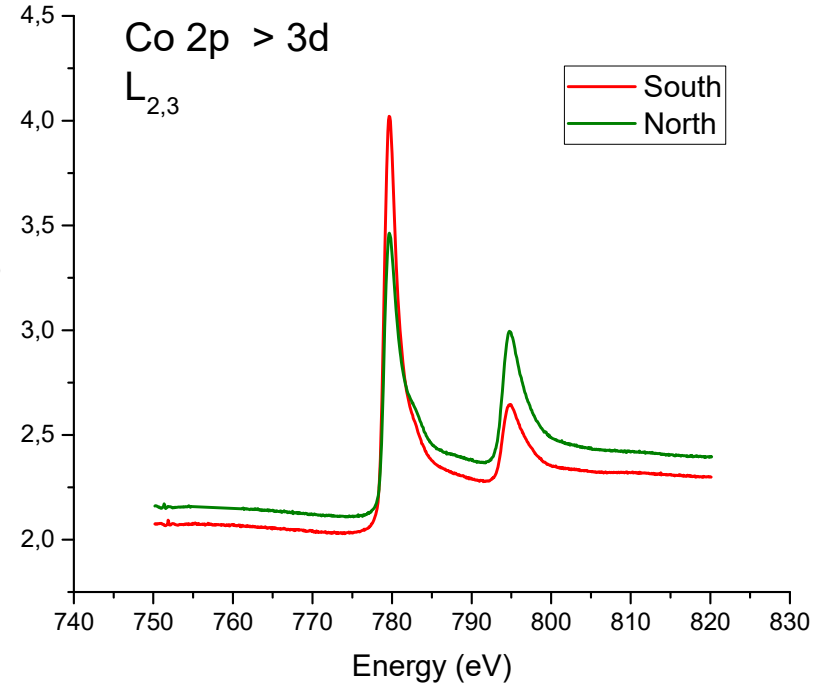
Data measurement and analysis: Co thin film!

Measure sample current I_1 and incoming intensity I_0 for north and south field

Step 1: Divide them I_1/I_0





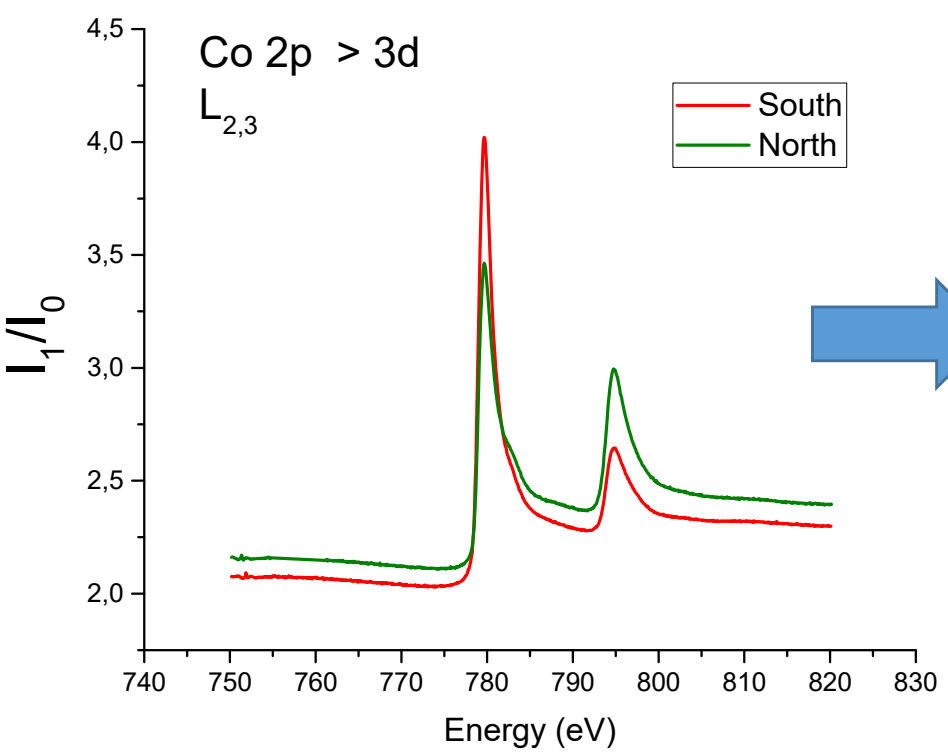


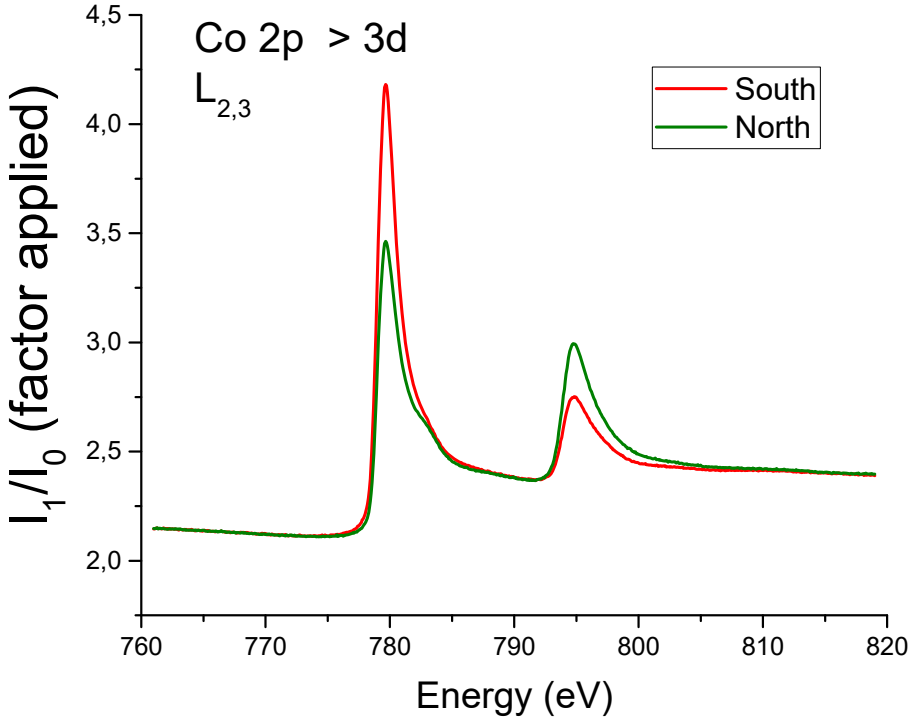
north and south means field orientation with respect to the photon beam!

Data measurement and analysis

Step 2: Remove „offset“ by a simple factor

Important: Make sure that pre- and Post-Edge region (without XMCD) are equal



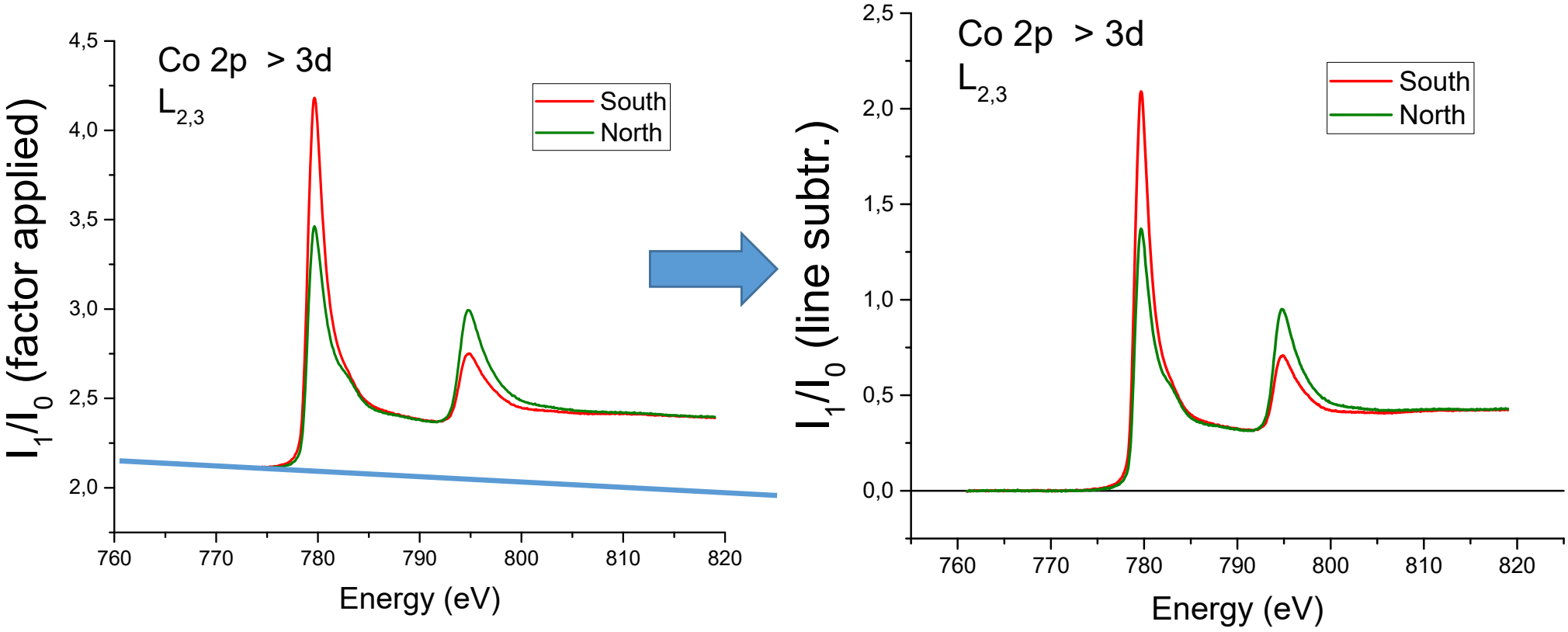


Here the factor is 1.04

Data measurement and analysis

Step 3: Subtract background by a linear approximation

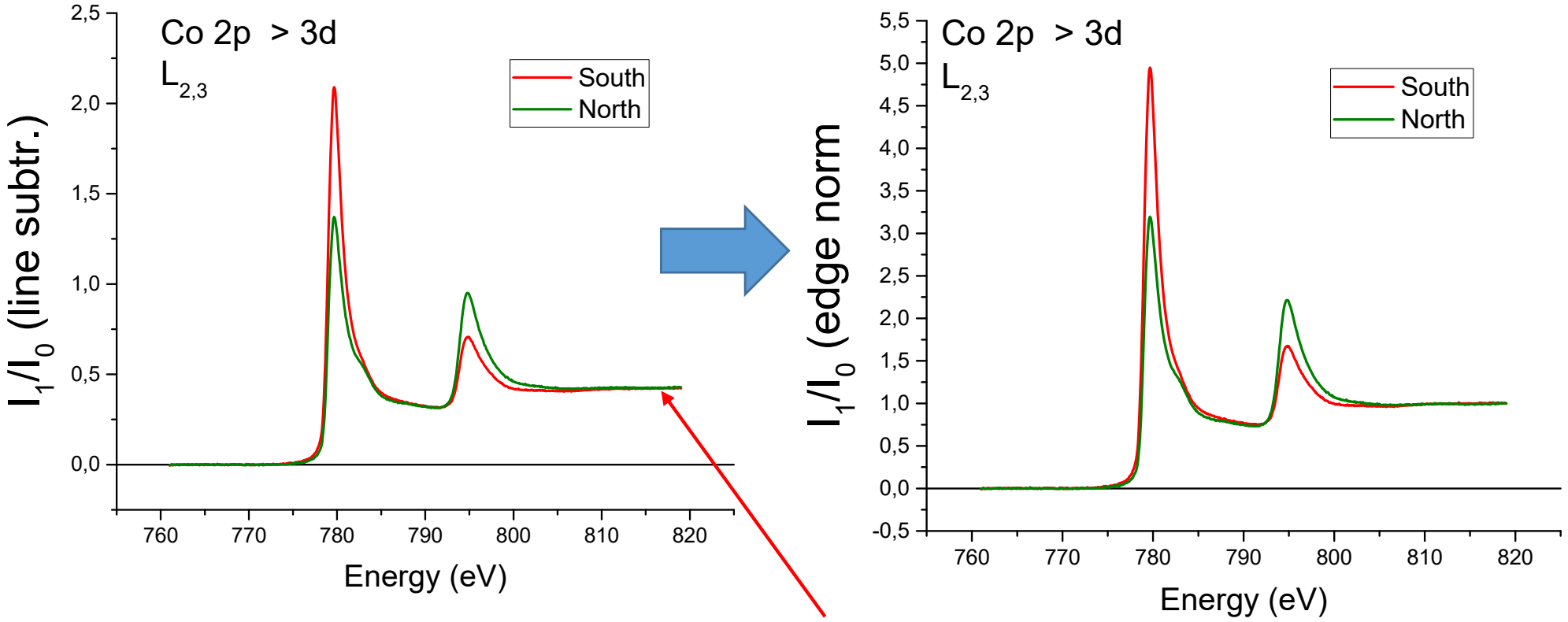
Important: Exactly the same for north and south spectra



Data measurement and analysis

Step 4: Devide by post edge value to normalize

Important: Exactly the same value for north and south spectra

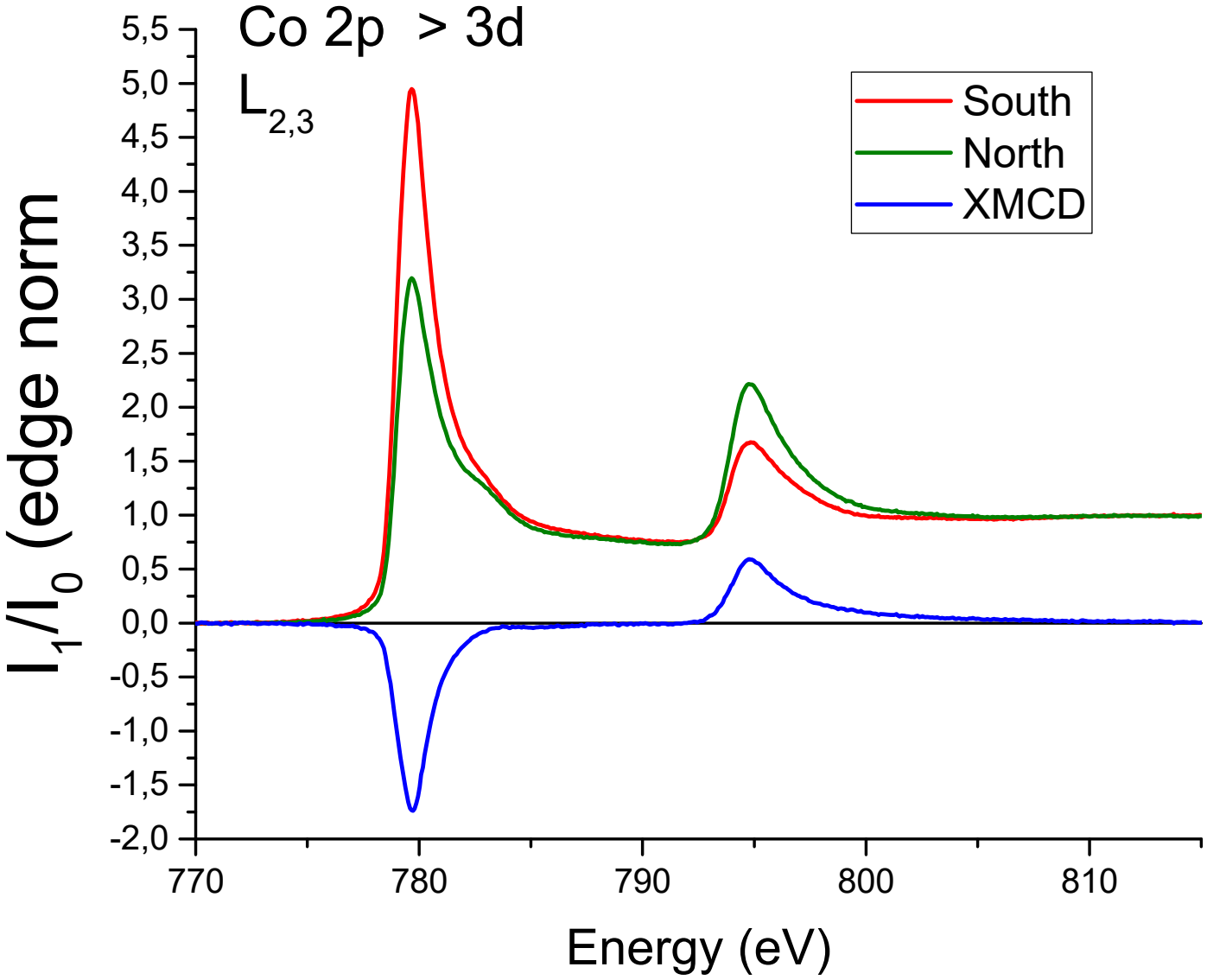


Here 0.425

Now the data is so called edge normalized!

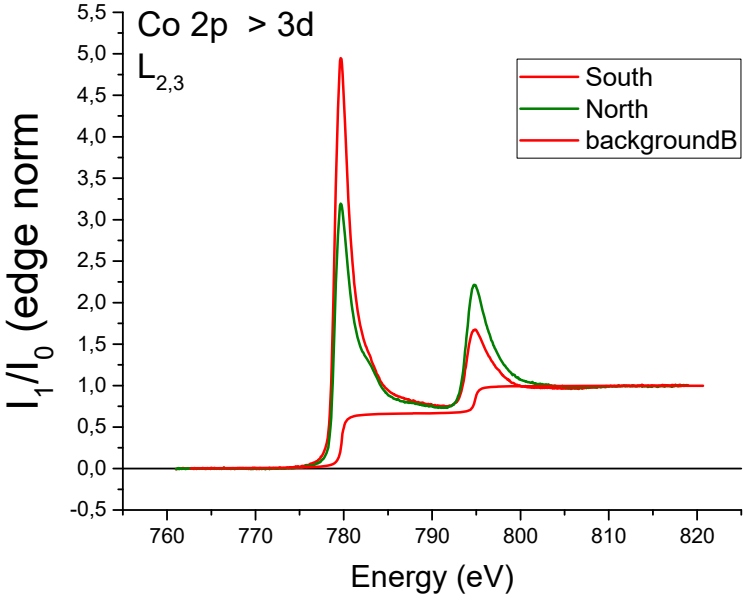
Data measurement and analysis

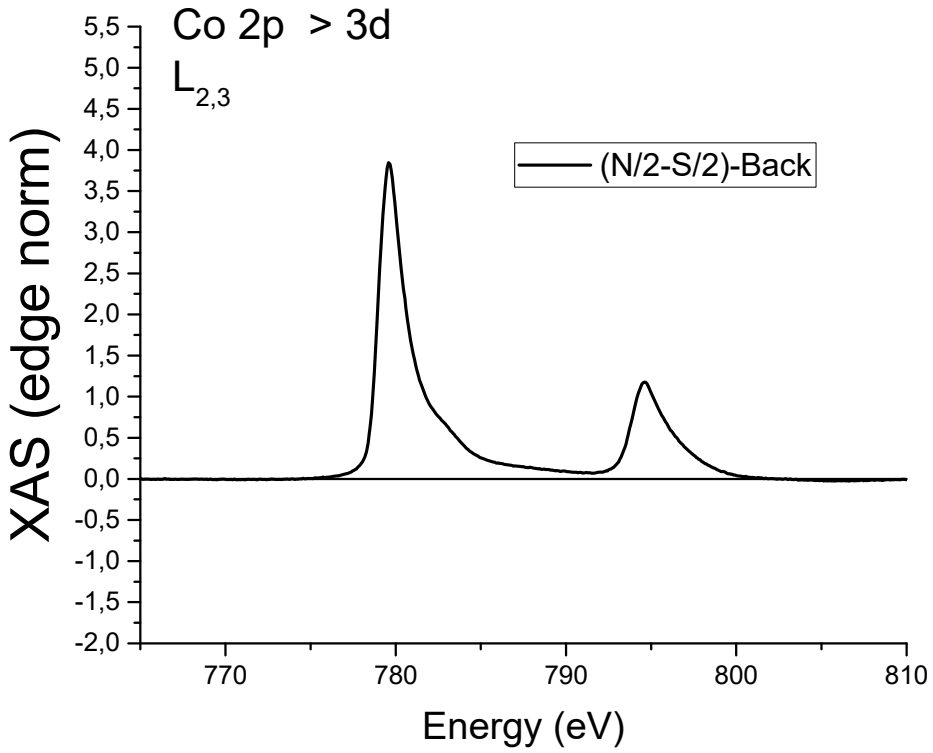
Step 5: Plot together with difference XMCD= North-South



Data measurement and analysis

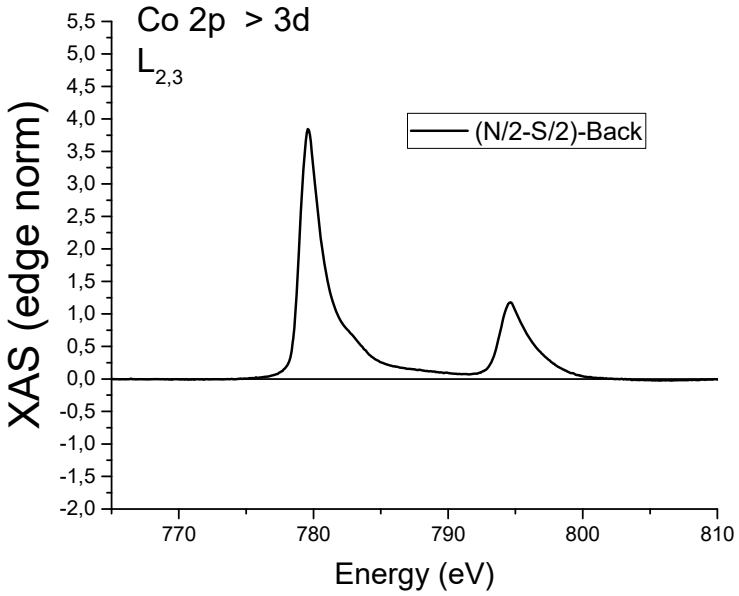
Step 6: For **sum rule** analysis remove non resonant background and calculate the “non magnetic” average. This does not change XMCD signal

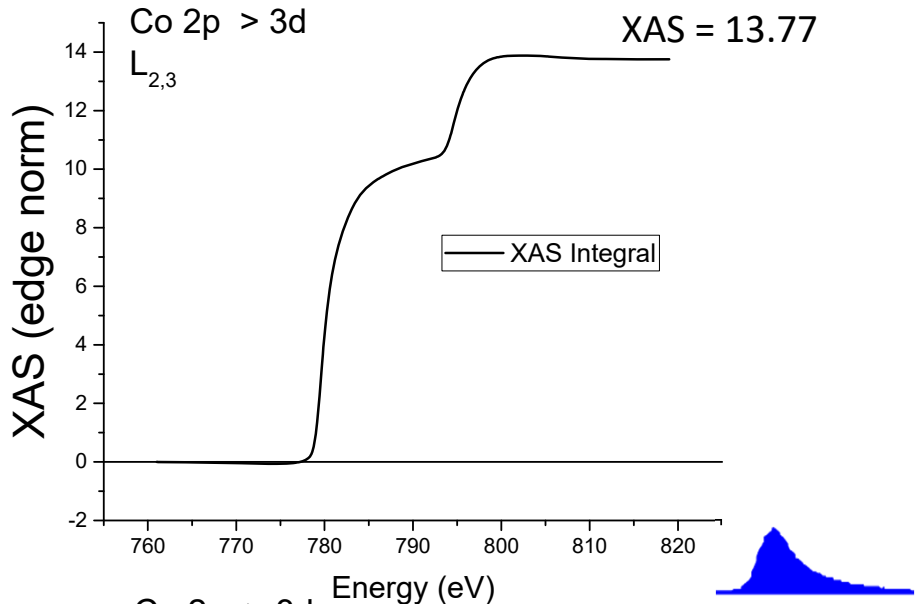


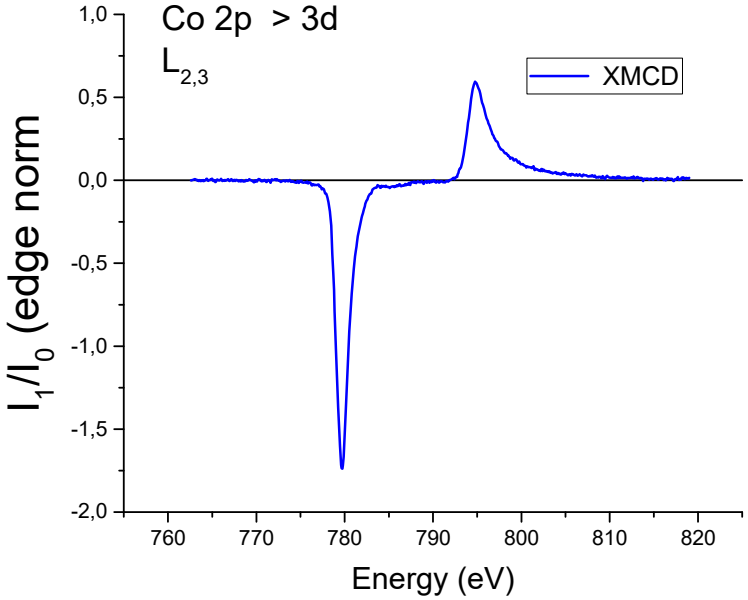


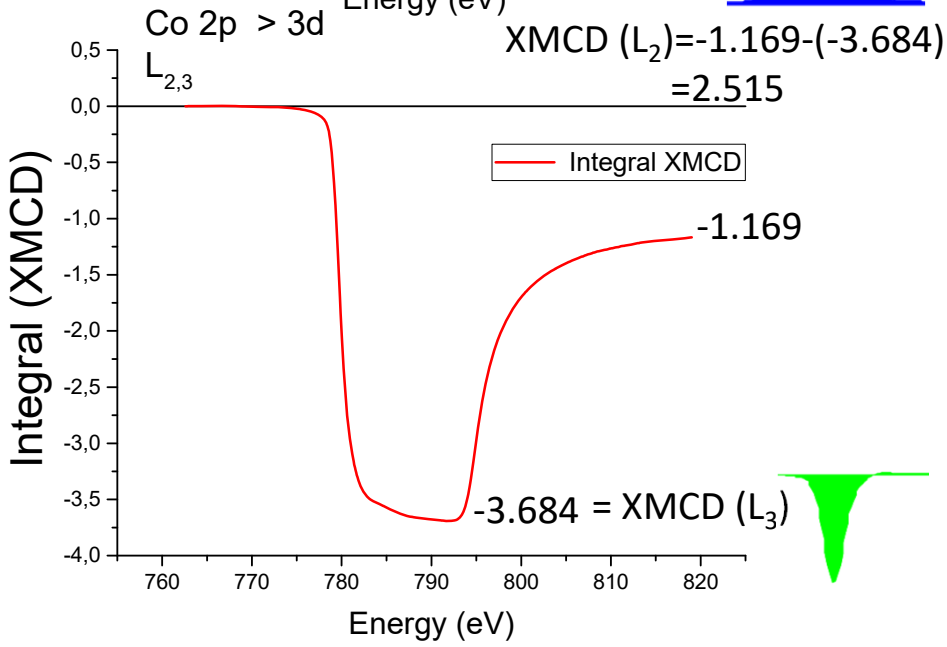
Data measurement and analysis

Step 7: Calculate the integrals for XAS (= nonmagnetic) and XMCD









Data measurement and analysis

Step 8: Sum Rules Calculation: Use values in formula

$$\langle L_z \rangle = -\frac{4}{3} \cdot \frac{+}{2\cdot} \cdot (10 - n_{3d})$$

$$\langle S_z \rangle + 7 \cdot \langle T_z \rangle = - \frac{-2\cdot}{2\cdot} \cdot (10 - n_{3d})$$

XAS = 13.77= 

XMCD (L_3)= -3.684 = 

XMCD (L_2)= 2.515 = 

$1 - n_{3d}(\mathrm{Co}) = 2.49$

$$\langle L_z \rangle = -\frac{4}{3} \cdot \frac{-3.64 + 2.515}{2 \cdot 13.77} \cdot 2.49 = 0.14$$

$$\langle S_z \rangle + 7 \cdot \langle T_z \rangle = - \frac{-3.64 - 2 \cdot 2.515}{2 \cdot 13.77} \cdot 2.49 = 0.785$$

Data measurement and analysis

Step 9: Correct for finite degree of circular polarization

Depends on Energy, setup, beamline, source as bending or undulator etc. etc. ➔ usually ask the beamline responsible

In our case here 84%!

Using the g-factor of 2 for the spin and transfer from angular momenta to magnetic moments

$$\langle m_L \rangle_z = \frac{\langle L_z \rangle}{0.84} \cdot \mu_B = \frac{0.14}{0.84}\,\mu_B = \underline{\underline{0.17\,\mu_B}} \qquad \langle m_S \rangle_z = 2 \cdot \frac{\langle S_z \rangle}{0.84} \cdot \mu_B = 2 \cdot \frac{0.785}{0.84} \cdot \mu_B = 1.87\,\mu_B$$

The deviation here is because of Tz!

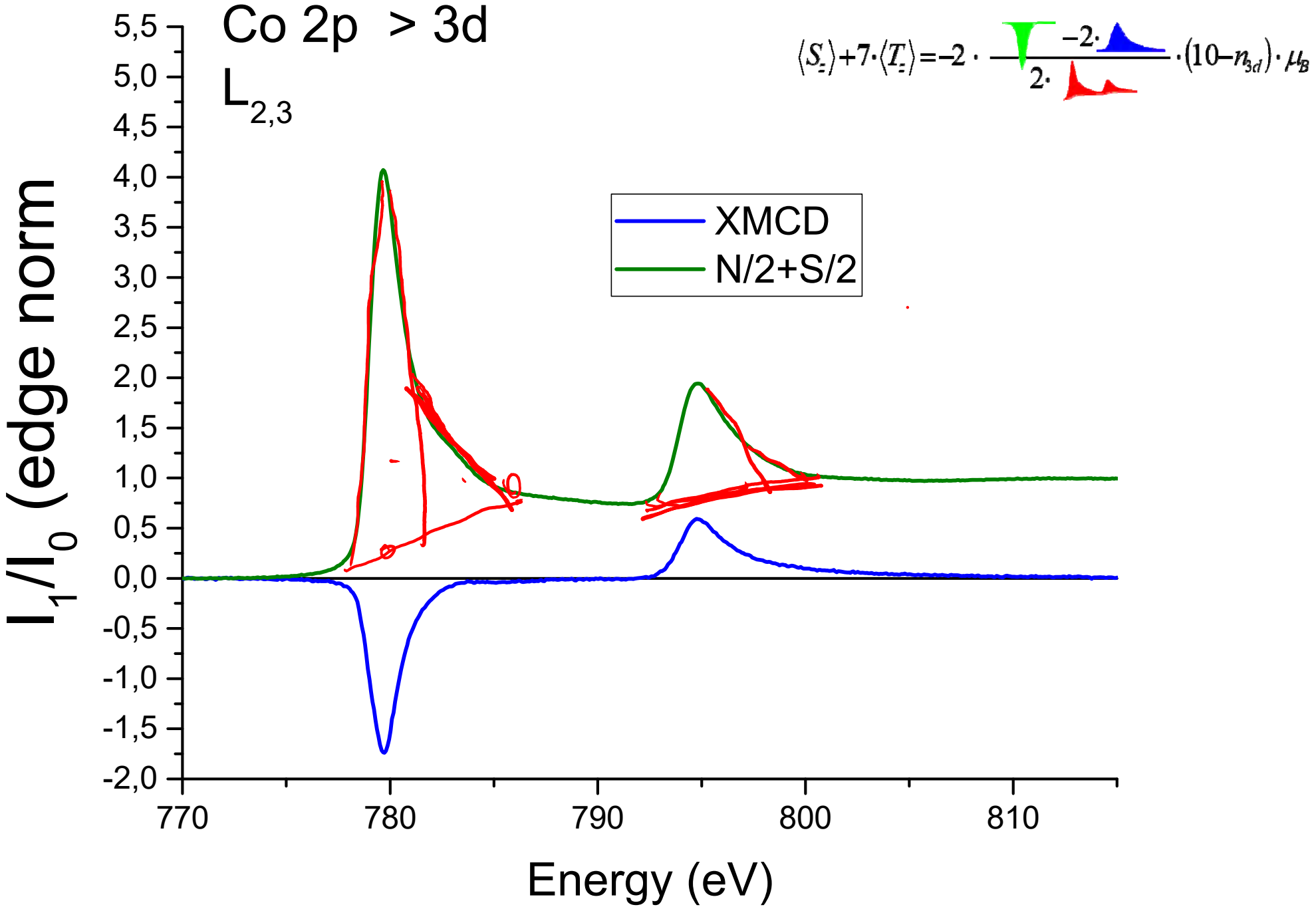
Element	exp. (XMCD)		theo.	
	m_s (μ_B)	m_l (μ_B)	m_s (μ_B)	m_l (μ_B)
Fe Chen PRL 75	1.98	0.085	2.19	≈ 0.059
Co Chen PRL 75	1.55	0.153	1.57	≈ 0.087
Ni Dhesi PRB 60	0.58	0.07	0.58	≈ 0.06

Sum-Rules Hands On

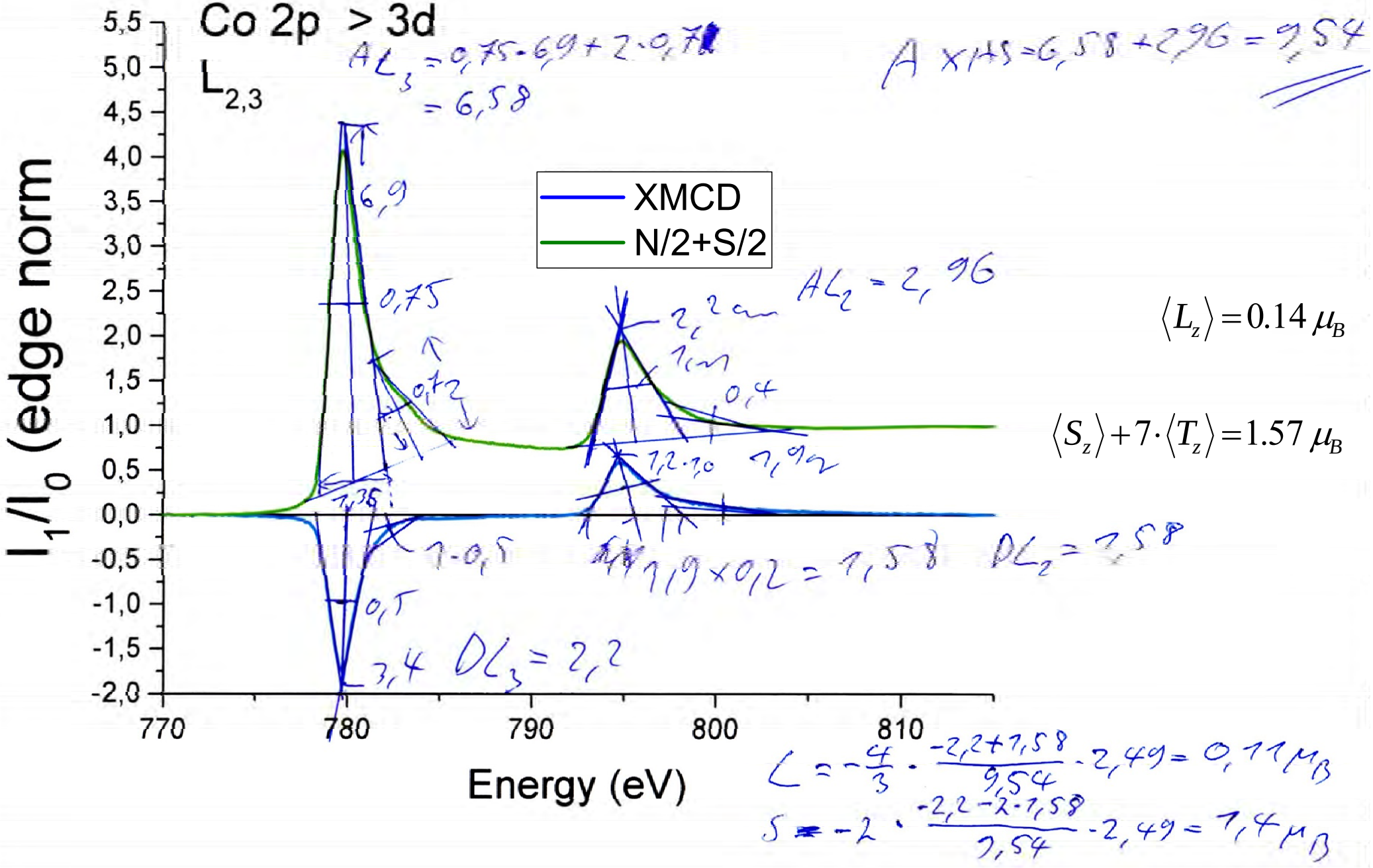
- Try to estimate the areas using a rule and a pen.

$$\langle L_z \rangle = -\frac{4}{3} \cdot \frac{+}{2\cdot} \cdot (10 - n_{3d}) \cdot \mu_B$$

$$\langle S_z \rangle + 7 \cdot \langle T_z \rangle = -2 \cdot \frac{-2\cdot}{2\cdot} \cdot (10 - n_{3d}) \cdot \mu_B$$

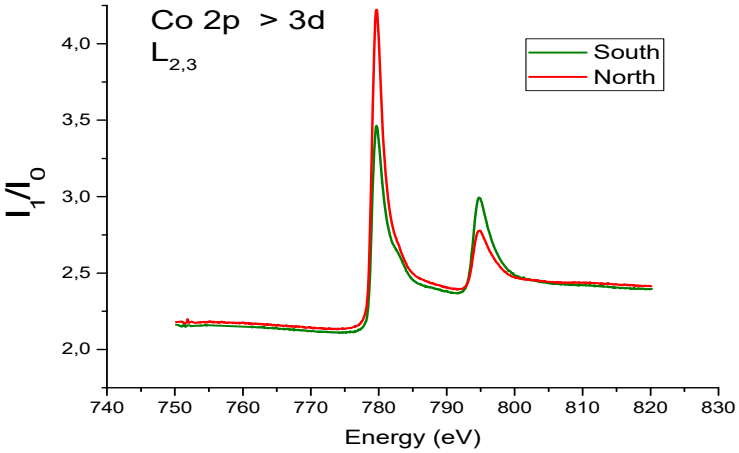


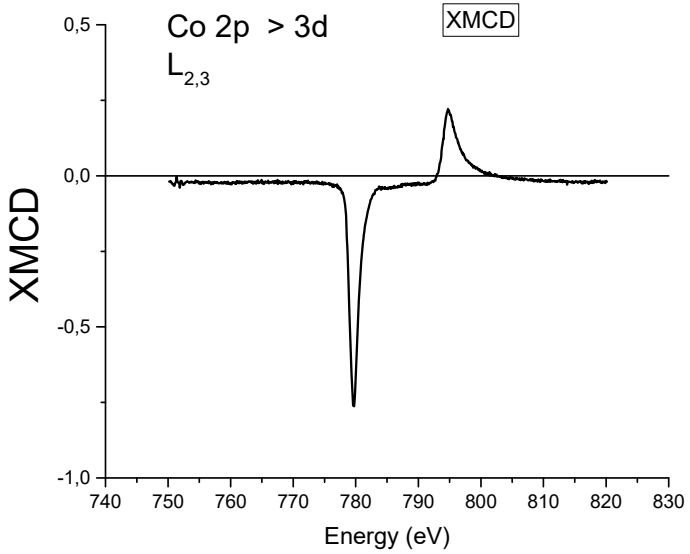
Estimating area by FWHM x Height or as you want

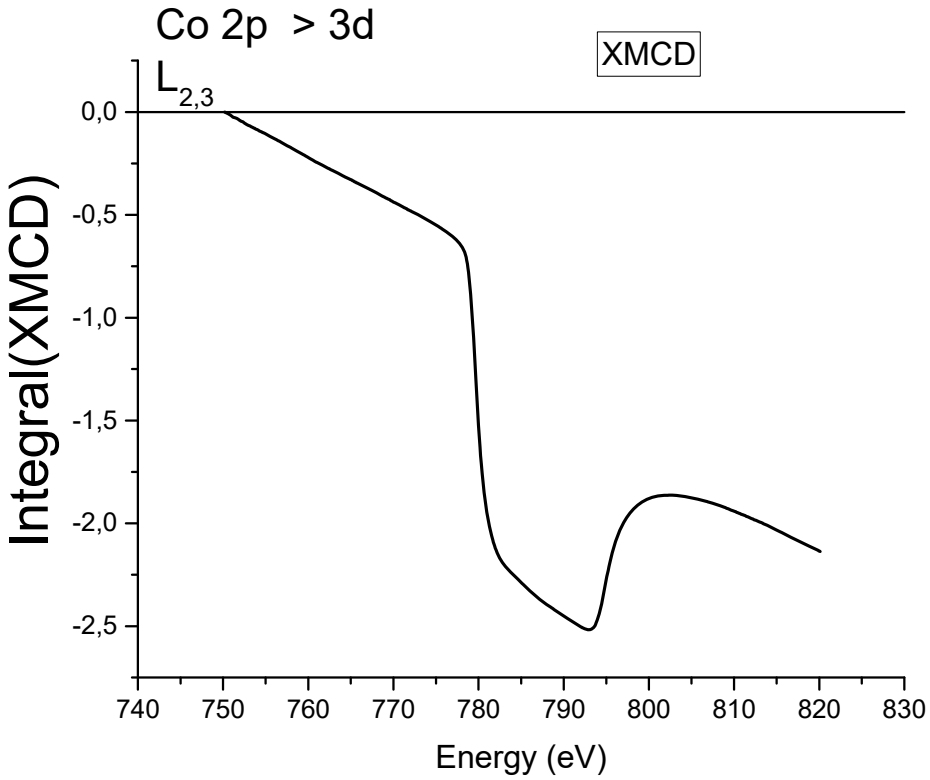


Data measurement and analysis

Typical pitfall: Offset corrected with wrong factor







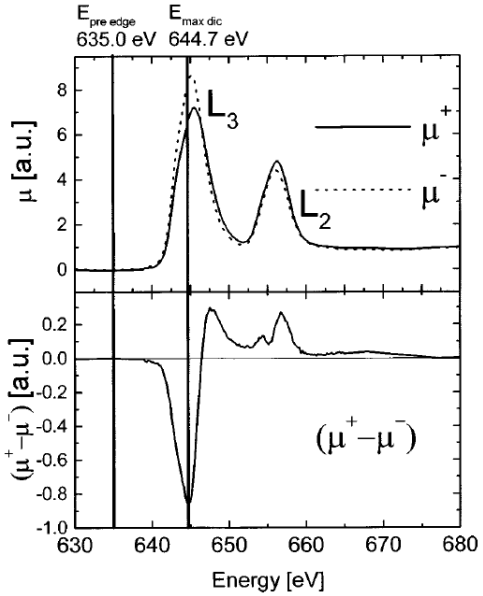
Best visible in a finite slope in the XMCD integral

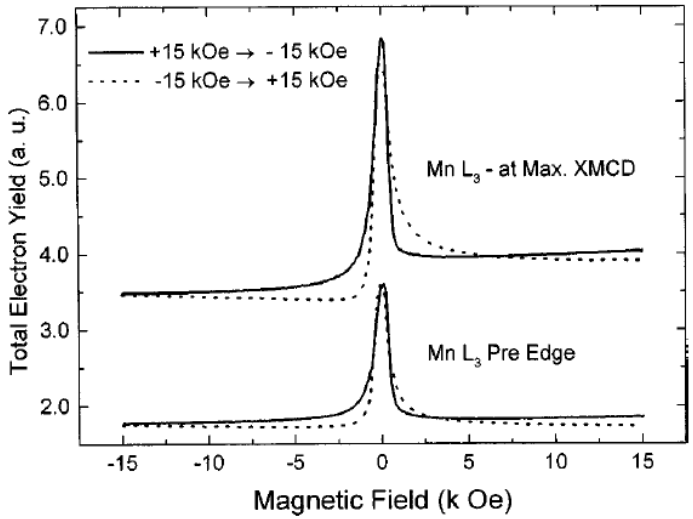
If present ➔ better factor

Why using a single factor for Offset correction?

Electron current depends on B-field dependent proportionality.

Could be asymmetric

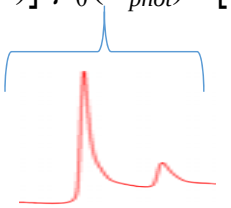


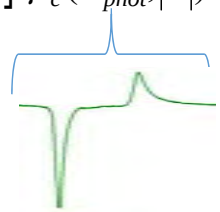


$$I(E_{phot},B) = f(B)\cdot\mu(E_{phot},B)$$

$$\mu(E_{phot},B^+) = \mu_0(E_{phot}) + \mu_c(E_{phot},|B|)$$
$$\mu(E_{phot},B^-) = \mu_0(E_{phot}) - \mu_c(E_{phot},|B|)$$

$$\Delta I(E_{phot};B) = f(B^+)\cdot\left[\mu_0(E_{phot}) + \mu_c(E_{phot},|B|)\right] - f(B^-)\cdot\left[\mu_0(E_{phot}) - \mu_c(E_{phot},|B|)\right]$$
$$= \left[f(B^+) - f(B^-)\right]\cdot\mu_0(E_{phot}) + \left[f(B^+) + f(B^-)\right]\cdot\mu_c(E_{phot},|B|)$$





if $f(B^+) = f(B^-) = f(B)$:

$$\Delta I(E_{phot};B) = 2\cdot f(B)\cdot\mu_c(E_{phot},|B|)$$ ✓

if $f(B^+) \neq f(B^-)$ choose k as $= f(B^+) = k\cdot f(B^-)$

As μ_0 is not a straight line, a line offset subtraction is wrong!

E. Goering et al., J.Sync.Rad. **8** (2001) 434-436 and J. Appl. Phys. **88** (2000) 5920

Sum Rules: In general for all edges!

J_+ is L+S and J- is L-S: Example L_3 edge: l=1 s=1/2 $J=J_+= 1+1/2 = 3/2$ and $J=J_-= 1-1/2 = 1/2$

$$\frac{-\int_{j_+ + j_-} \left(\mu^+(E) - \mu^-(E)\right) \cdot \mathrm{d}E}{\int_{j_+ + j_-} \left(\mu^+(E) + \mu^-(E) + \mu^0(E)\right) \cdot \mathrm{d}E} = a \cdot \frac{\langle L_z \rangle}{n_h}$$

this is the absorption sum for all absorption channels: μ^-= left, μ^+= right, and μ^0= z-polarized light

$$\frac{-\left(\int_{j_+} \left(\mu^+(E) - \mu^-(E)\right) \cdot \mathrm{d}E - b \cdot \int_{j_-} \left(\mu^+(E) - \mu^-(E)\right) \cdot \mathrm{d}E\right)}{\int_{j_+ + j_-} \left(\mu^+(E) + \mu^-(E) + \mu^0(E)\right) \cdot \mathrm{d}E} = \frac{c \cdot \langle S_z \rangle + d \cdot \langle T_z \rangle}{n_h}$$

angular momenta for the i=initial and f=final states

Table 1. •.

l_i	l_f	a	b	c	d
s:0	p:1	1	–	–	–
p:1	d:2	1/2	2	2/3	7/3
d:2	f:3	1/3	3/2	2/3	2

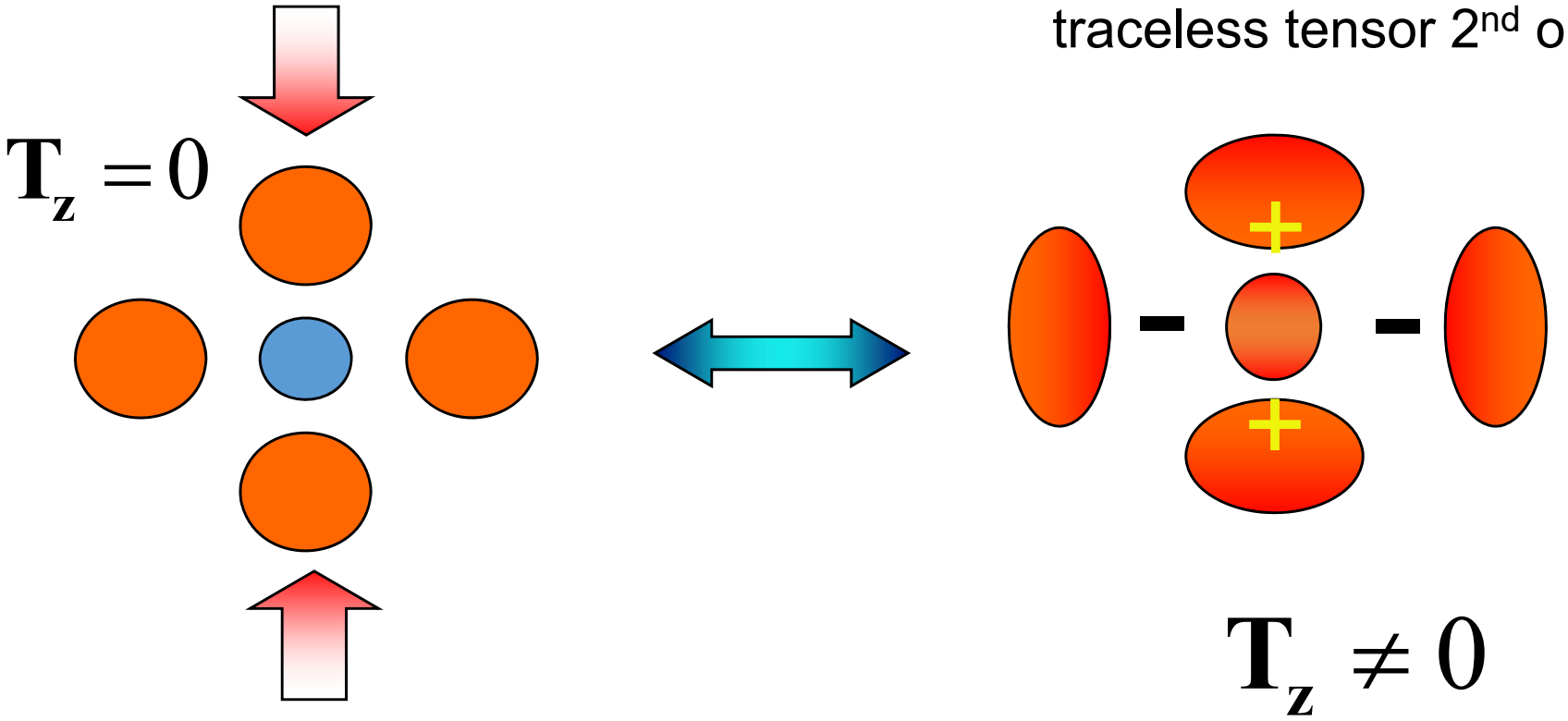
From Schütz, Stoll, and Goering Handbook of Magnetism (Wiley)
based on T. Thole, P. Carra *et al.* : PRL **86** (1992) 1943 ; PRL **70** (1993) 694

What is this T_z?

perturbation theory provides: $\mathbf{T}_z \approx -\frac{2}{7} \cdot \mathbf{Q} \cdot \hat{\mathbf{S}}$

G. van der Laan, J. Phys.: Condens. Matter **10** (1998) 3239

Q: quadrupolar charge distribution
traceless tensor 2nd order



Is important in less than cubic systems, with oriented crystals, in 4f metals, and in ultra thin films and interfaces

Something more about Tz: König and Stöhr, PRL **75** (1995) 3748; Buck and Fähnle, JMMM **166** (1997) 297

Further “Problems”

- For the light 3d transition metals, its hard to separate $P_{3/2}$ and $P_{1/2}$ excitations → excitations “mix”

  see: E. Goering, Phil. Mag. **85** (2005) 2897-2911 and references therein

- In 4f systems, as supermagnets, the spin-sum-rule is not „simply“ valid anymore (orbital works fine)

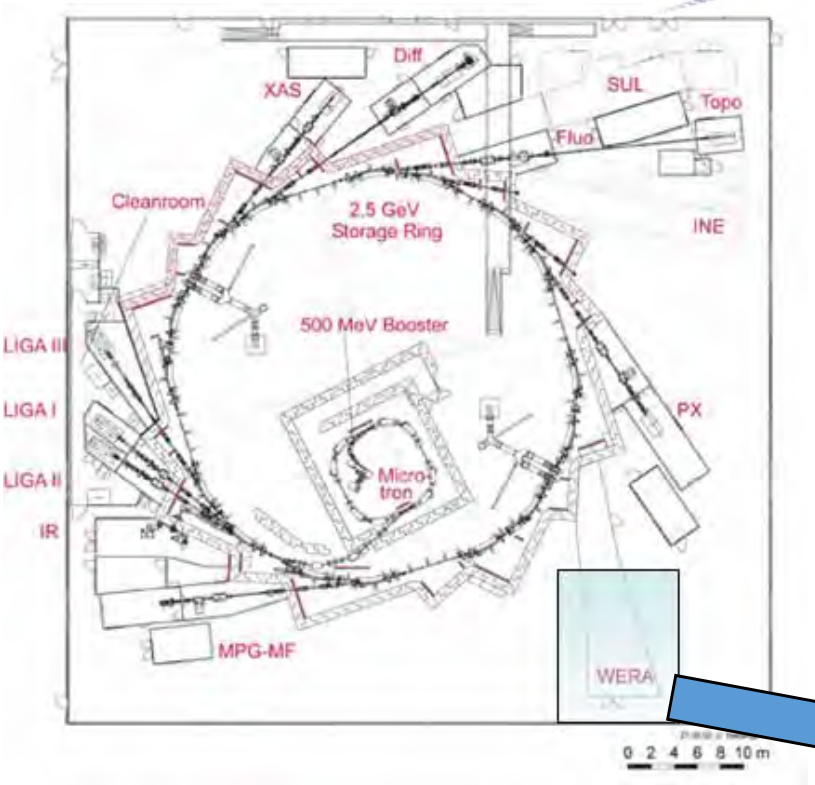
  see: Y. Teramura et al, J.Phys.Soc **65** (1996) 3056 and T. Jo, J.El.Spec.Rel.Phenom, **86** (1997) 73

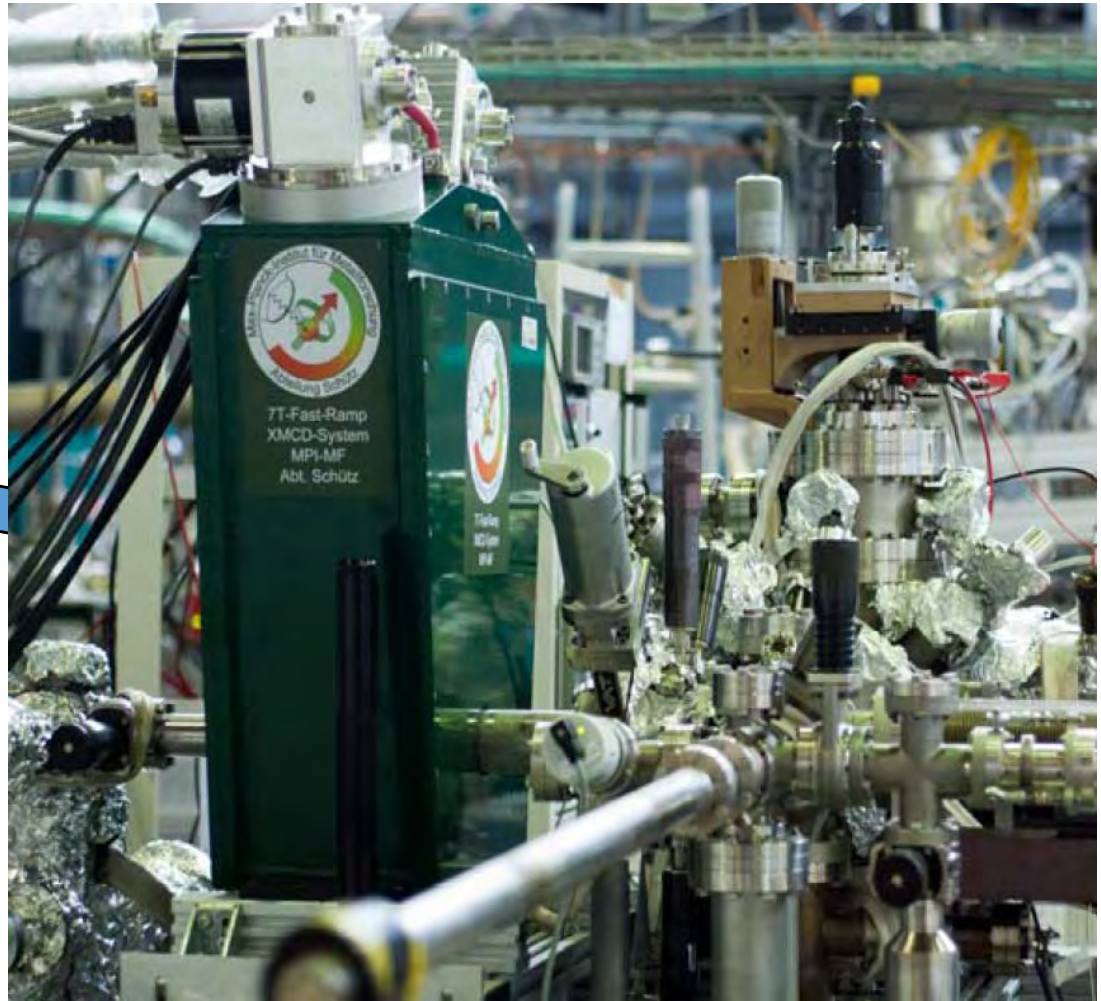
  - Actually, we are working on this at the moment, and it looks to be solvable, at least in a practical way.

2013 we could inaugurate our “new” 7T XMCD system!

- ANKA-Karlsruhe

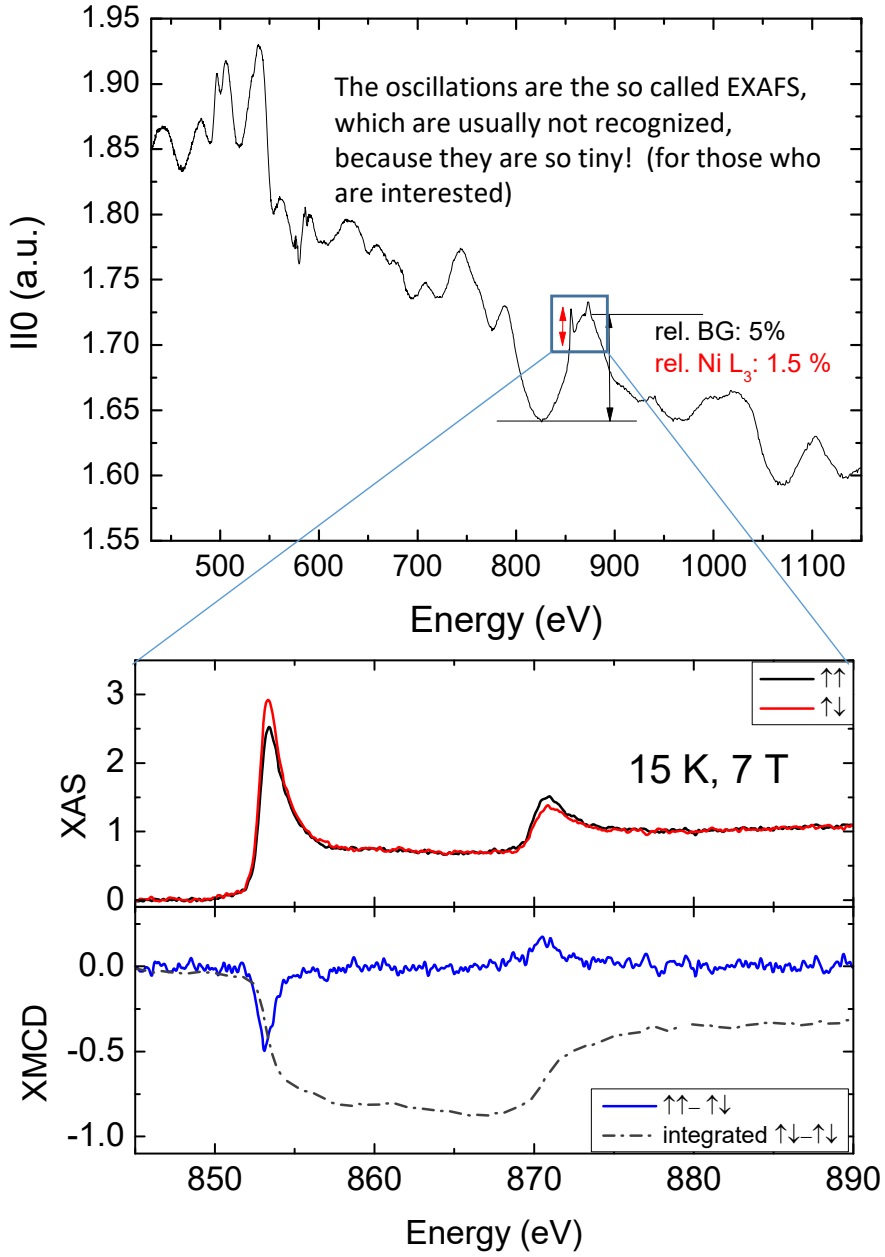
@ WERA-Beamline





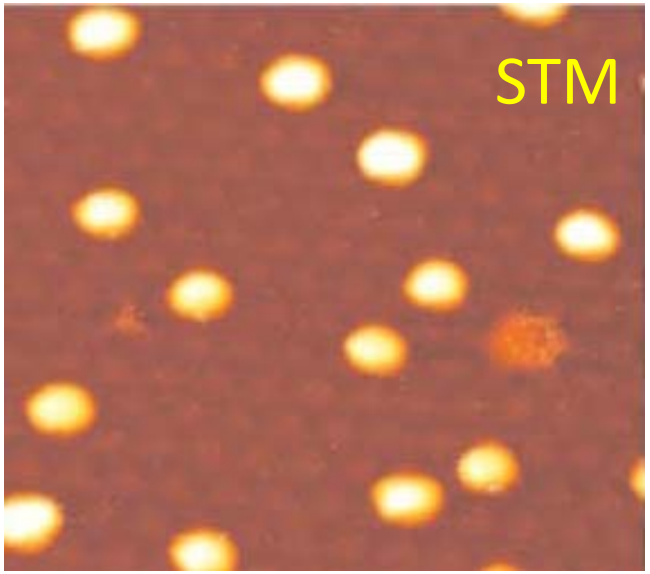
- **Unique superconducting magnet system**
- **7T ramped with 1.5T/s! (-5T ➔ +5T in 6,6s)**
  - low temperatures, portable, “load lock”
  - TEY, FY, Transmission ➔ parallel
  - No L-He refill ➔ two “cryo-coolers”
  - Gives anough signal to detect paramgnetism of diluted systems ➔ now 0.0002μ_B sensitivity
  - Fast XMCD measurements with highest quality ➔ **2-5 min/spectra**

XMCD at the „recent“ limit: 0.2ML paramagnetic Ni on Graphen



In-situ prepared Ni nanostructures (3nm height) :
0.2 ML nominal (@ 200 K) on Graphen/Ir Moiré-template

Cooperation with group of
M. Fonin, Univ.- Konstanz



Sicot et. al.: APPLIED PHYSICS LETTERS **96**, 093115 2010

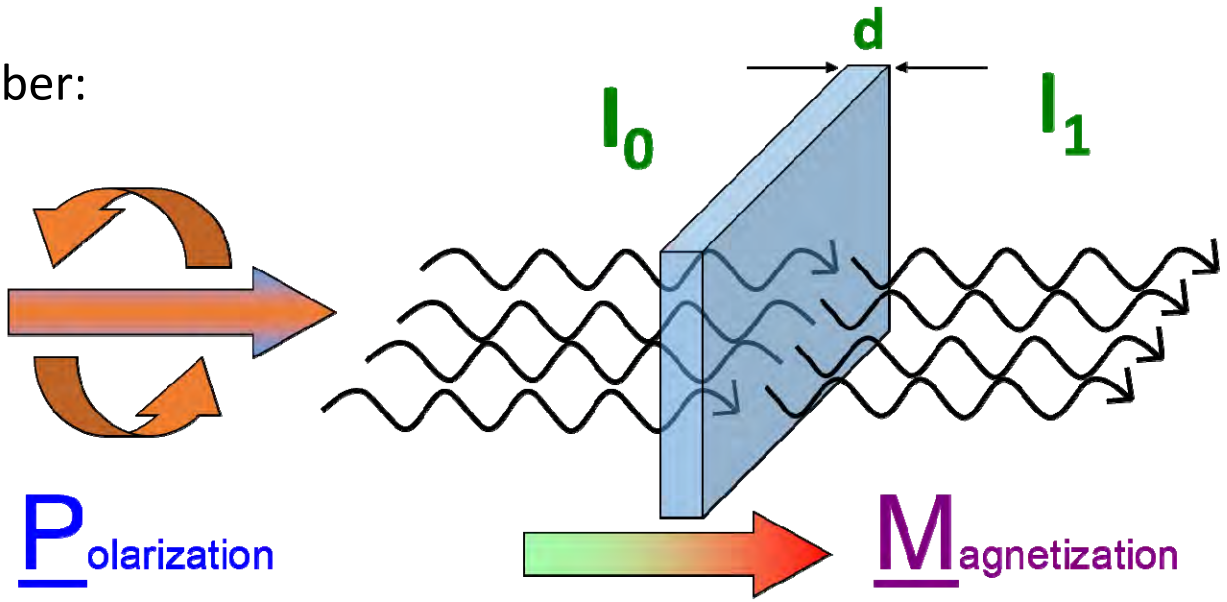
Questions:

1: Can we distinguish between pinned and rotatable moments?

2: Do we get a XMCD signal for a sample with permanent magnetic moments but disordered?

3: What do we get, if we have the same magnetic atoms, but half the amount? As Fe-XMCD for Fe ➔ FeCo alloy

Remember:



Measured quantity: $\Delta\mu=\mu^{+}-\mu^{-} \sim \Delta(\underline{P}\cdot\underline{M})$

X-ray magnetic circular dichroism: XMCD