放射光実験、XAFSとその周辺

-これからXAFSを始める人のために-

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Outline

- 放射光
- 軟X線領域のXAFS: NEXAFS, XMCD
- 蛍光X線分析 (XRF, XFA)
- （硬X線領域の）XAFS
  - 原子間距離を求める、“長さを測る”、ことについて
  - EXAFSの式、それを得るまでの理論的概念の整理
  - XAFS測定
- Some topics

放射光（Synchrotron Radiation）

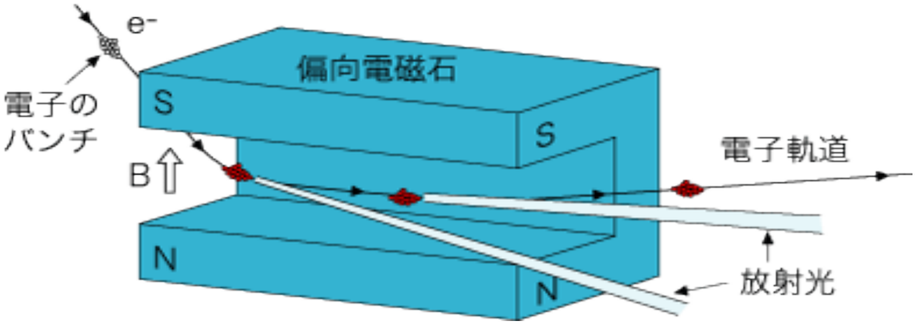
高エネルギーの電子が磁場の中を運動

└── 偏向電磁石（Bending Magnet）,etc.

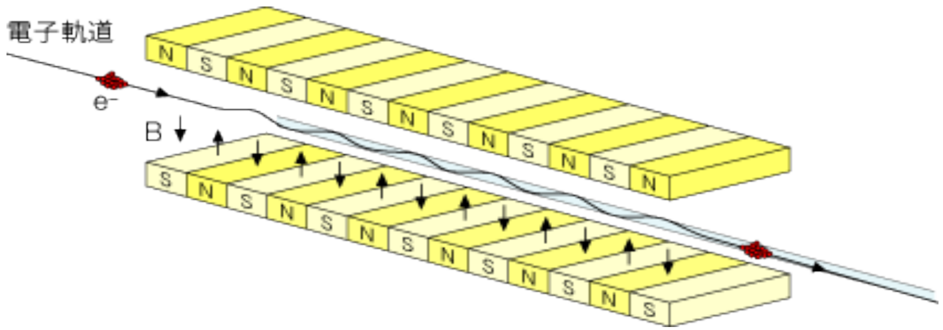
電子：円運動の中心に向かって力を受け，軌道が曲げられる

↓

電磁波が円軌道の接線方向に放射される；放射光

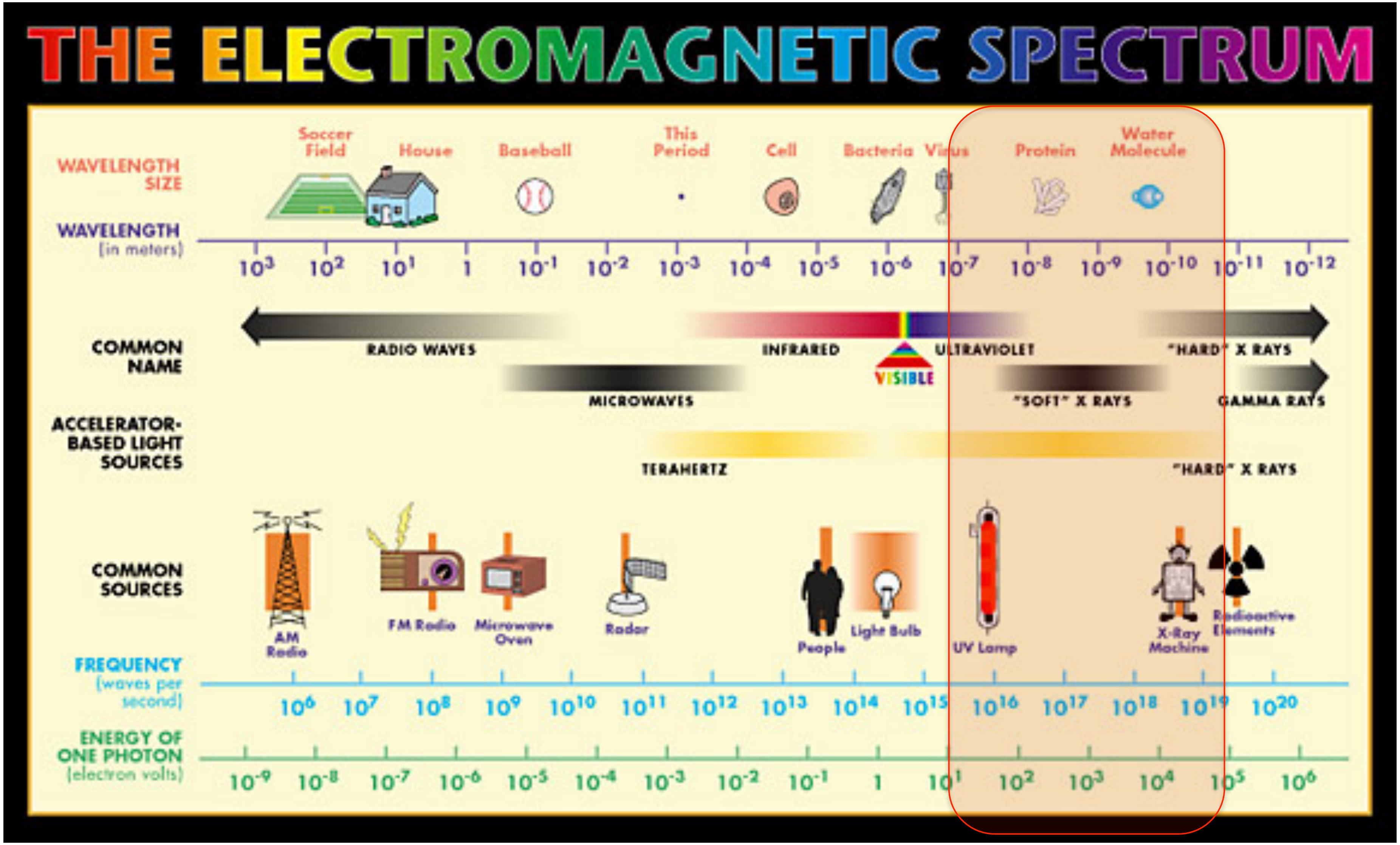


偏向電磁石（Bending Magnet）



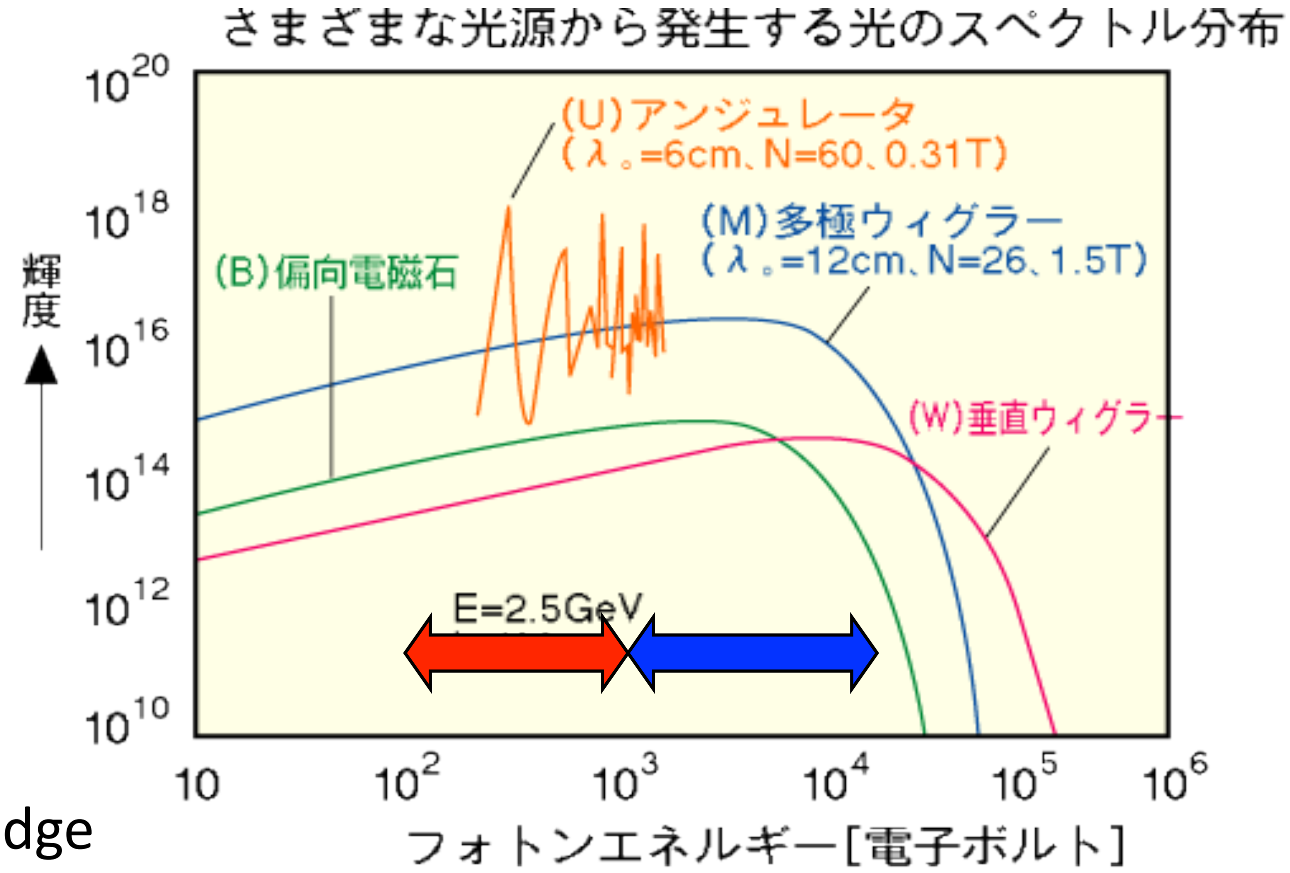
挿入光源（Insertion Device）
Undulator, Wiggler

pfwww.kek.jp



THE ELECTROMAGNETIC SPECTRUM
WAVELENGTH SIZE
Soccer Field
House
Baseball
This Period
Cell
Bacteria
Virus
Protein
Water Molecule
WAVELENGTH (in meters)
10^3 10^2 10^1 1 10^-1 10^-2 10^-3 10^-4 10^-5 10^-6 10^-7 10^-8 10^-9 10^-10 10^-11 10^-12
COMMON NAME
RADIO WAVES
INFRARED
VISIBLE
ULTRAVIOLET
"HARD" X RAYS
MICROWAVES
"SOFT" X RAYS
GAMMA RAYS
ACCELERATOR-BASED LIGHT SOURCES
TERAHERTZ
"HARD" X RAYS
COMMON SOURCES
AM Radio
FM Radio
Microwave Oven
Radar
People
Light Bulb
UV Lamp
X-Ray Machine
Radioactive Elements
FREQUENCY (waves per second)
10^6 10^7 10^8 10^9 10^10 10^11 10^12 10^13 10^14 10^15 10^16 10^17 10^18 10^19 10^20
ENERGY OF ONE PHOTON (electron volts)
10^-9 10^-8 10^-7 10^-6 10^-5 10^-4 10^-3 10^-2 10^-1 1 10^1 10^2 10^3 10^4 10^5 10^6

Light sources and spectra



C, N, O *K*-edge

250-600 eV

Fe, Co, Ni... *L*-edge

650-900 eV

...Fe, Co, Ni,... *K*-edge

4-10 keV

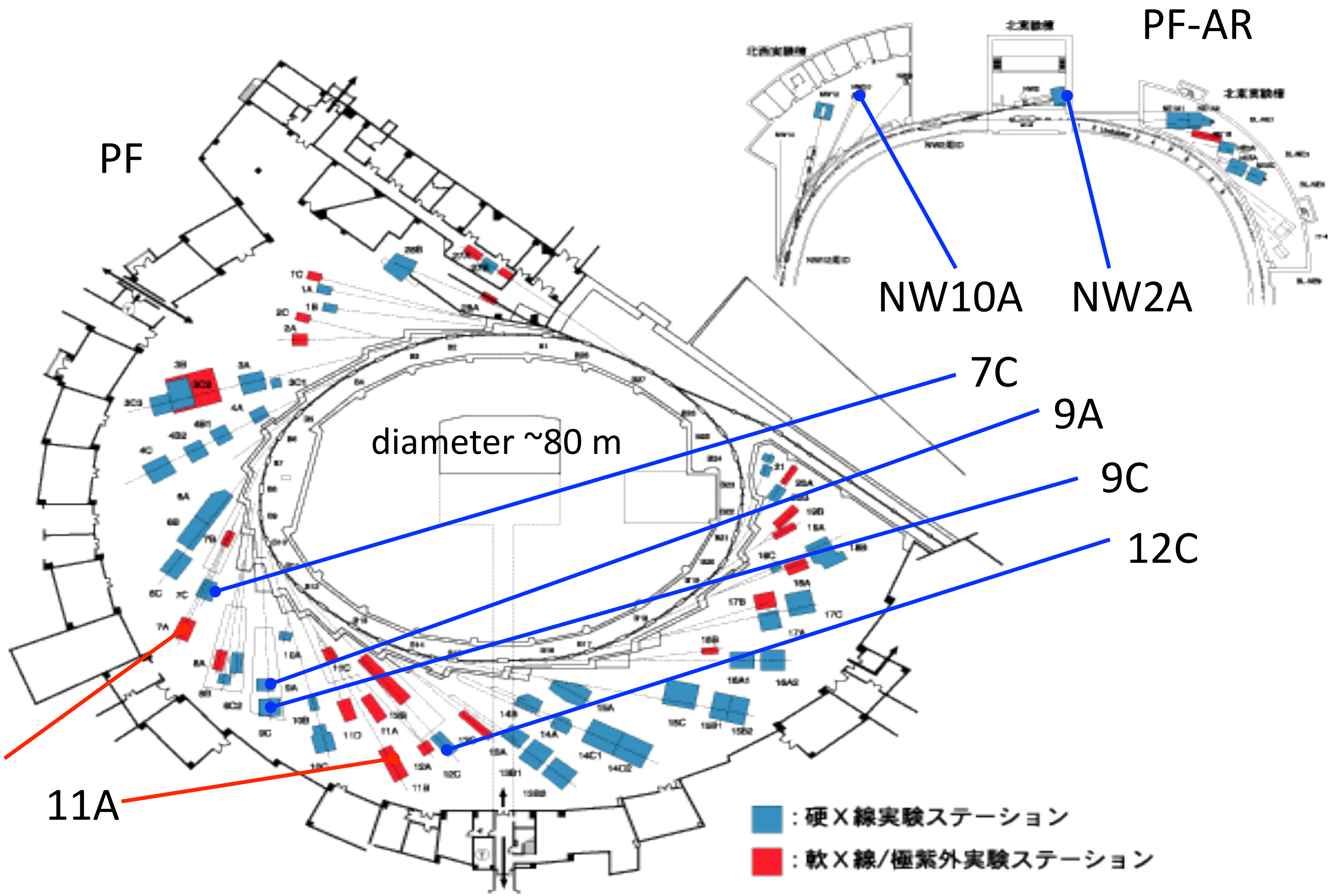
Pd *K*-edge

23 keV

軟X線 (Soft x-ray)

硬X線 (Hard x-ray)

Beamlines



PF
PF-AR
NW10A
NW2A
diameter ~80 m
7C
9A
9C
12C
7A
11A
：硬X線実験ステーション
：軟X線/極紫外実験ステーション

XAFS

XAFS: X-ray Absorption Fine Structure, X線吸収微細構造

軟X線領域 : ~200 – 2000 eV ← *超高真空が必要*

(Soft x-ray) (~10^{-8} Pa)

XAS (X-ray Absorption Spectroscopy) とも言う

硬X線領域 : ~2 keV – どこまでも

(Hard x-ray)

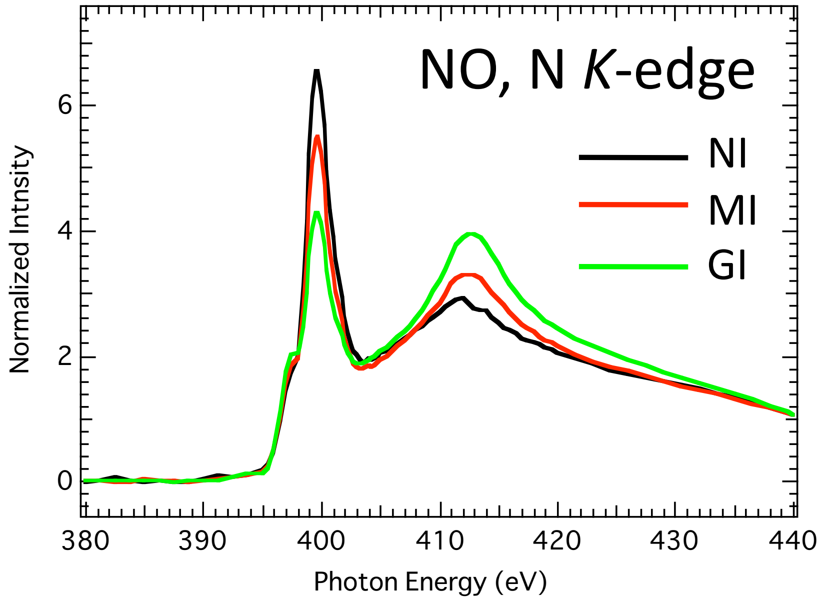
~42 keV (at PF-AR NW10A)

~60 keV, 113 keV (at SPring-8 BL01B1)

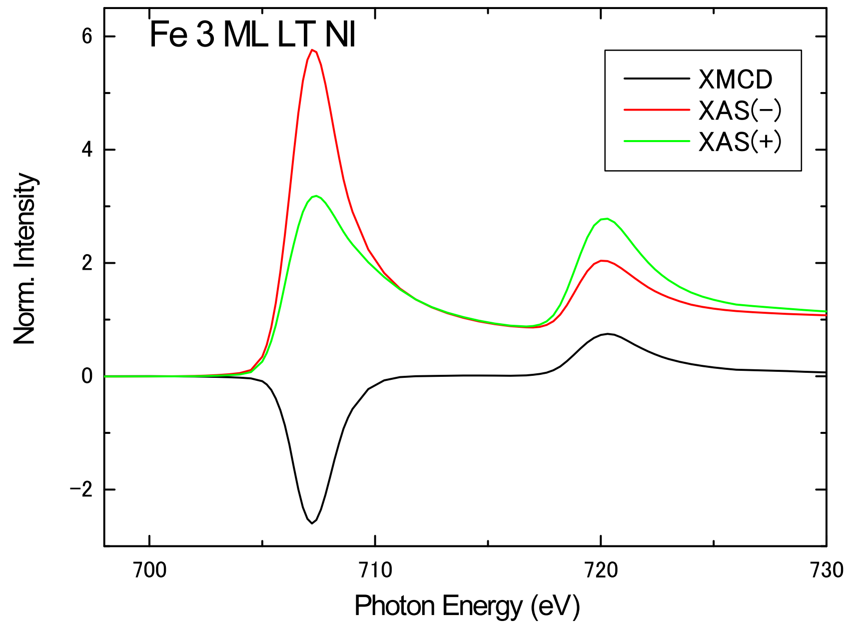
~2 keV – 4 keV: Hard x-rayの中では、"Soft"と呼ばれる

軟X線領域のX線吸収分光

NEXAFS: Near Edge X-ray Absorption Fine Structure



XMCD: X-ray Magnetic Circular Dichroism



NEXAFSから分かること

- 空準位のエネルギーと部分状態密度

  ⇒ LUMO, LUMO+1・・など空軌道の情報

- 空準位への遷移モーメントの方向

  ⇒ 吸着分子や固体の配向情報

- ある空準位への遷移モーメントを持つものの量

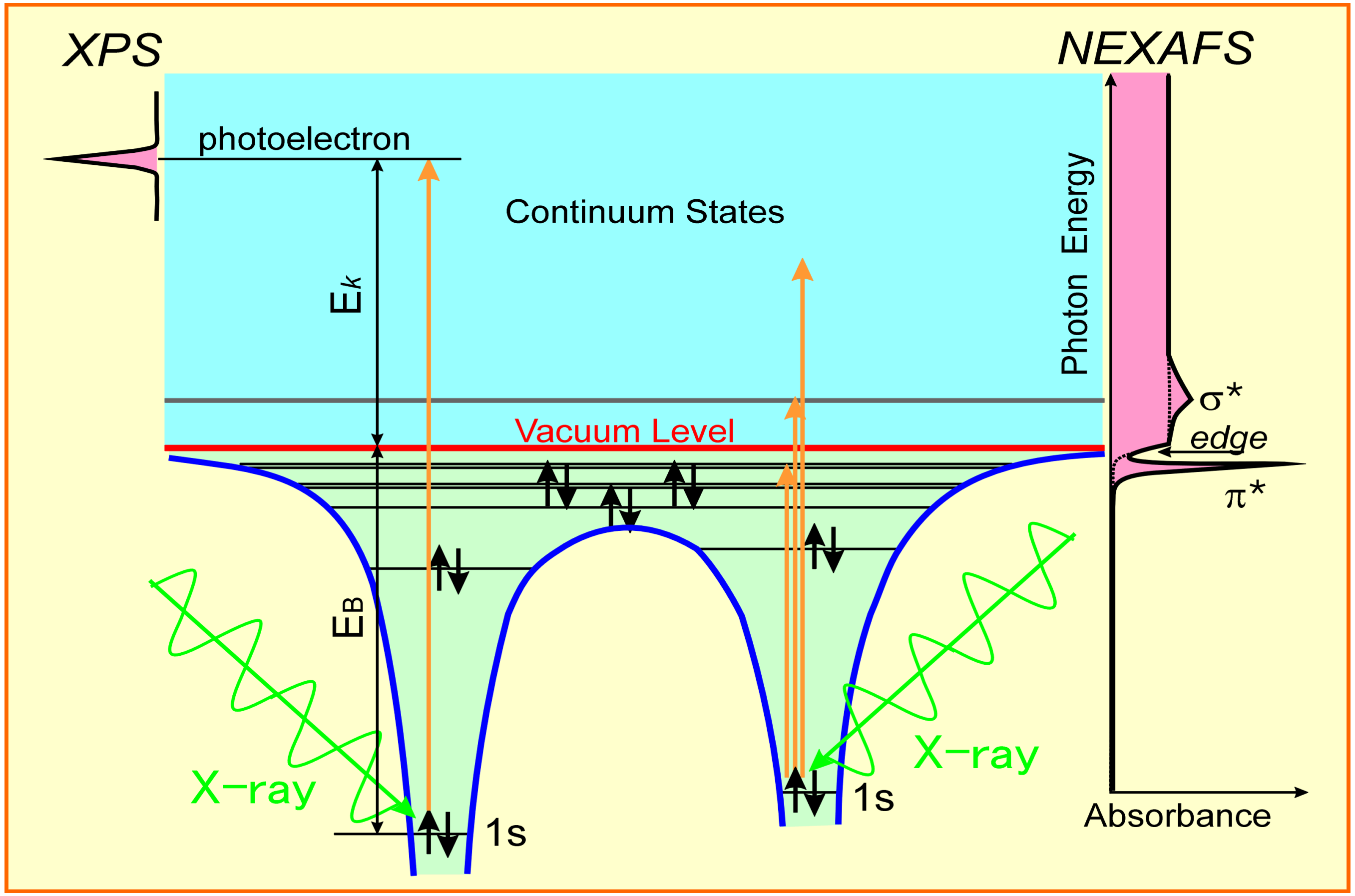
  ⇒ 吸着分子の被覆率

Basics of NEXAFS

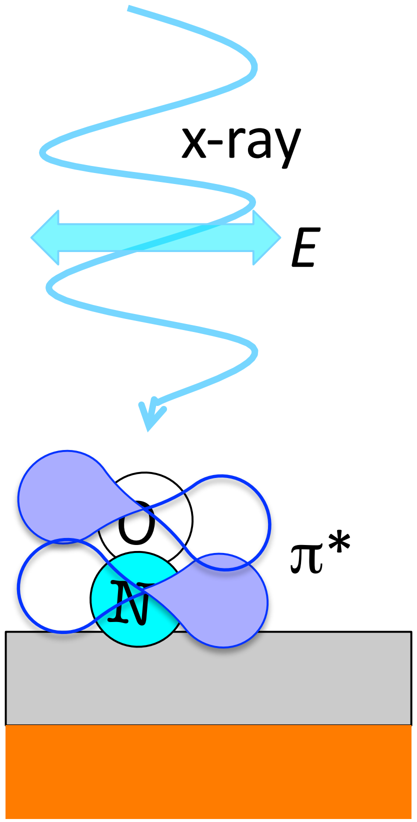
Near-Edge X-ray Absorption Fine Structure (NEXAFS)

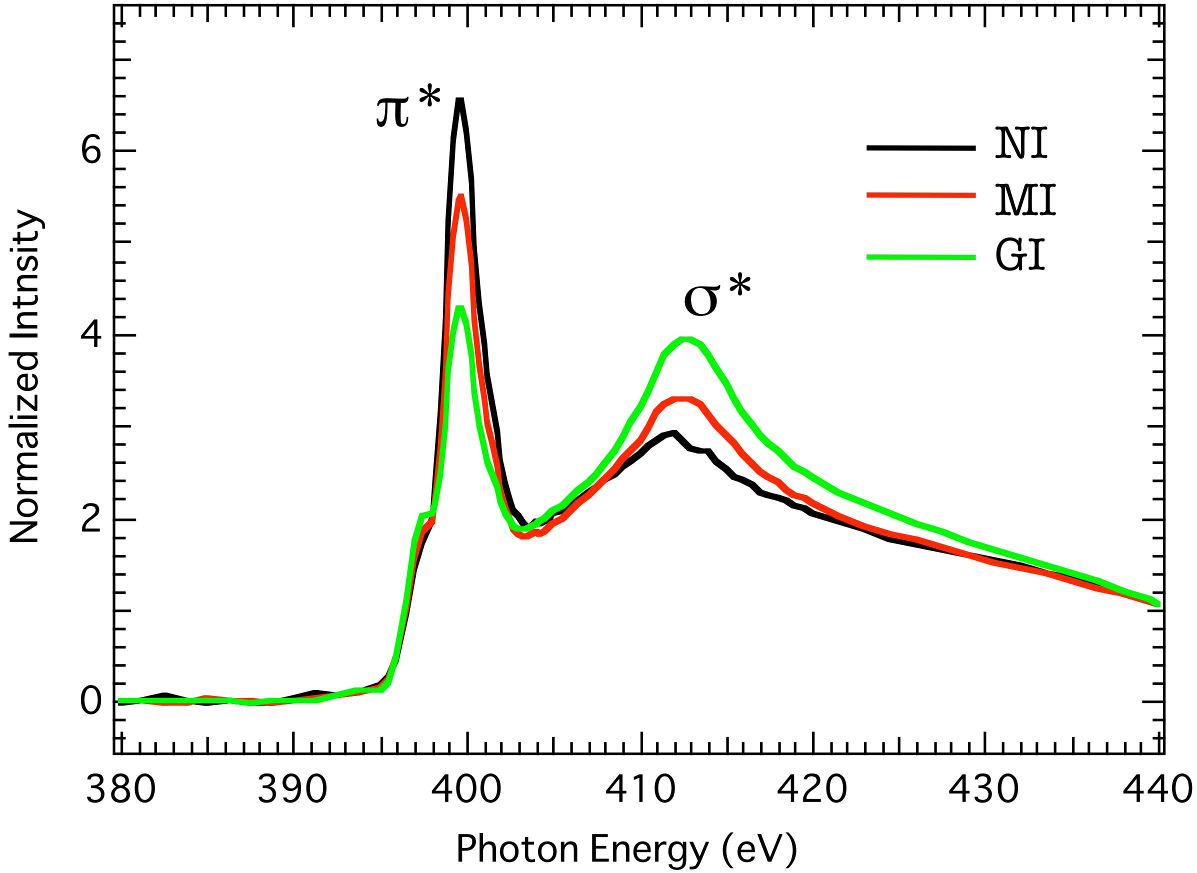
特徴

- 元素選択性
- （表面で）1 ML以下の分子を定量的に観測できる
- 局所的な分子の配向構造が見える (偏光依存性から)
- 局所電子構造が見える (unoccupied states)



N-*K* NEXAFS of NO: NO/Fe/Cu(001)





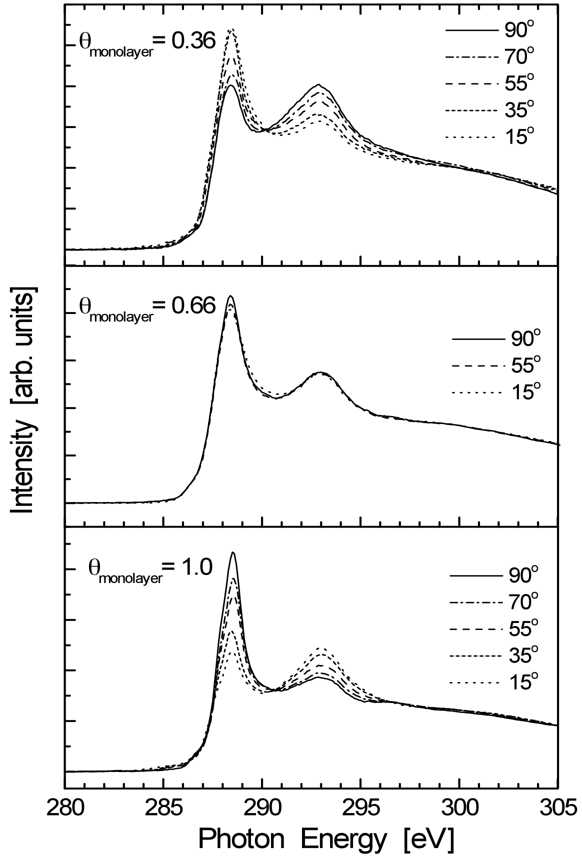
large π* peak for Normal incidence (NI)

NO molecules: nearly perpendicular to the plane

NEXAFSの応用例　（吸着分子の配向情報）

多層C_6H_{14}/単層$C_6H_{13}S$/Au(111)に対するC-K NEXAFSによって観測された

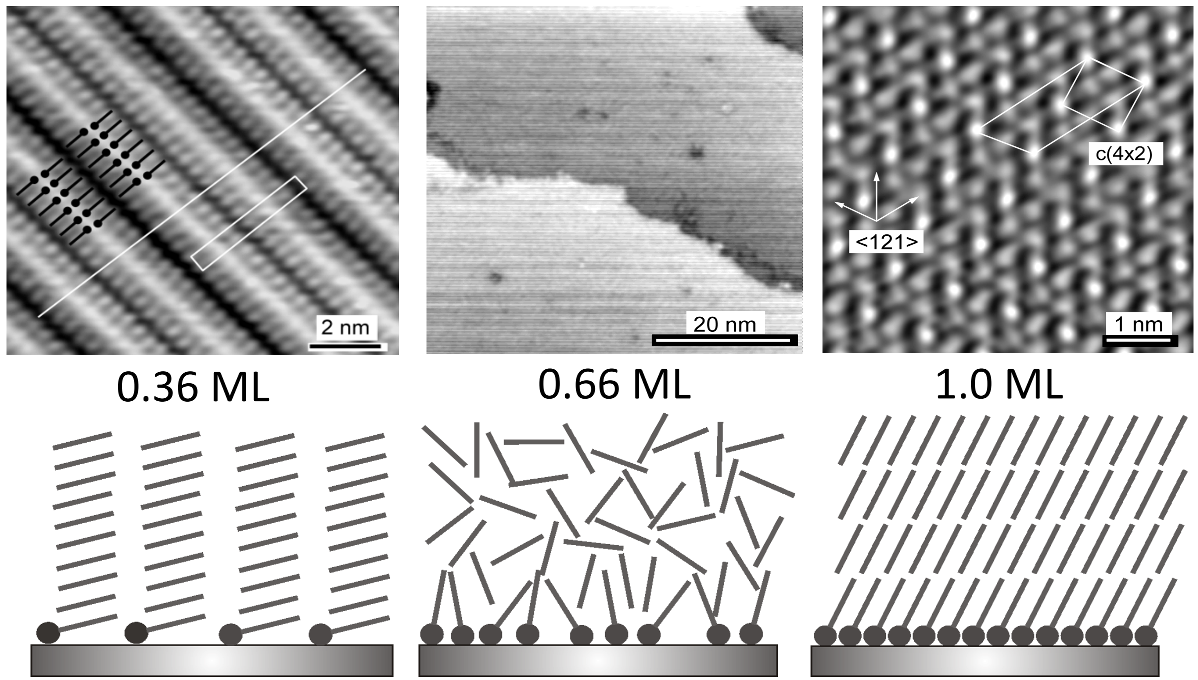
表面第1層をtemplateとする多層配向



表面第1層の分子密度（配向）を変えたときの

$C_6H_{14}/C_6H_{13}S$/Au(111)に対するC-K NEXAFS

表面第1層のチオレート単分子膜のSTM像

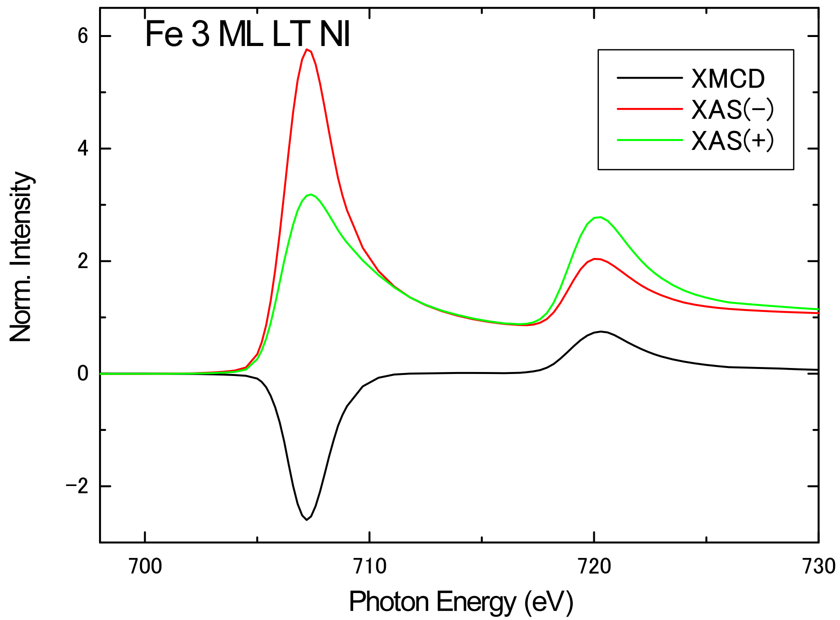


第1層： 73±5°	第1層： ランダム	第1層： 35±5°
多層　： 75±5°	多層　： ランダム	多層　： 35±5°

配向モデル

H. Kondoh et al. *Langmuir* **17**, 8178 (2001).

Basics of XMCD



XMCDで分かること

元素選択的に

- 磁化の向き
- スピンと軌道の磁気モーメント

What is XMCD?

- Normal one photon absorption (NEXAFS)
- Absorption spectroscopy with circularly polarized light
- Take the difference of the "+" and "-" XAS

$$\vec{r} = x\vec{e}_x + y\vec{e}_y + z\vec{e}_z$$

$$\vec{e} = \mp\frac{1}{\sqrt{2}}\left(\vec{e}_x \pm i\vec{e}_y\right)$$

$$P_1^{(1)} = \vec{e}\cdot\vec{r} = -\frac{1}{\sqrt{2}}(x+iy) = r\sqrt{\frac{4\pi}{3}}Y_1^1 \quad : Right$$

$$P_{-1}^{(1)} = \vec{e}\cdot\vec{r} = \frac{1}{\sqrt{2}}(x-iy) = r\sqrt{\frac{4\pi}{3}}Y_1^{-1} \quad : Left$$

selection rules:

orbital angular momentum quantum number: $\Delta l = \pm 1$

magnetic quantum number: $\Delta m_l = +1$ (Right), -1 (Left)

XMCD signal intensity

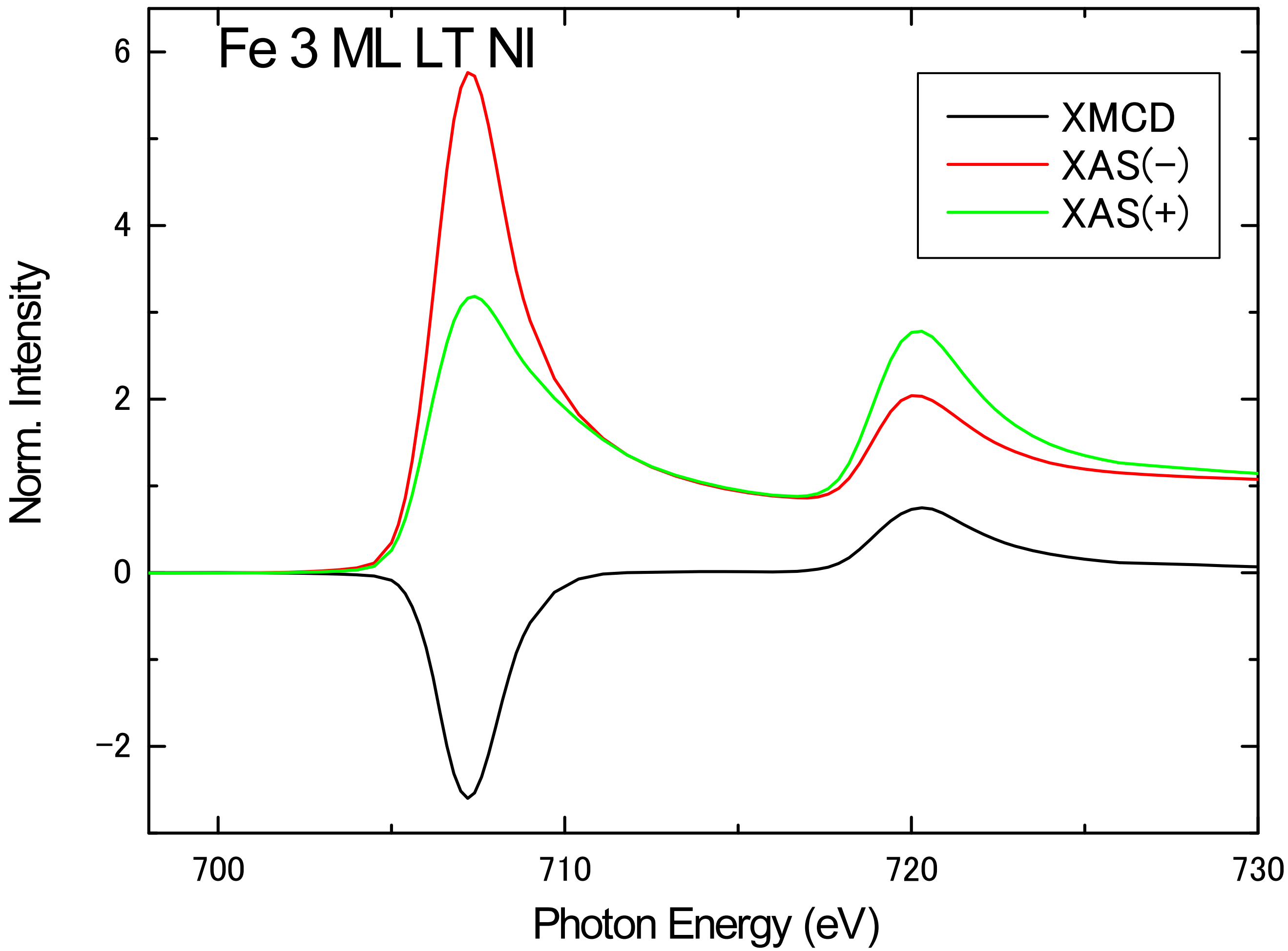
$\Delta I = I(+) - I(-)$

$I(+)$: XAS with photon spin parallel to majority spin

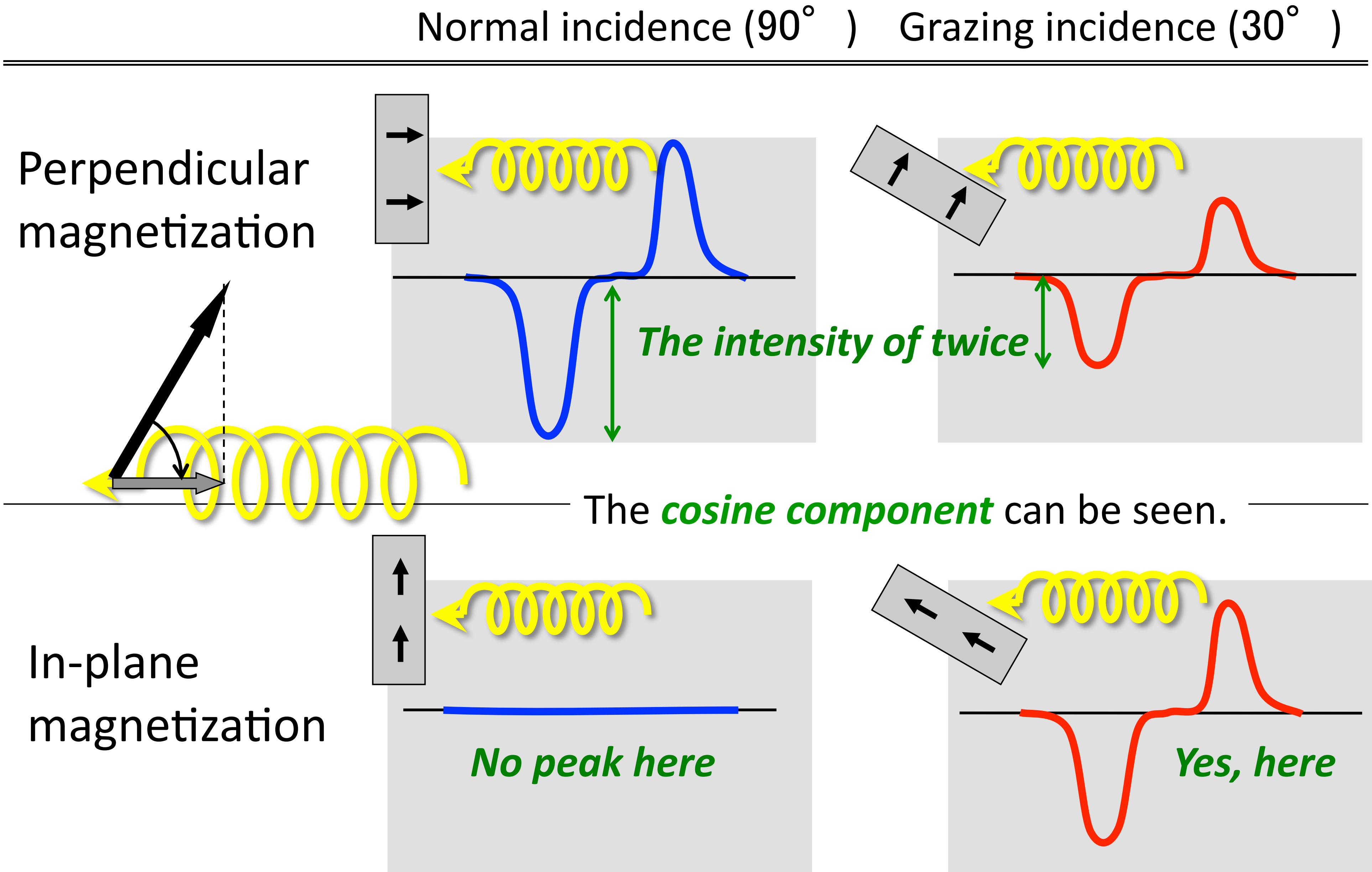
$I(-)$: XAS with photon spin antiparallel to majority spin

XAS(+) - XAS(-) = XMCD

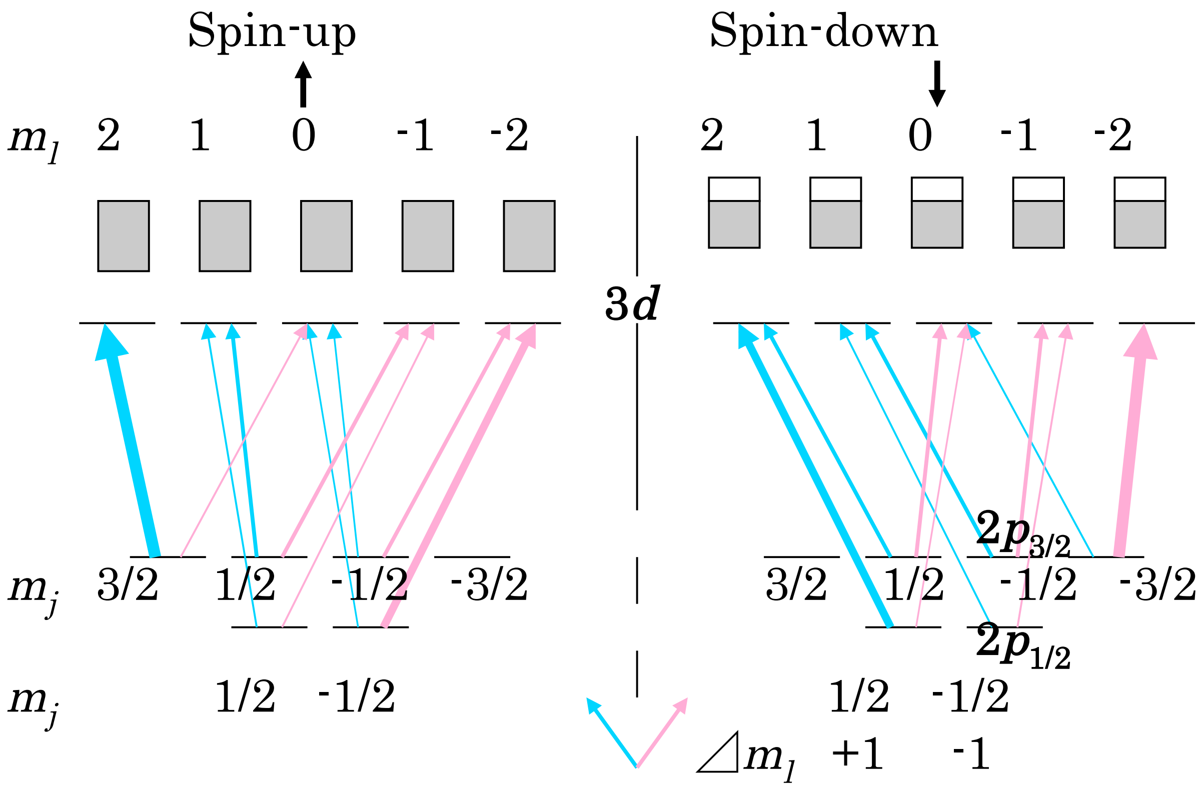
X-ray Absorption Spectrum X-ray Magnetic Circular Dichroism



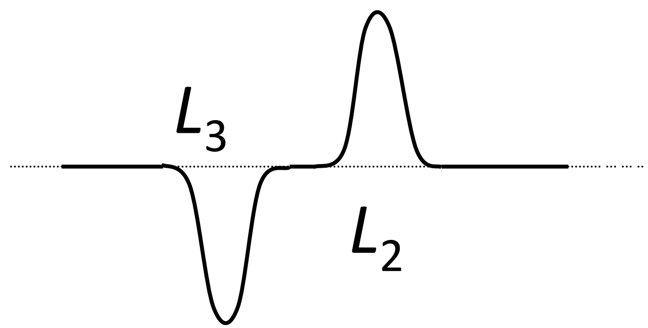
XMCD spectra and magnetization direction



XMCD: *d* orbitals without s-o interaction



$|\Delta L3| = |\Delta L2|$



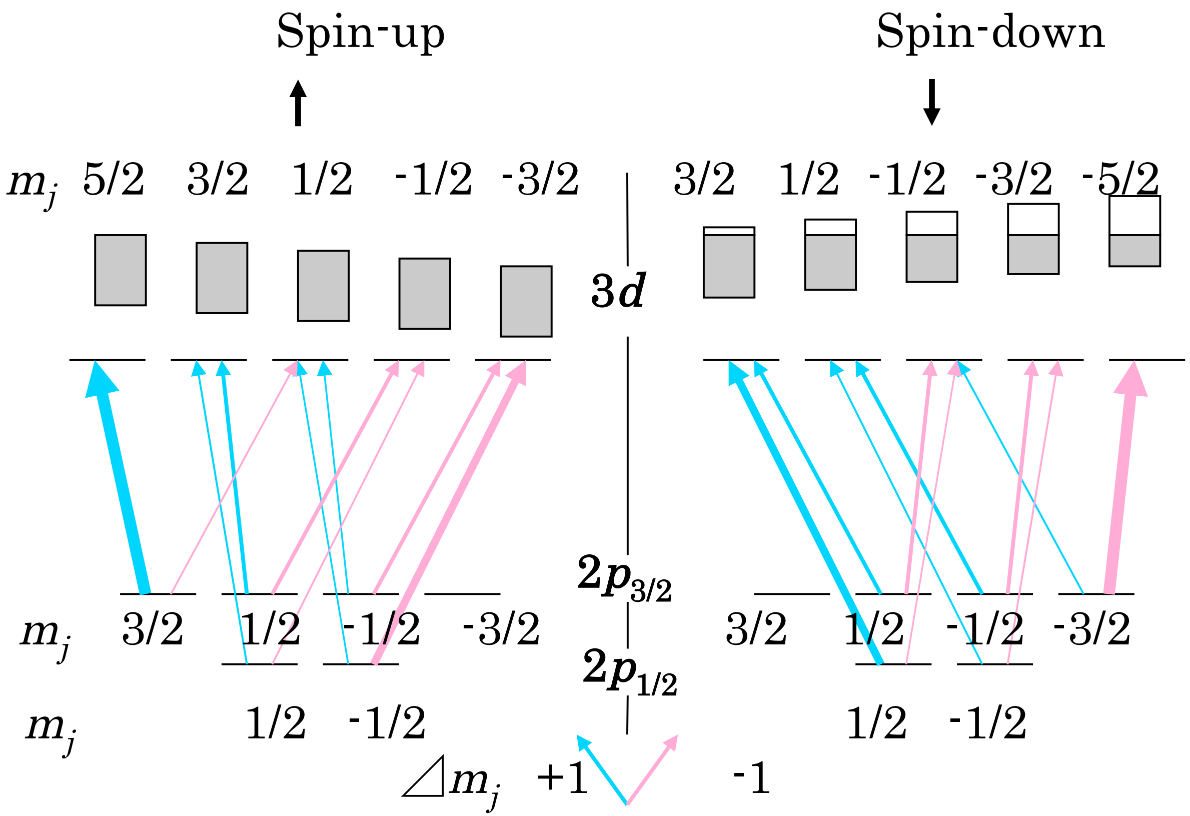
d orbitals without spin-orbit interaction

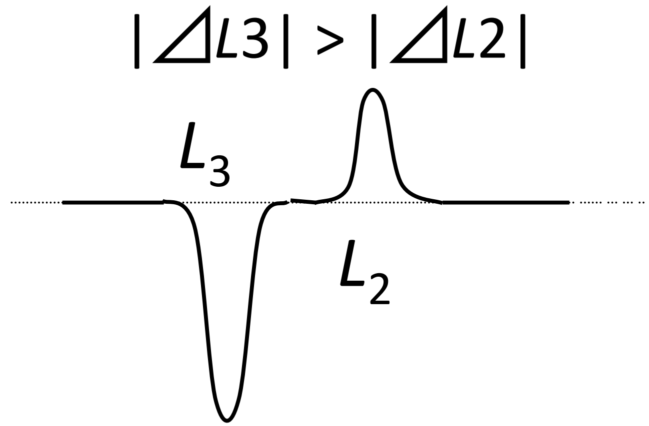
Quenched orbital magnetic moment ⇨

Symmetric shape of XMCD

The same XMCD intensities both at L_3 edge and L_2 edge

XMCD: *d* orbitals with s-o interaction

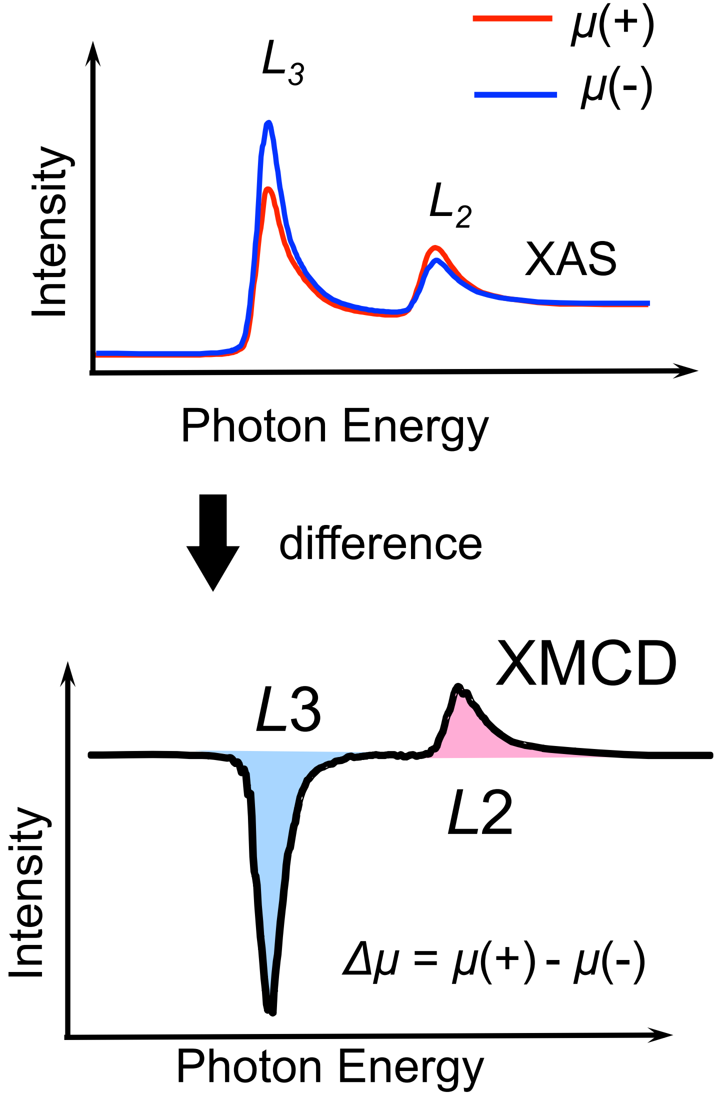


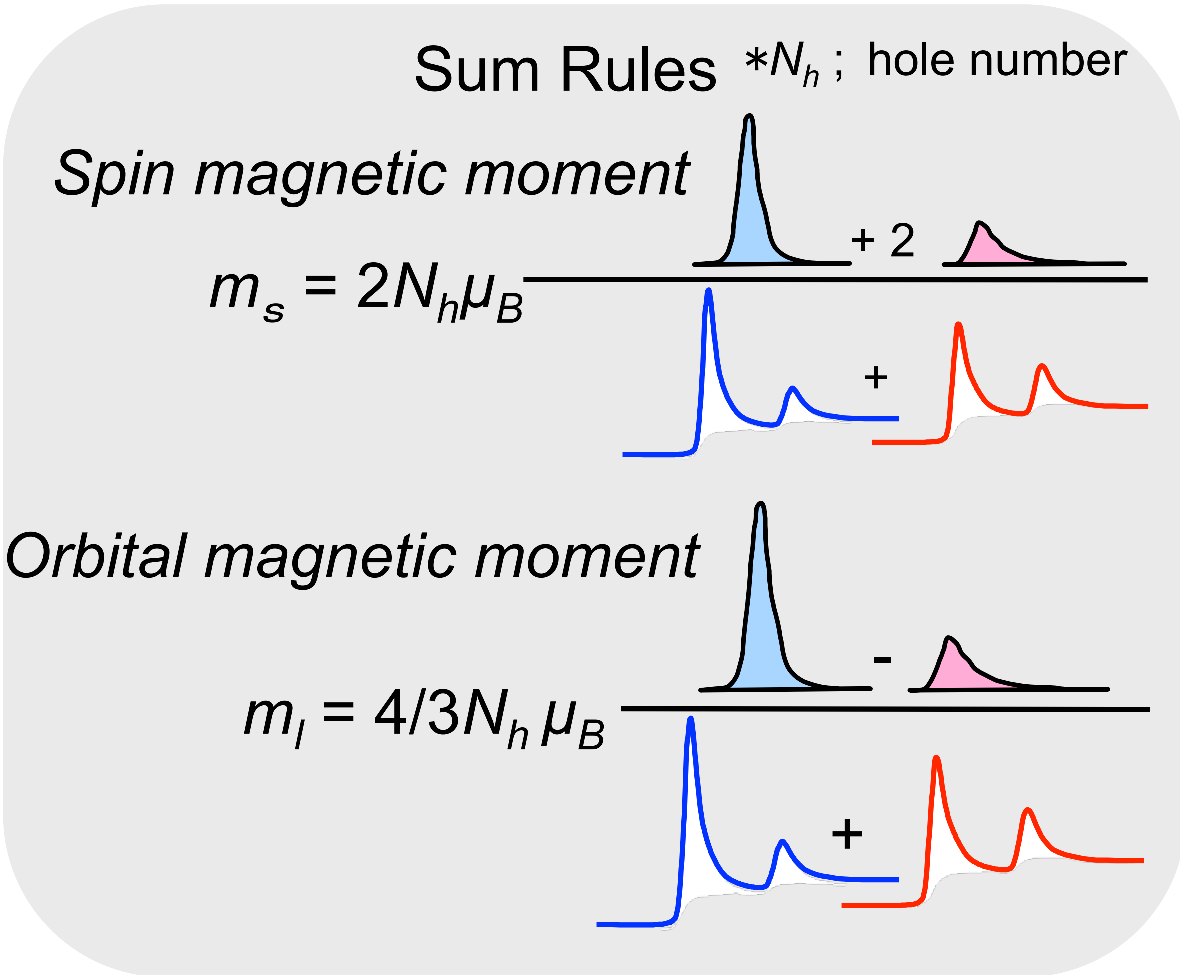


d orbitals with spin-orbit interaction

Survived orbital magnetic moment ⇨ Asymmetric shape of XMCD

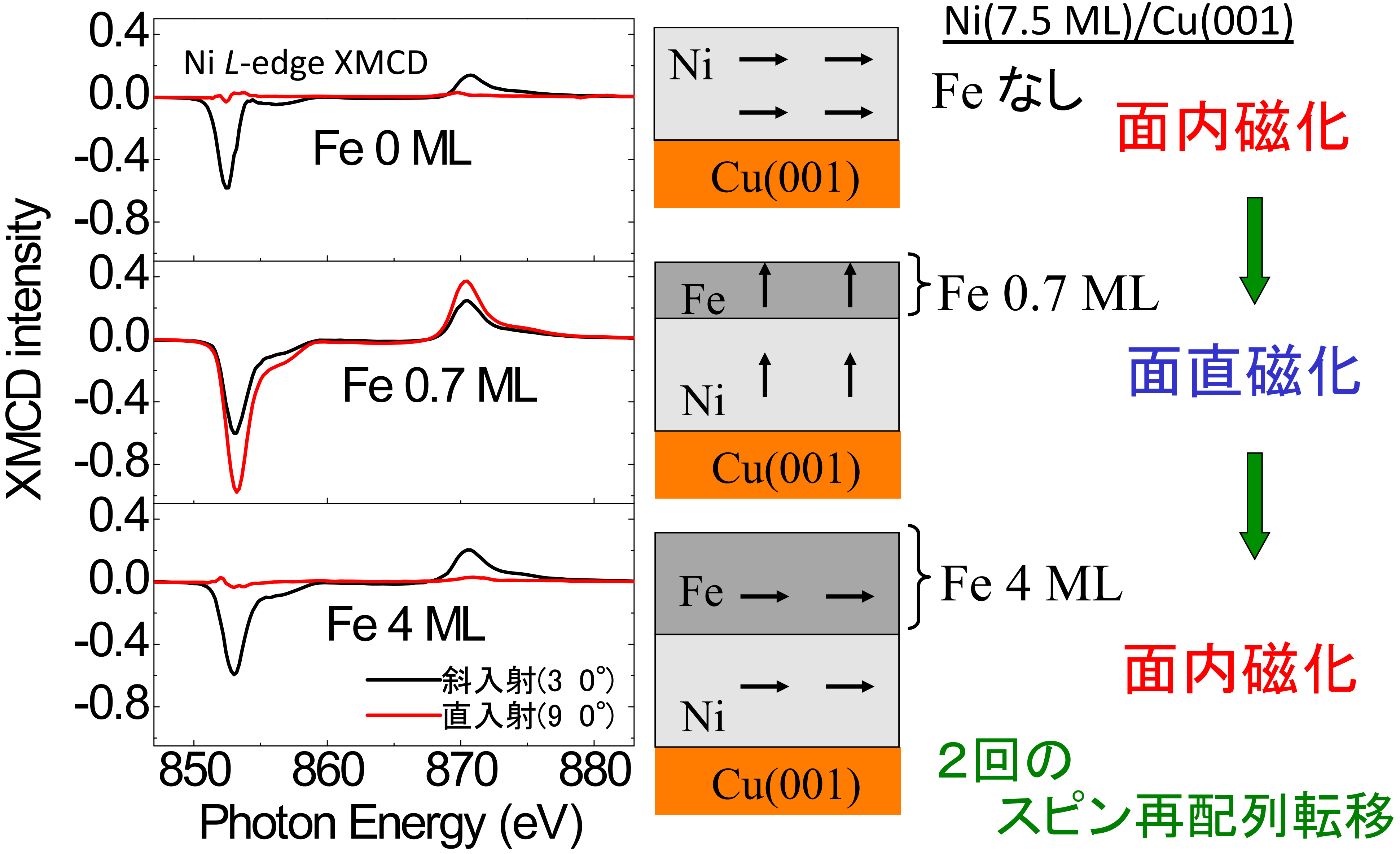
Sum rules: XMCD spectra and magnetic moments



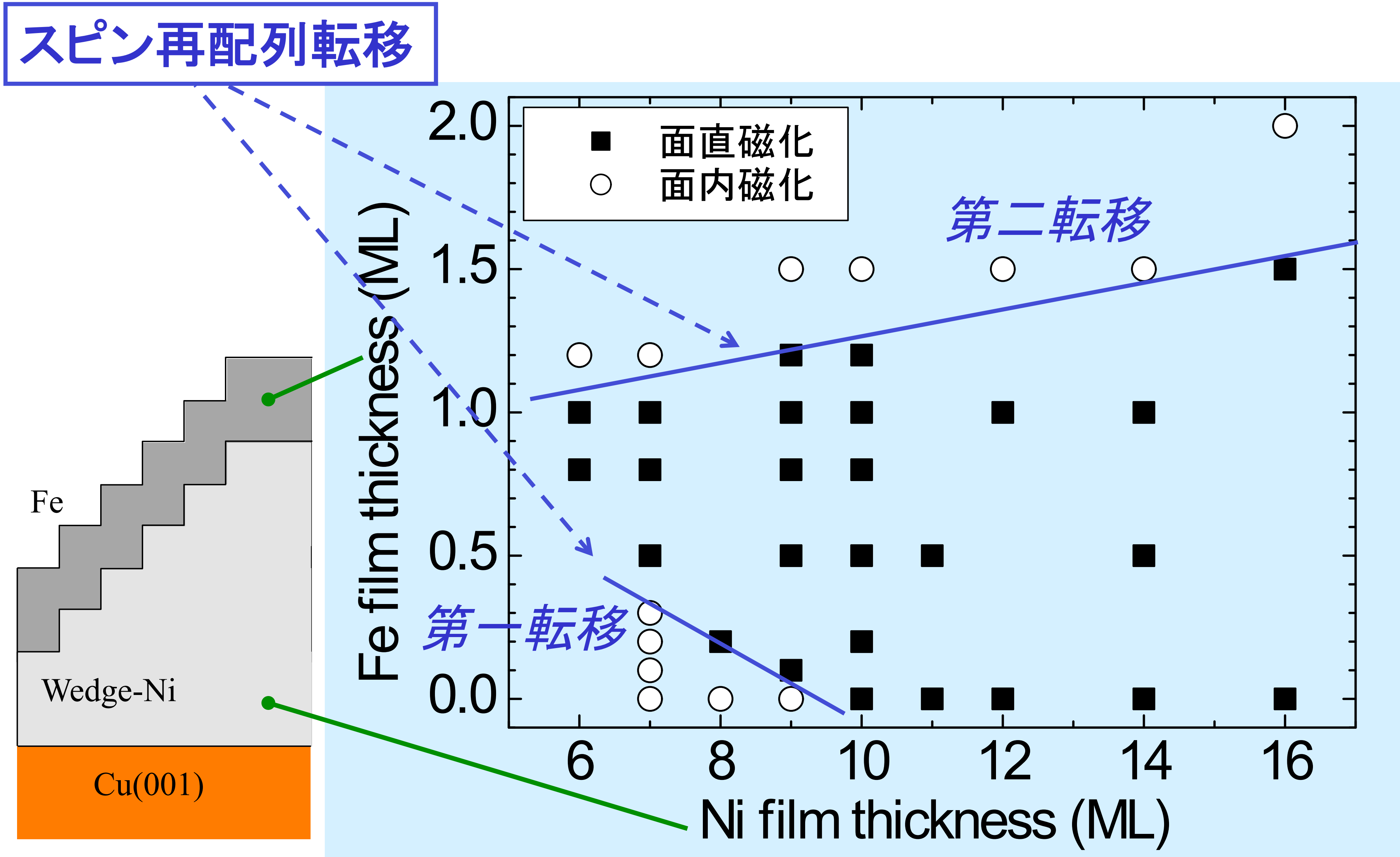


B. T. Thole, *et al.*, Phys. Rev. Lett. **68**, 1943 (1992)
P. Carra, *et al.*, Phys. Rev. Lett. **70**, 694 (1993)

Ni/Cu(001)にFeを蒸着していくと…



Fe/Ni/Cu(001)の磁気異方性相図



NEXAFS, XMCDでわかること

We can get from...

元素選択的に

NEXAFS:

- どんな分子が（表面近傍に）存在するか
- その分子がどんな方向を向いているか
- その分子がどのくらいあるか

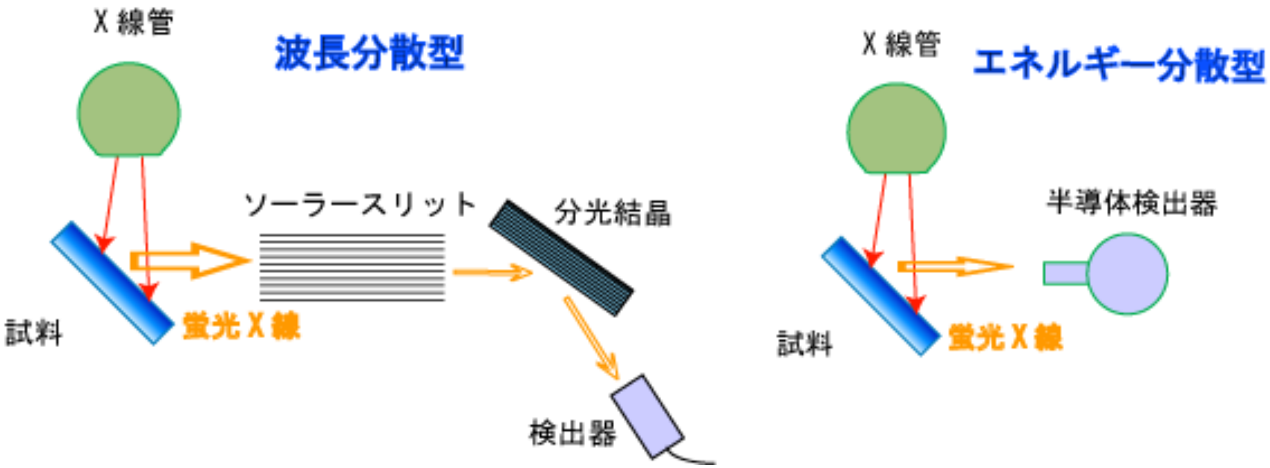
XMCD:

- 磁化の方向
- スピンと軌道の磁気モーメント

蛍光X線分析

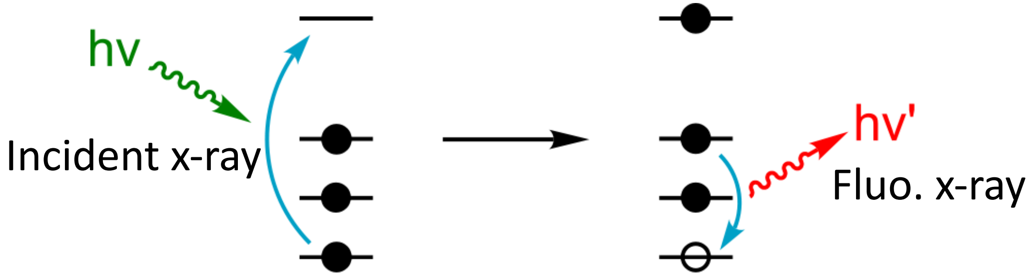
(X-ray Fluorescence Analysis, XRF)

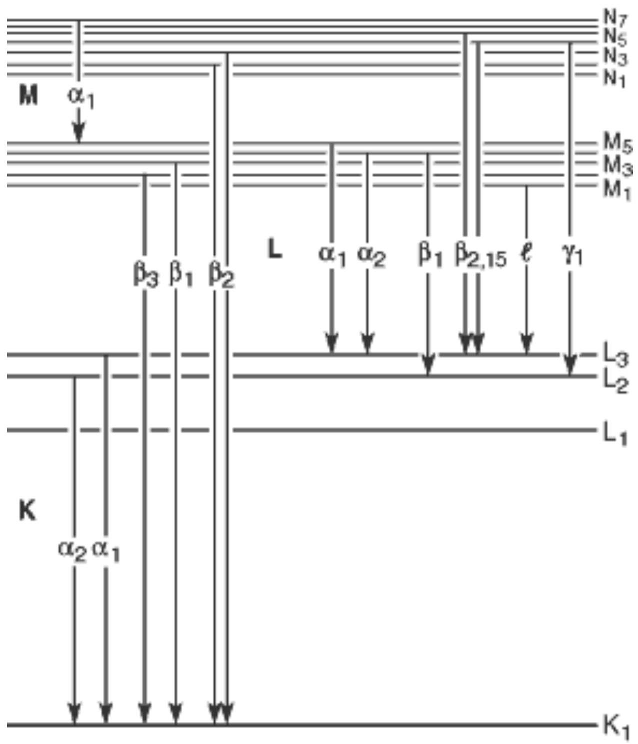
(1) 試料の化学的処理は不要（非破壊分析）。
(2) 適用元素はNaからUまでの全元素で、測定時間も短い。多元素分析も可能。
(3) 分析可能範囲が、1ppm程度から100%までと広い。しかも分析精度が高い。



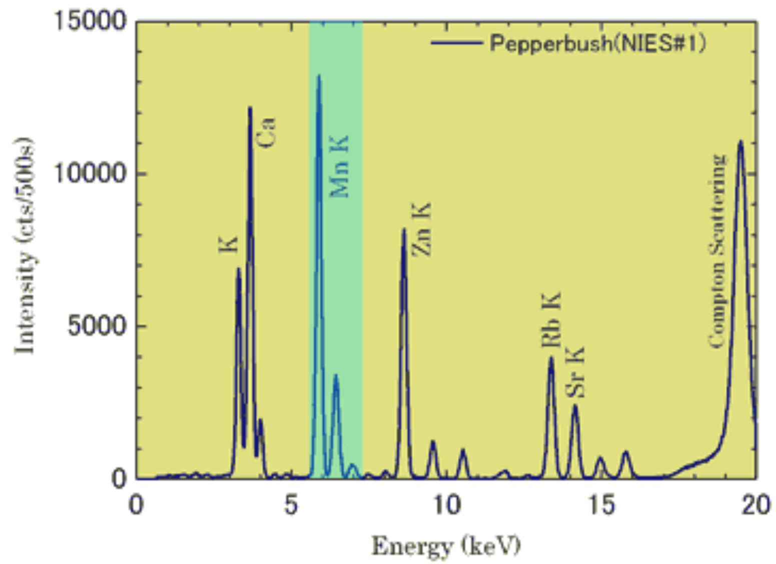
http://pfwww.kek.jp/iida/xrf.htm

Element specific emission: Fluorescent x-ray





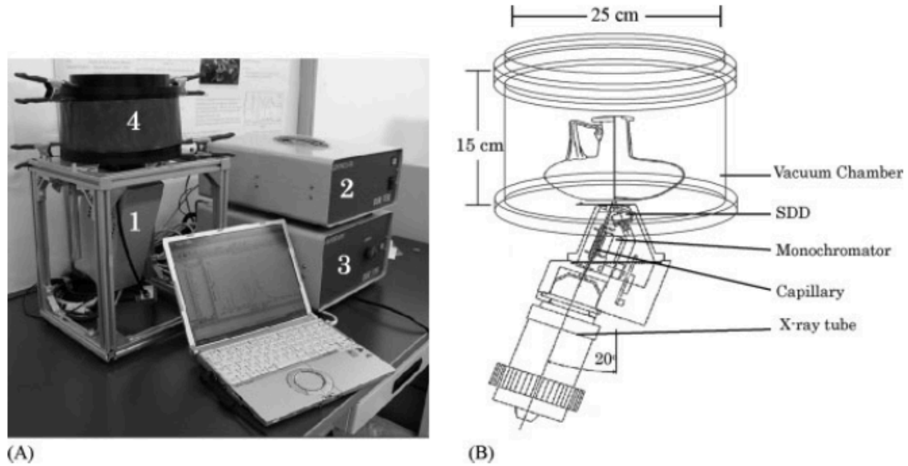
Element	$K\alpha_1$	$K\alpha_2$
22 Ti	4,510.84	4,504.86
23 V	4,952.20	4,944.64
24 Cr	5,414.72	5,405.509
25 Mn	5,898.75	5,887.65
26 Fe	6,403.84	6,390.84
27 Co	6,930.32	6,915.30
28 Ni	7,478.15	7,460.89
29 Cu	8,047.78	8,027.83
30 Zn	8,638.86	8,615.78

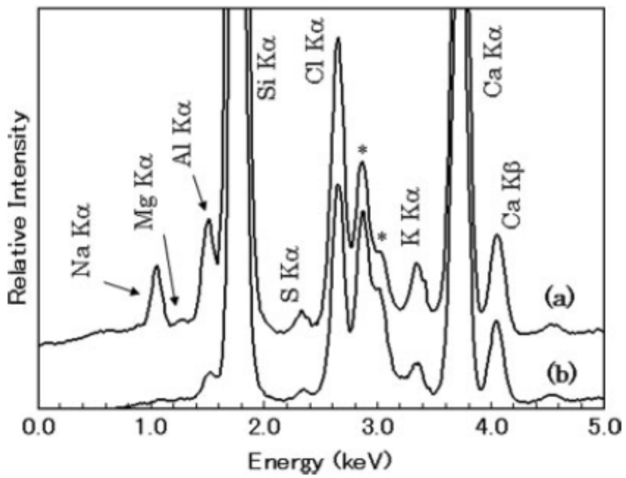


XRFを使った研究例: 古代のガラス

Archaeological analysis of Roman glass excavated from Zadar, Croatia, by a newly developed portable XRF spectrometer for glass

K. Tantrakarn,[a] N. Kato,[a] A. Hokura,[a] I. Nakai,[a]* Y. Fujii[b] and S. Gluščević[c]





Na_2O, MgO, Al_2O_3, PdO, CuO, ...

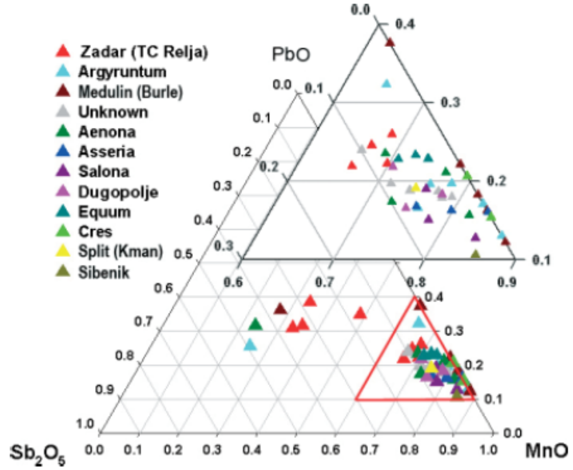
各元素の含有量がわかる

X-ray Spectrometry **38**, 121 (2009)

数十%からppmという幅広い濃度で分析できる

Table 3. Glass types and their average chemical compositions

	Bell-shaped flask		Depression flask		Square jug		Cinerary urn		Glass ingot
	Mn decolorizers N = 40	Sb decolorizers N = 8	Mn decolorizers N = 15	Sb decolorizers N = 4	Mn decolorizers N = 4	Sb decolorizers N = 3	Mn decolorizers N = 5	Sb decolorizers N = 1	N = 1
Na_2O (wt%)	14.6 ± 4.5	11.5 ± 6.3	16.4 ± 0.6	24.9 ± 5.5	20.0 ± 3.2	19.6 ± 3.9	18.7 ± 5.8	9.2	14.8
MgO (wt%)	0.60 ± 0.06	0.65 ± 0.05	0.59 ± 0.02	0.66 ± 0.02	0.49 ± 0.24	0.09 ± 0.03	0.16 ± 0.24	0.02	0.06
Al_2O_3 (wt%)	1.28 ± 0.19	1.21 ± 0.33	1.98 ± 0.69	1.73 ± 0.17	1.26 ± 0.17	1.10 ± 0.05	1.10 ± 0.13	1.30	1.11
K_2O (wt%)	0.19 ± 0.06	0.20 ± 0.06	0.23 ± 0.11	0.27 ± 0.02	0.26 ± 0.08	0.26 ± 0.04	0.19 ± 0.06	0.22	0.15
CaO (wt%)	4.25 ± 0.50	3.58 ± 0.53	3.96 ± 0.33	4.64 ± 0.04	4.16 ± 0.44	3.68 ± 0.22	3.85 ± 0.54	3.22	3.32
MnO (wt%)	1.10 ± 0.15	1.05 ± 0.18	1.00 ± 0.12	1.05 ± 0.10	0.70 ± 0.09	0.80 ± 0.05	0.15 ± 0.01	0.15	0.82
Fe_2O_3 (wt%)	0.29 ± 0.05	0.32 ± 0.05	0.30 ± 0.05	0.39 ± 0.01	0.32 ± 0.08	0.34 ± 0.01	0.27 ± 0.06	0.30	0.24
PbO (ppm)	100 ± 30	360 ± 100	190 ± 70	470 ± 30	200 ± 190	1620 ± 360	250 ± 230	1000	90
SrO (ppm)	680 ± 90	580 ± 80	690 ± 20	700 ± 30	635 ± 85	560 ± 40	580 ± 50	530	550
CuO (ppm)	1100 ± 240	1220 ± 300	1410 ± 120	1640 ± 40	1480 ± 800	2070 ± 400	1640 ± 1320	1740	1020
Zr (ppm)	3580 ± 220	3520 ± 370	3800 ± 60	3840 ± 160	3630 ± 280	3560 ± 70	3550 ± 100	3700	3510
Sb_2O_3 (ppm)	1650 ± 1270	26300 ± 9800	2560 ± 1790	22500 ± 6300	2200 ± 1090	23500 ± 1900	2790 ± 2240	22000	1390

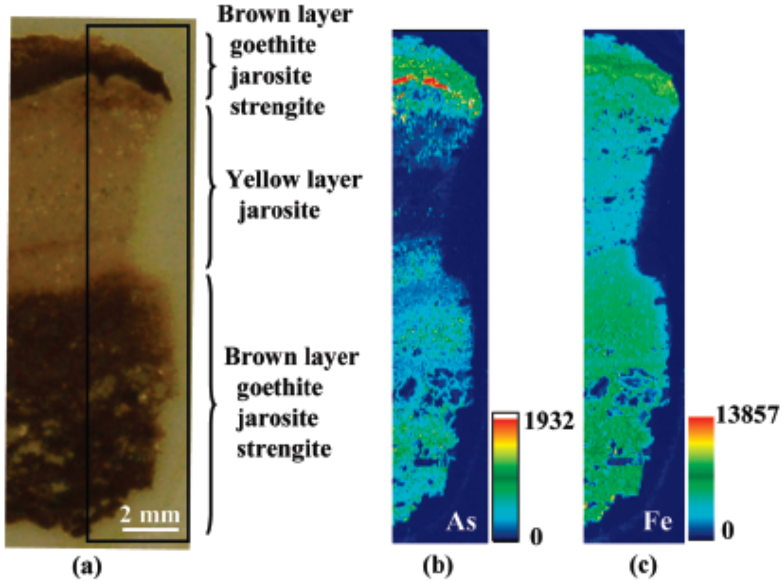


μ-XRFを使って元素マッピングの例

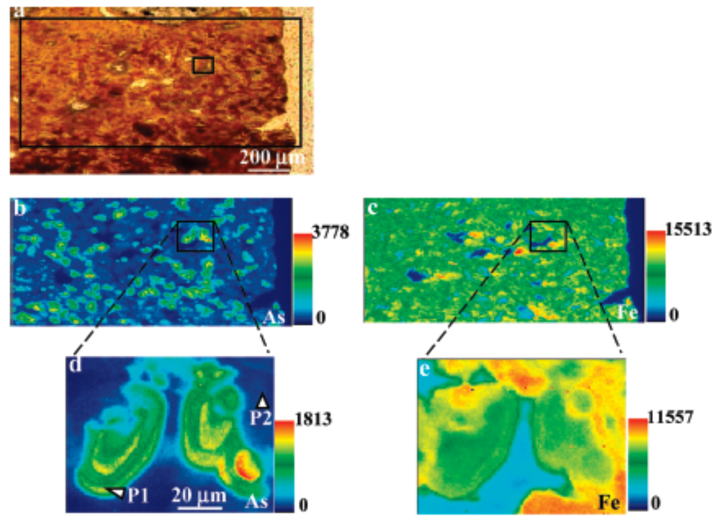
Chemical Speciation of Arsenic-Accumulating Mineral in a Sedimentary Iron Deposit by Synchrotron Radiation Multiple X-ray Analytical Techniques

SATOSHI ENDO,† YASUKO TERADA,‡ YASUHIRO KATO,§ AND IZUMI NAKAI*,†

鉱物中の元素の濃度分布が見える



As　　Fe



As　　Fe

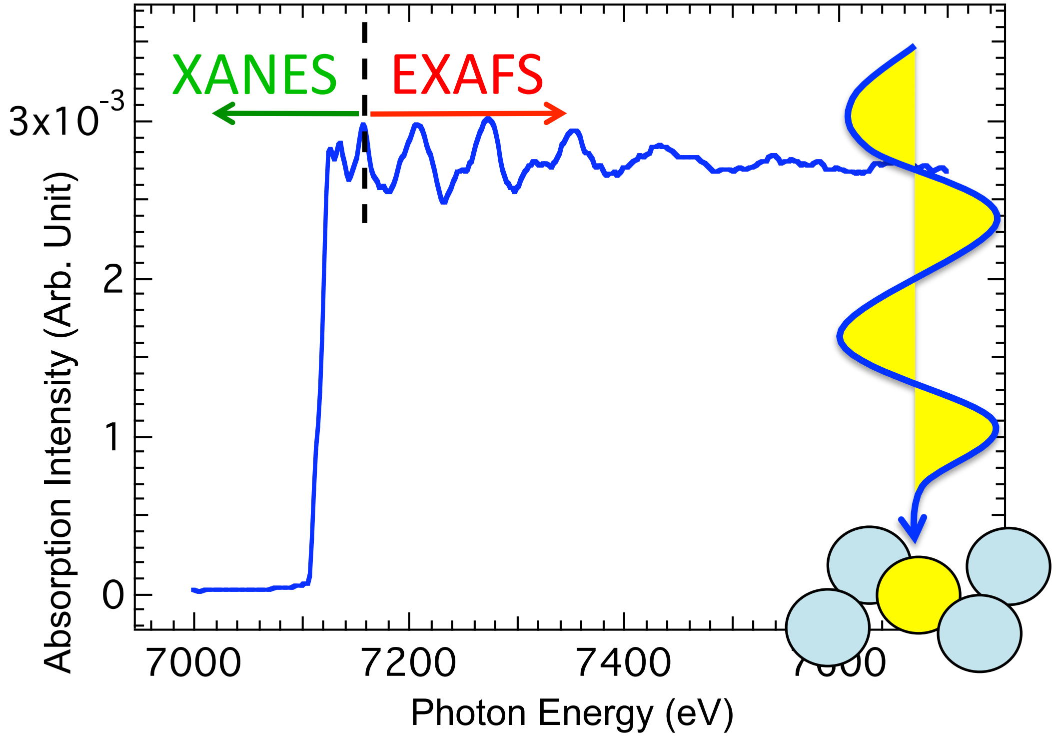
Environ. Sci. Technol. **42**, 7152 (2008)

XAFSって？ -XAFSデータが含むもの-

X-ray Absorption Fine Structure
（X線吸収微細構造）

電子状態
（価数）
対称性

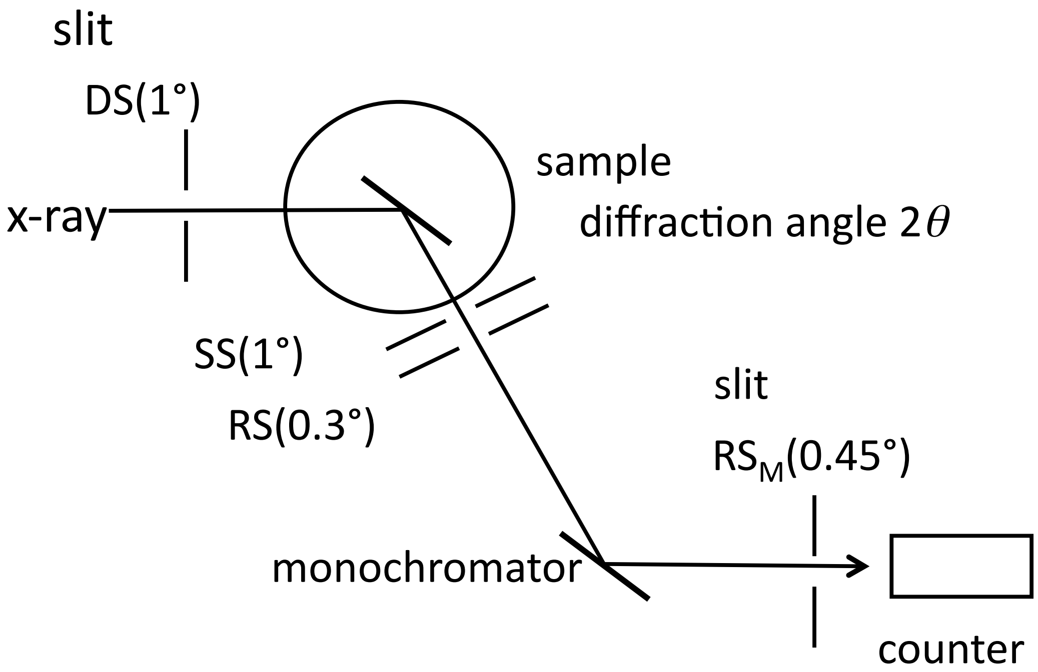
吸収原子と周辺の散乱原子との結合距離
周辺原子の数（配位数）、種類
周辺原子の分布の様子、熱振動



元素選択的に情報が得られる
局所構造を観測する
　結晶のような周期性がなくてもOK
固相、液相、気相、何でも測定できる

XANES: X-ray Absorption Near Edge Structure
EXAFS: Extended X-ray Absorption Fine Structure

X-ray diffraction (XRD)



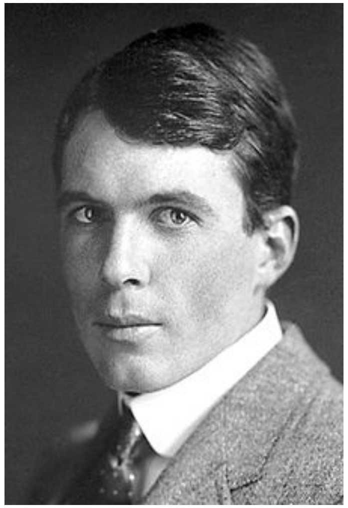
a machine for XRD measurements

RINT-TTR III, Rigaku

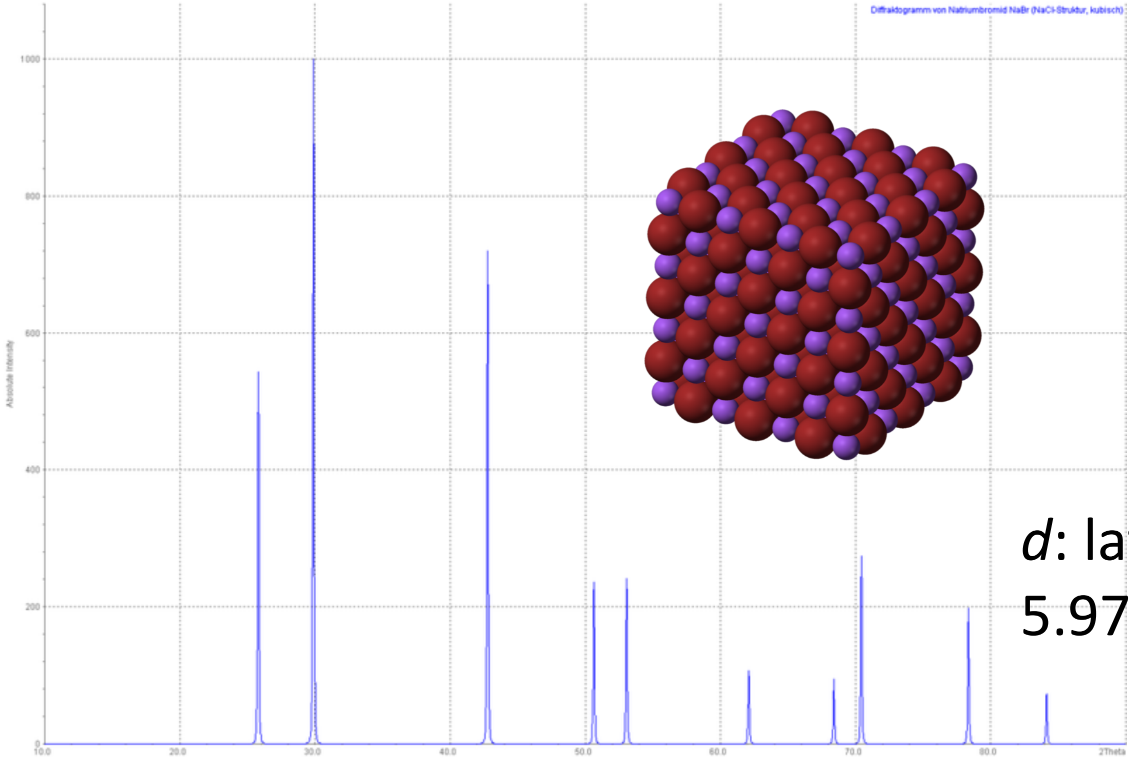
an XRD spectrum of NaBr

What is the ruler here?

The wave length of the x-ray is used as **a ruler** to measure the lattice constant.



W. L. Bragg
(1890-1971)



2θ

Bragg's law

$$2d\sin\theta = n\lambda$$

d: lattice constant
5.97 Å

***Long range order is required** for XRD measurements.*

結合距離でなぜX線なのか？

モノの長さを測る時、どうする？

定規：　目盛りがあって、好きな長さが測れる。

定規がなかったら？

背の高さ、腕を広げた長さ、手の大きさ、…などを使う

測りたいモノによって、適した基準のモノがある

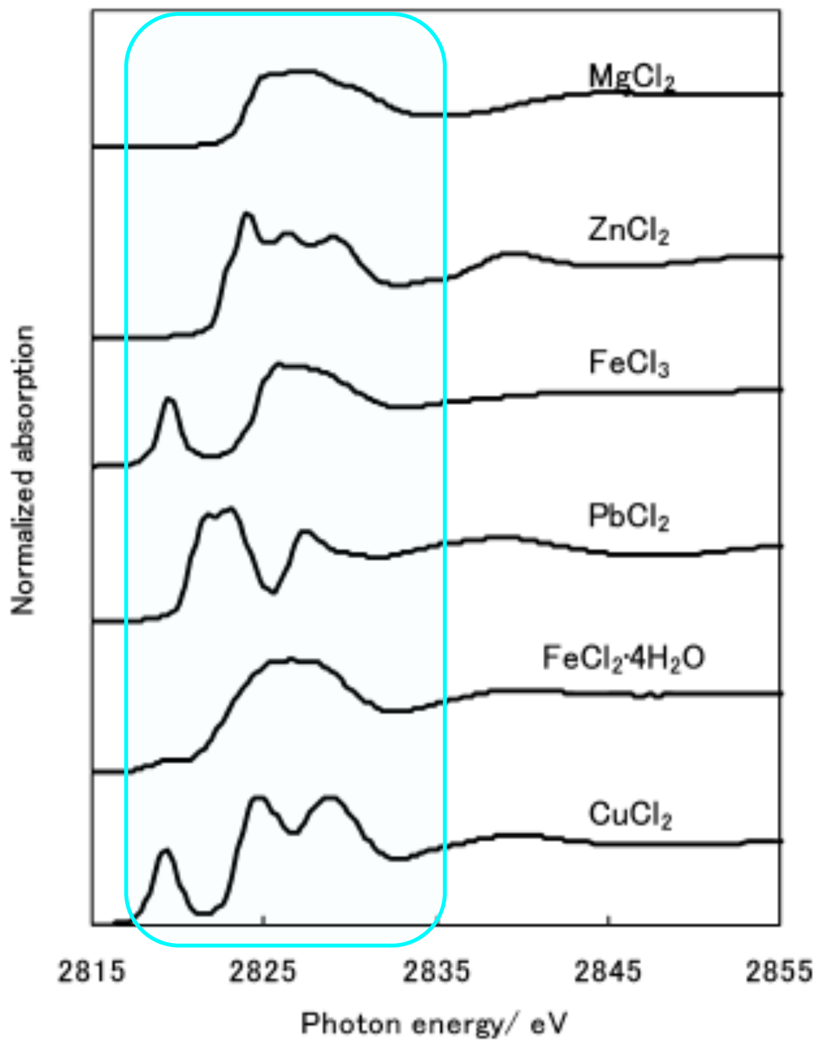
（背の高さでペンの長さは測らない）

測りたいモノ：　結晶周期、原子間距離、…

適した基準のモノ：　X線の波長、電子の波動性、…

XANES tells us what your sample is.

Cl *K*-edge XANES



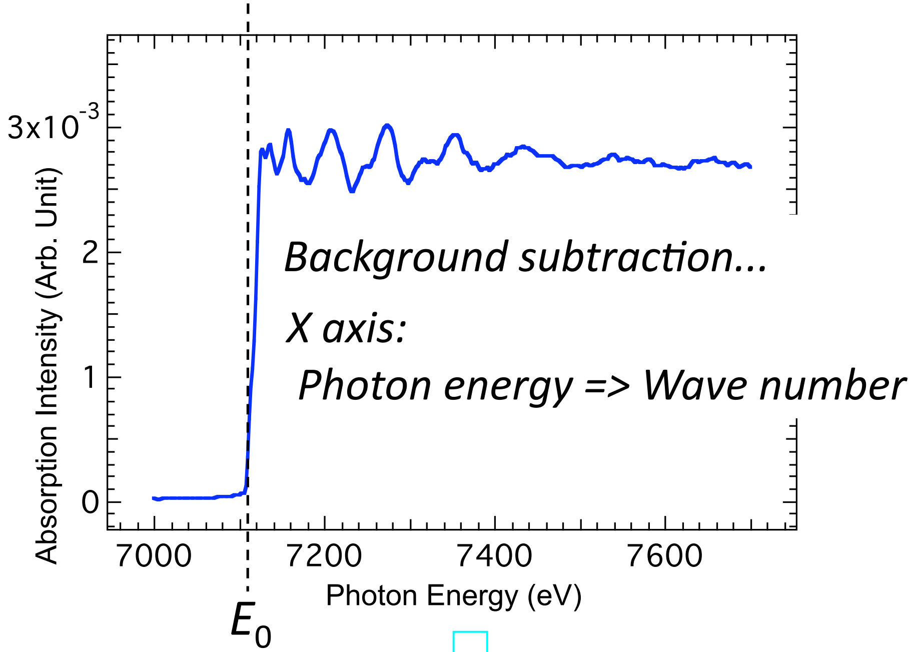
All these are metal chlorides.

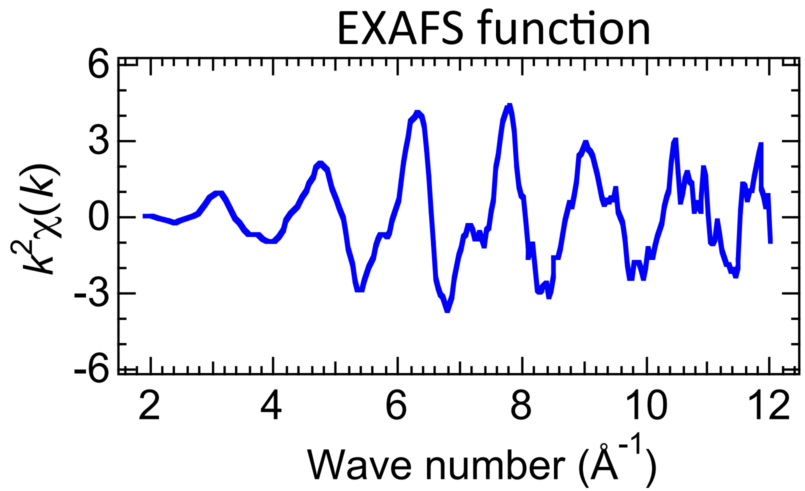
But you can see some specific features in each spectrum.

So you would recognize what your sample is.

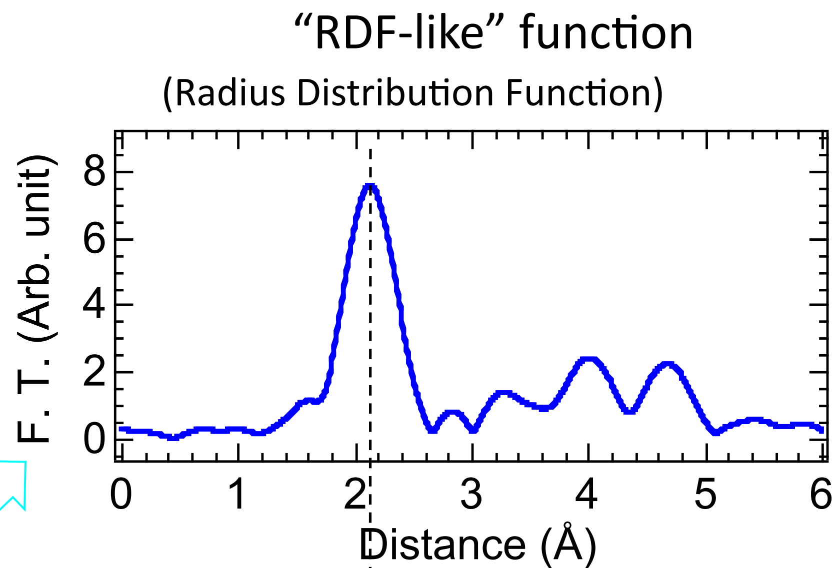
F. Zhu, *et al.,* Environ. Sci. Technol. **42**, 3932 (2008)

How to Obtain Bond Length by EXAFS





Fourier Transform



Nearest neighbor atomic distance

\+ *phase shift*

→ Bond length

Peak area

→ Coordination number

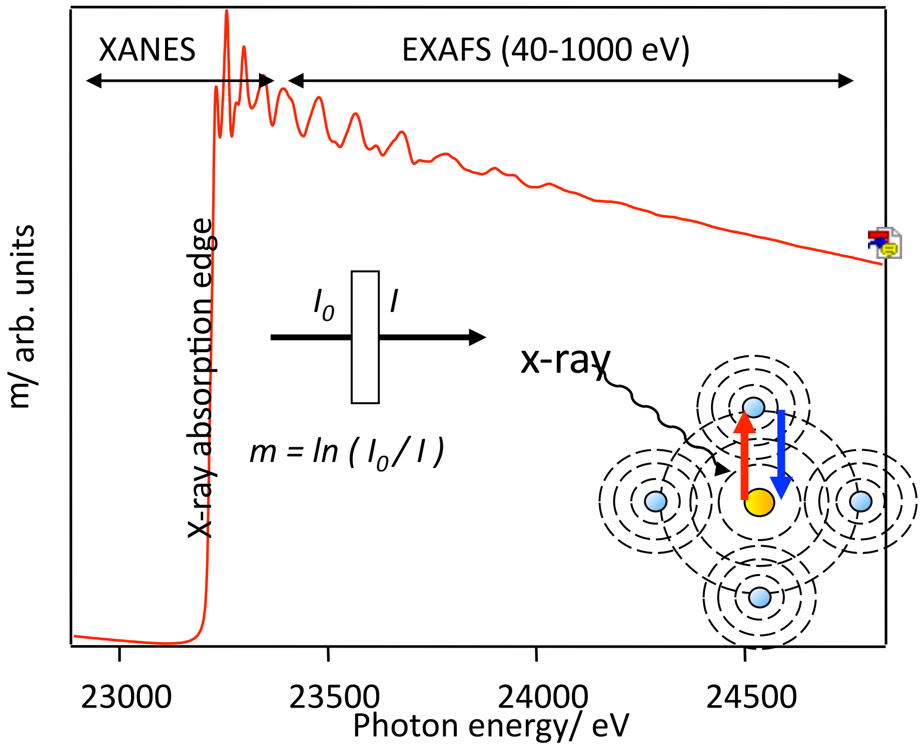
Simple things XAFS spectra give us

- XANES gives us... with element specificity
  - Valence state
    - We can determine our sample as a certain molecule or material.
  - Symmetry

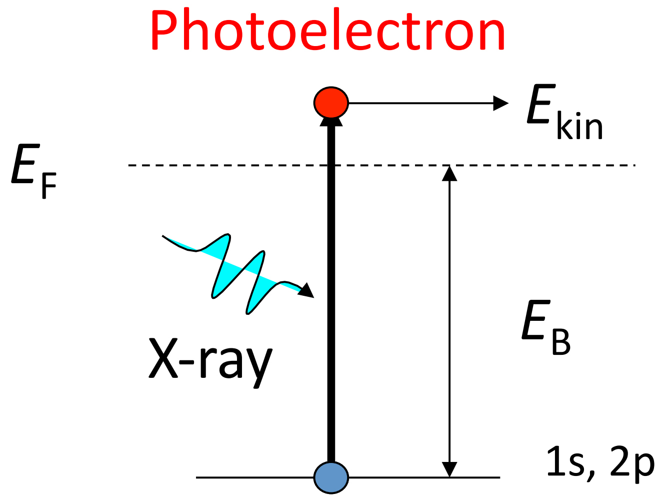
- EXAFS gives us...
  - Bond length
    - **A local structure** is given.
    - **Crystallinity, or long range order is not required**.
  - Coordination number (CN)
    - Simply, the number of atoms around the atom.
    - CN enables us to estimate sizes of nano clusters.

XAFS

- X-ray Absorption Fine Structure(XAFS)
  - XANES(X-ray Absorption Near Edge Structure)
  - EXAFS(Extended X-ray Absorption Fine Structure)



X-ray absorption spectrum

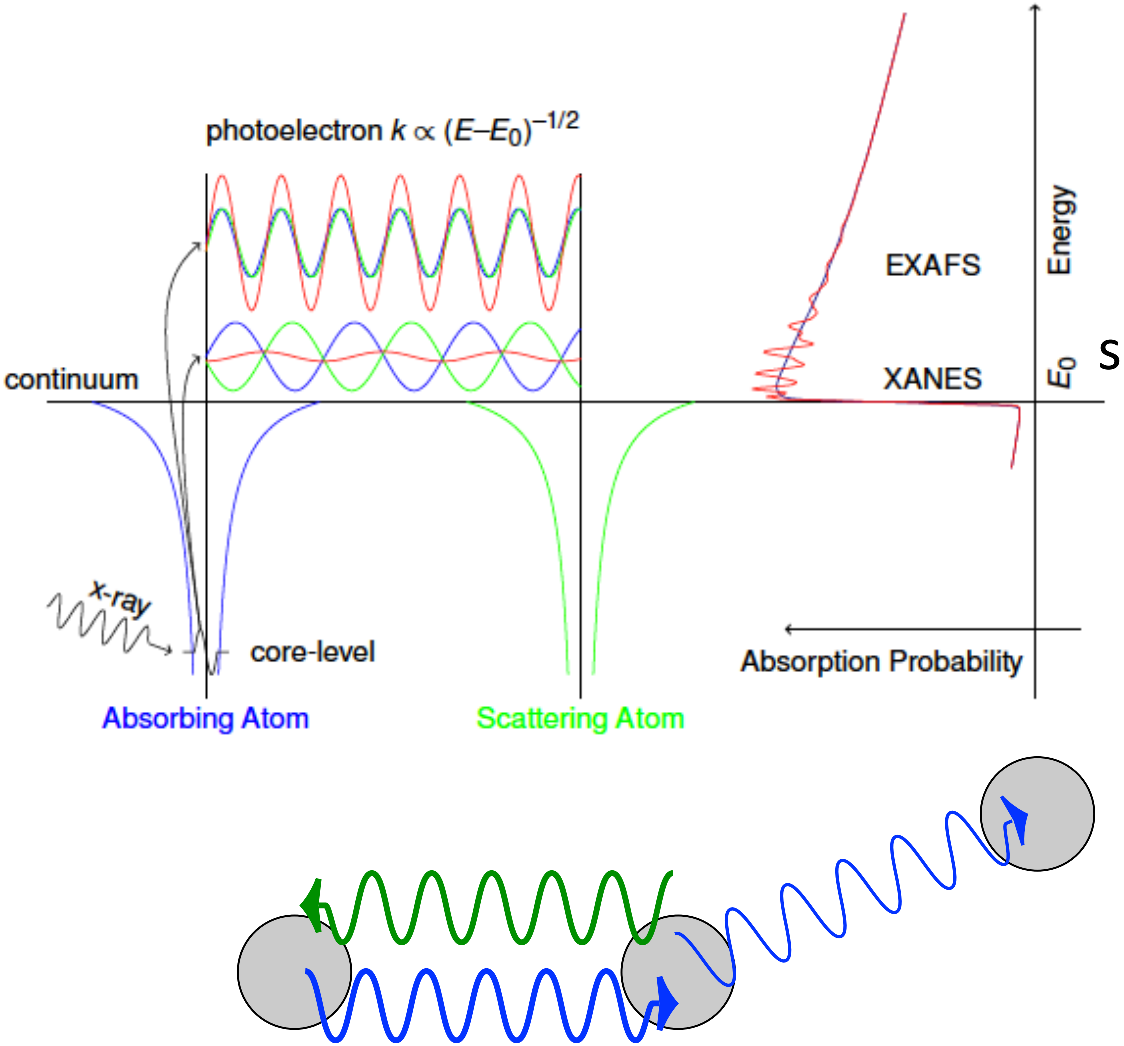


$E_{kin} = h\nu - E_B$

1s electron *K* shell

2p electron *L* shell

Picture of the wave function of final state in EXAFS



“Photoelectron (wave)” emitted

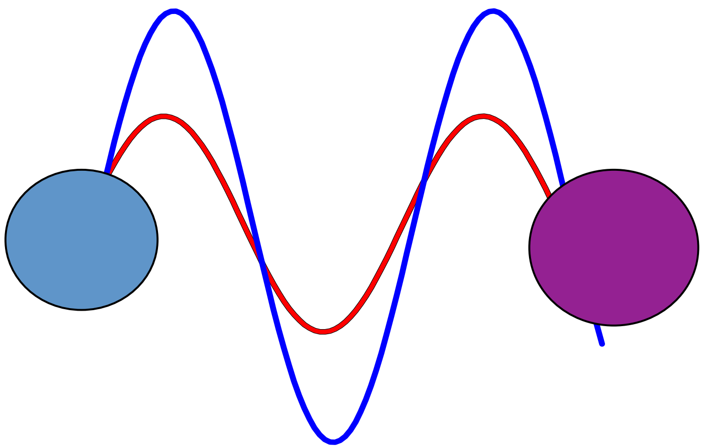
scattered by the surrounding atoms

Wave function of the final state pictured by “quantum theory of scattering”

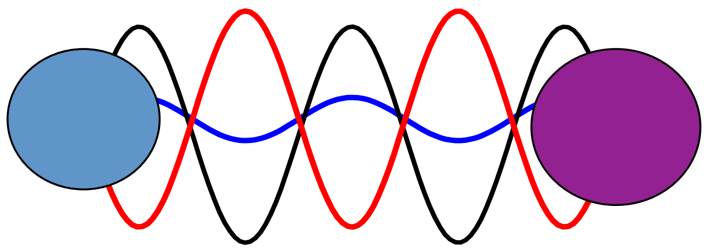
Scattering of electron and interference

$$\frac{\hbar^2 k^2}{2m} = E - E_0$$

K : wave vector
$\hbar$: Plank Const.
E : Photon energy
E_0 : threshold (edge)

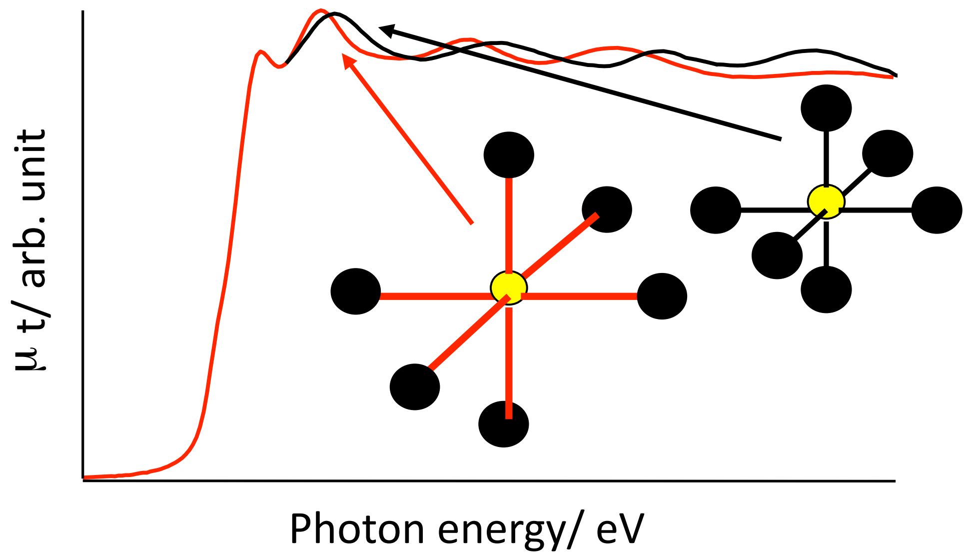


Enhancement



suppression

Bond length and Coordination number

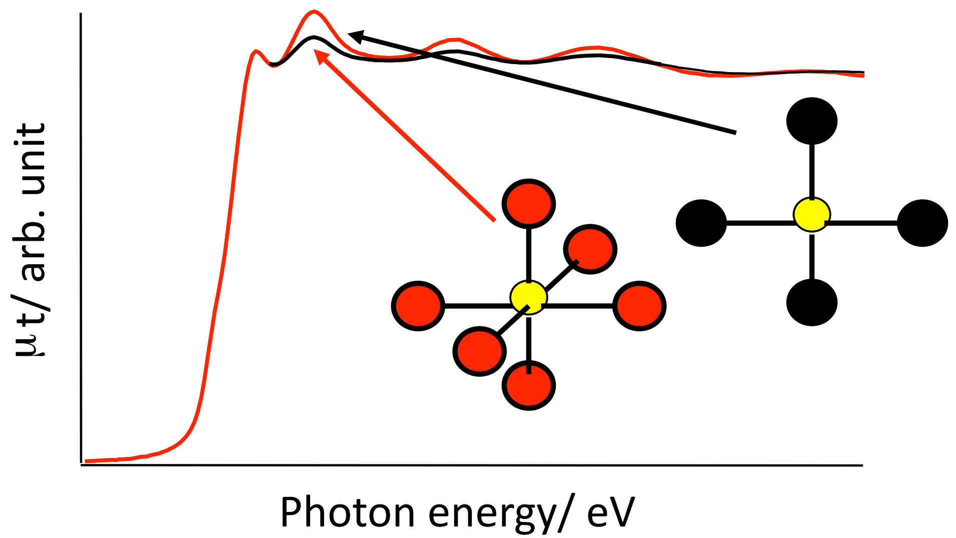


Higher frequency

(Shorter Period of Oscillation)

⇩

Longer Bond Length

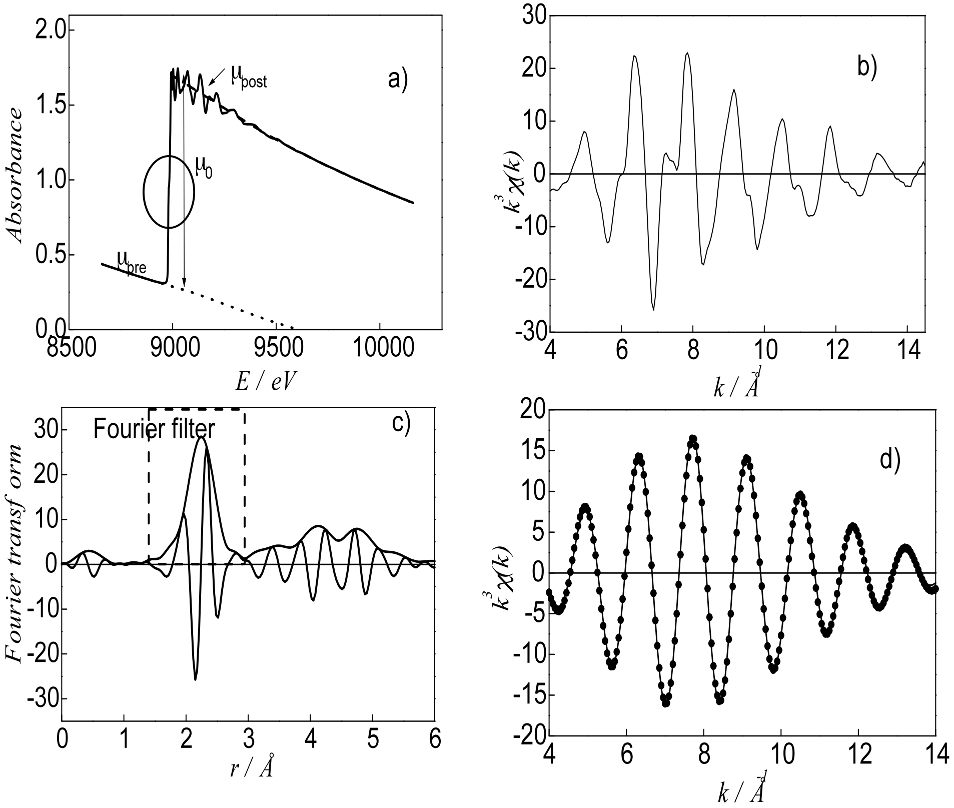


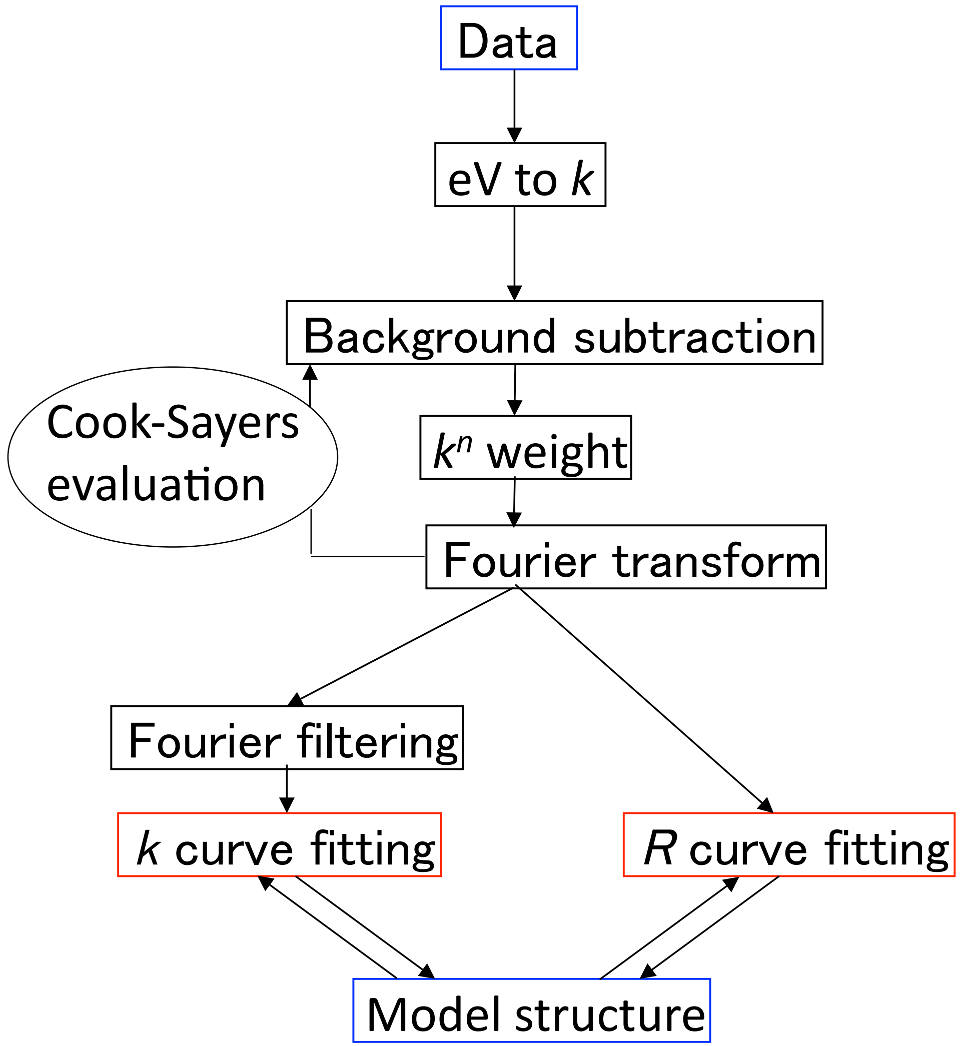
Larger Amplitude

⇩

Larger Coordination Number

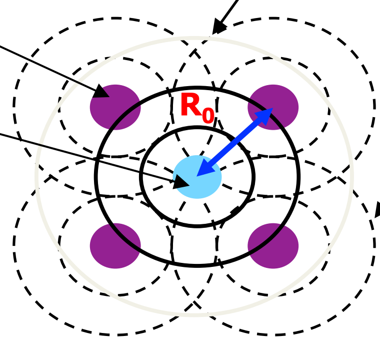
Sketch of XAFS analysis





The EXAFS equation

1. **leaving the absorbing atom**
2. **scattering from the neighbor atom**
3. **returning to the absorbing atom**



XAFS oscillation — Absorbance — Smooth backgroun — Edge-jump

$$\chi(k) = \frac{\mu(E) - \mu_s(E)}{\mu_0(E)} = S_0^2 \sum_i \frac{N_i F_i(k_i)}{k_i r_i^2} e^{-2k_i^2\sigma_i^2} \sin(2k_i r_i + \phi_i(k_i))$$

$$k = \sqrt{2m_e(E - E_0)/\hbar}$$

Theorptically or empirically derived Parameters

F_i : Backscattering amblitude

$* e^{-2r_i/\lambda(k_i)}$

ϕ_i : Phase shift

Curve-Fitting Parameters

N_i Coordination number

σ_i^2 DWfactor

E_0 energy shift

r distance

Fermi's Golden Rule to express μ of XAFS

- Born-Oppenheimer approximation
  - velocity of nuclear motion << that of electronic motion
  - (due to the high ratio between nuclear and electronic masses)
- Time-dependent Perturbation theory

Fermi's Golden Rule

$$\mu \propto \sum_f \left| \left\langle \Psi_f \middle| H' \middle| \Psi_i \right\rangle \right|^2 \delta\left(E_f - E_i - \hbar\omega\right) \quad \text{...(1)}$$

$$H' = -\frac{e}{mc} A(r) \cdot P$$

- $A(r)$: vector potential of X-ray
- P: momentum of electron

$$A(r) = \hat{e} A_0 e^{ik \cdot r}$$

- $\hat{e}$: unit vector of electric field
- r: position of electron
- k: wave number vector of X-ray

One-electron approx. & Dipole approx.

$$\mu \propto \sum_f \left|\left\langle \Psi_f \middle| H' \middle| \Psi_i \right\rangle\right|^2 \delta\left(E_f - E_i - \hbar\omega\right) \quad \text{...(1)}$$

One-electron approx.: $\left\langle \Psi_f \middle| H' \middle| \Psi_i \right\rangle \cong \left\langle \psi_f \middle| H' \middle| \psi_i \right\rangle$

All-electron wave function => One-electron wave function

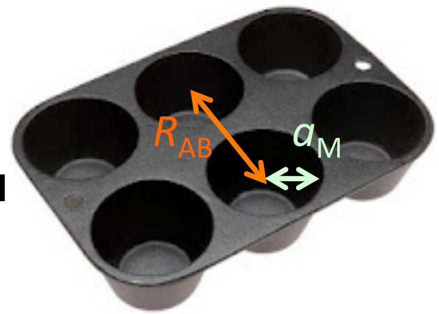
Dipole approx.: $e^{ik\cdot r} \cong 1$ for $k \cdot r << 1$

$$\mu \propto \sum_f \left|\left\langle \psi_f \middle| \hat{e} \cdot r \middle| \psi_i \right\rangle\right|^2 \delta\left(E_f - E_i - \hbar\omega\right) \quad \text{...(2)}$$

fundamental equation to express XAFS

Assumptions to depict EXAFS eq.

- [1] 一光子吸収
- [2] 一電子近似 & 双極子近似
- [3] (K殻) 電子放出 & 一電子散乱近似
- [4] kR_{AB} >> 1 近似.
  - 各散乱の素過程は主要項で近似（高次項は無視できる）
- [5] Muffin-tinポテンシャル近似
  - ポテンシャルは半径a_Mの球内で球対称で、その中間領域では一定であるとする
- [6] 平面波近似.
  - 最近接原子間距離R_{AB}に対し、a_M << R_{AB}なので、散乱は平面波で記述できるとする



Eq. of single scattering EXAFS

Amplitude — Oscillation (phase)

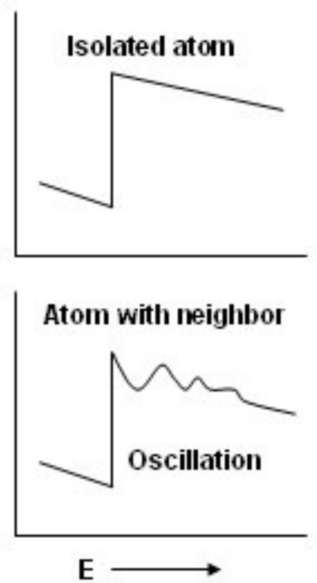
$$\chi(k) = -S_0^2 \sum_j \frac{N_j}{kR_j^2} F_j(k) \exp\left(-2\sigma_j^2 k^2\right) \sin\left(2kR_j + 2\delta_{A,1}(k) + \varphi_j(k)\right)$$

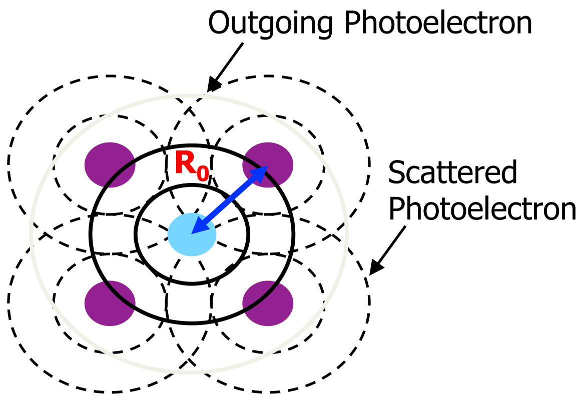
"Round trip" of the wave

Phase shift

of absorbing atom

of scattering atom





Fourier Transform...

Bond length R_j , etc.,

(Parameters high-lightened by yellow are fitting parameters.)

de Broglie wave as a Ruler

A particle with the momentum of *p*
having the wave character described by the below Eq.

as for Electron

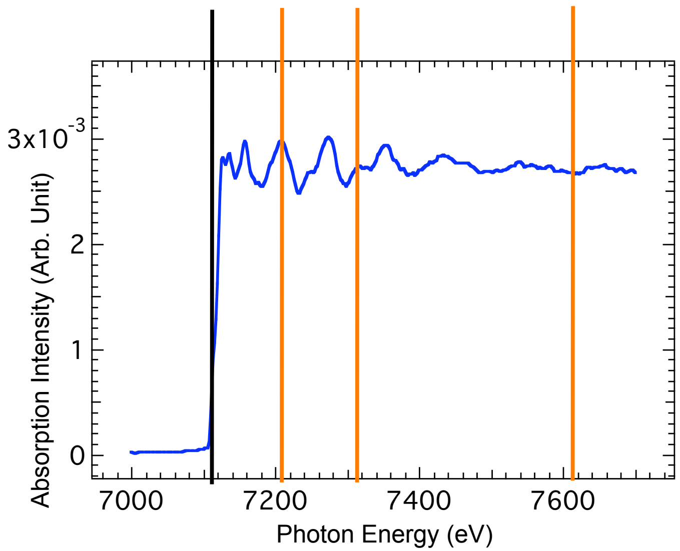
$$\lambda = \frac{h}{p} = \frac{h}{(2m_e eV)^{1/2}}$$

considering a bond length of ~2.5 Å

100 eV: 1.226 Å	2 waves
200 eV: 0.867 Å	3 waves
500 eV: 0.548 Å	4-5 waves

EXAFS

We use **de Broglie wave of electron** as a **Ruler**, in order to measure bond length

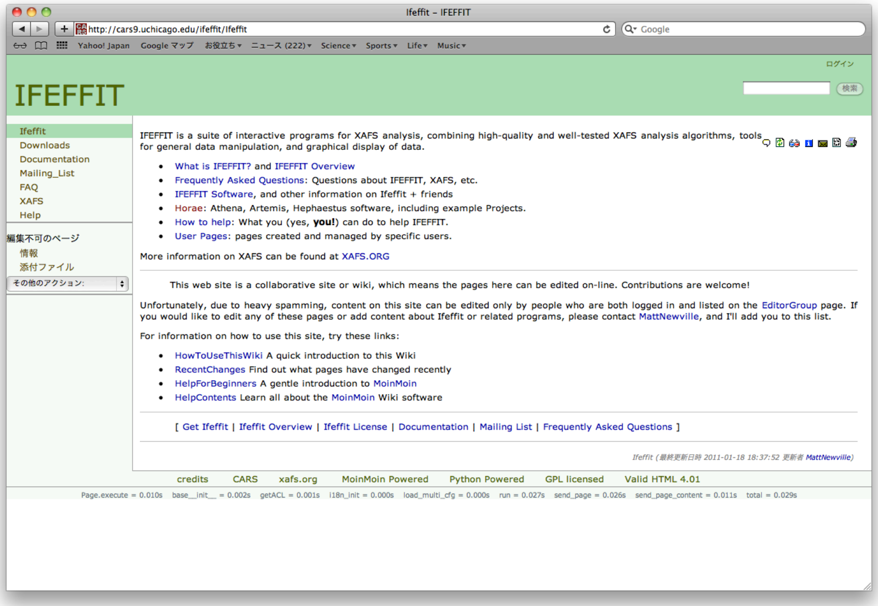


Software for XAFS analyses

Athena, Artemis (Ifeffit)

by a group at U. Chicago

http://cars9.uchicago.edu/ifeffit/Ifeffit



REX2000

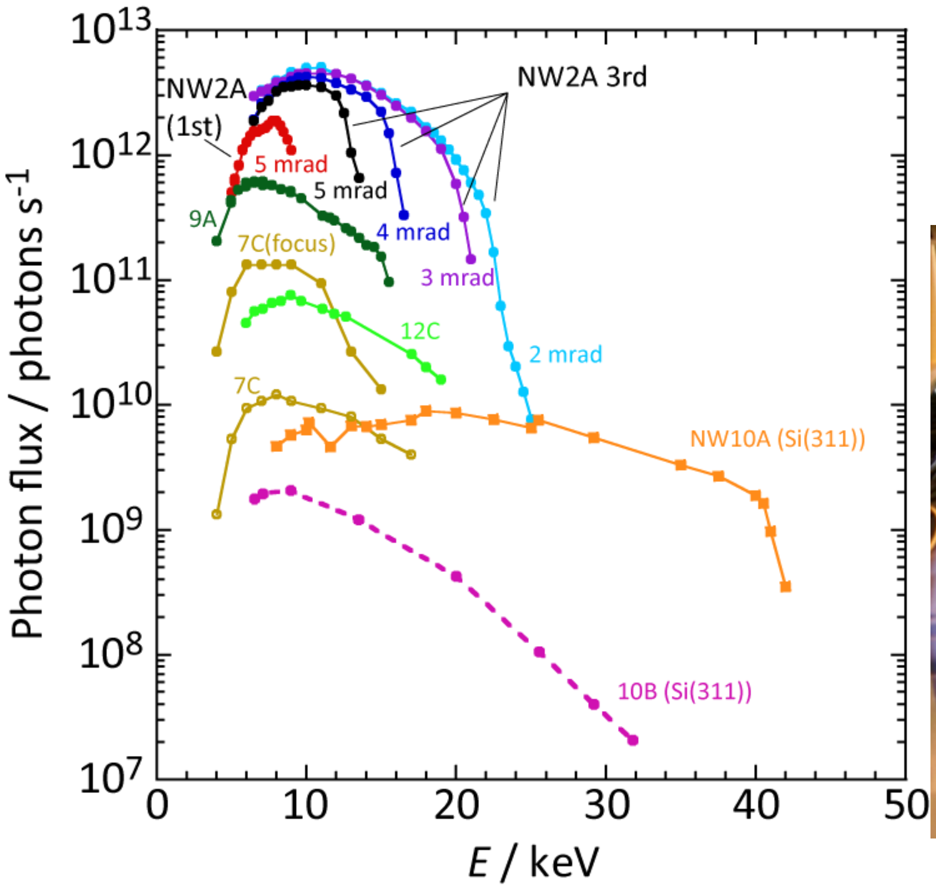
by RIGAKU corp.

http://www.rigaku.co.jp/products/p/xdxa0020/

Of course, there are many other softwares, and you can use what you'd like to.

Experiments of XAFS

Stations of XAFS experiments at PF

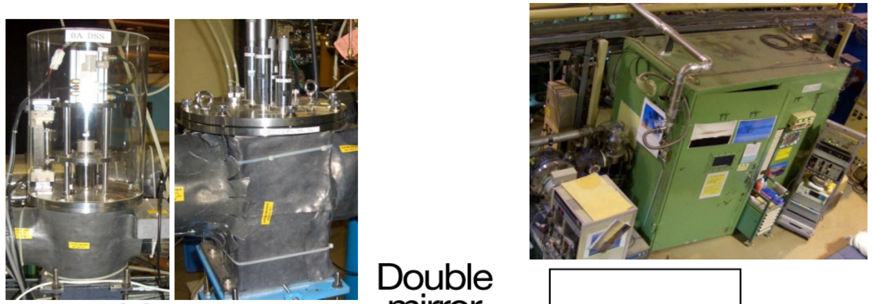


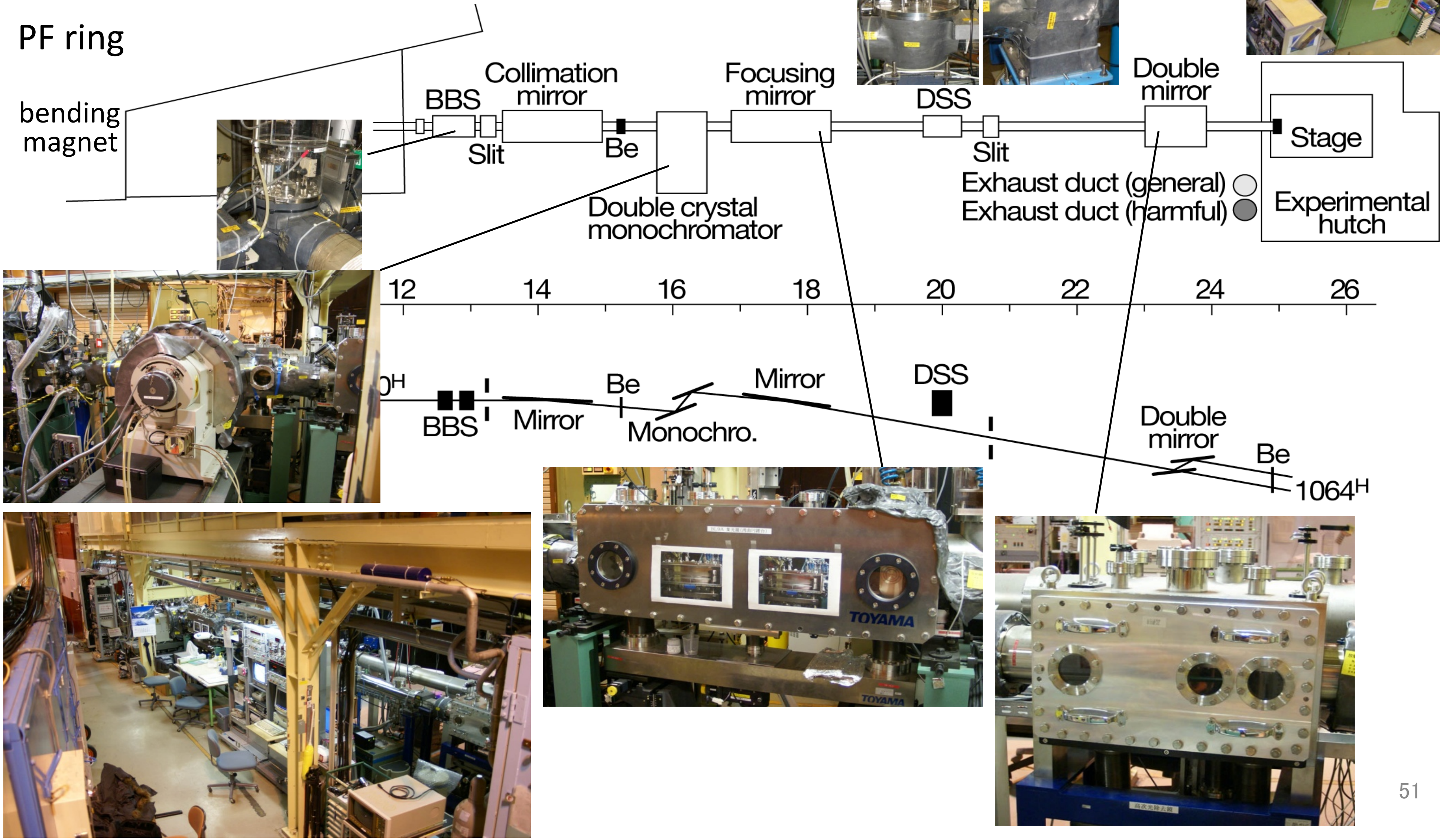
PF BL-9A

K edges: from P (~2.1 keV) to Ce (~40 keV)

L edges: from Mo (~2.5 keV) to U (~21 keV)

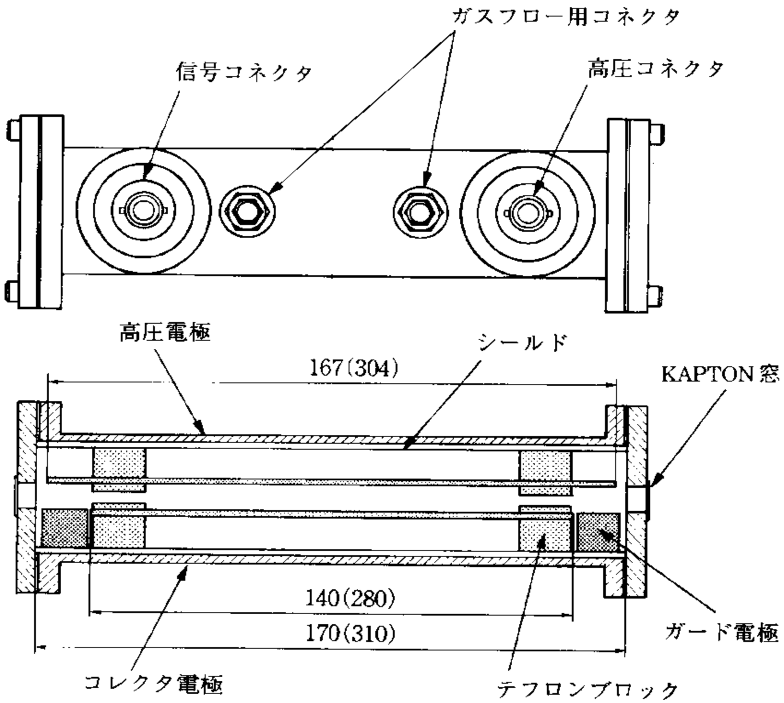
Schematic of BL-9A





Ionization chamber for x-ray detection

We measure the current produced by ionization of gas by incoming x-ray.



Current i ; measuring wih N_2 flowing Ion chamber to detect x-ray of 8 keV;

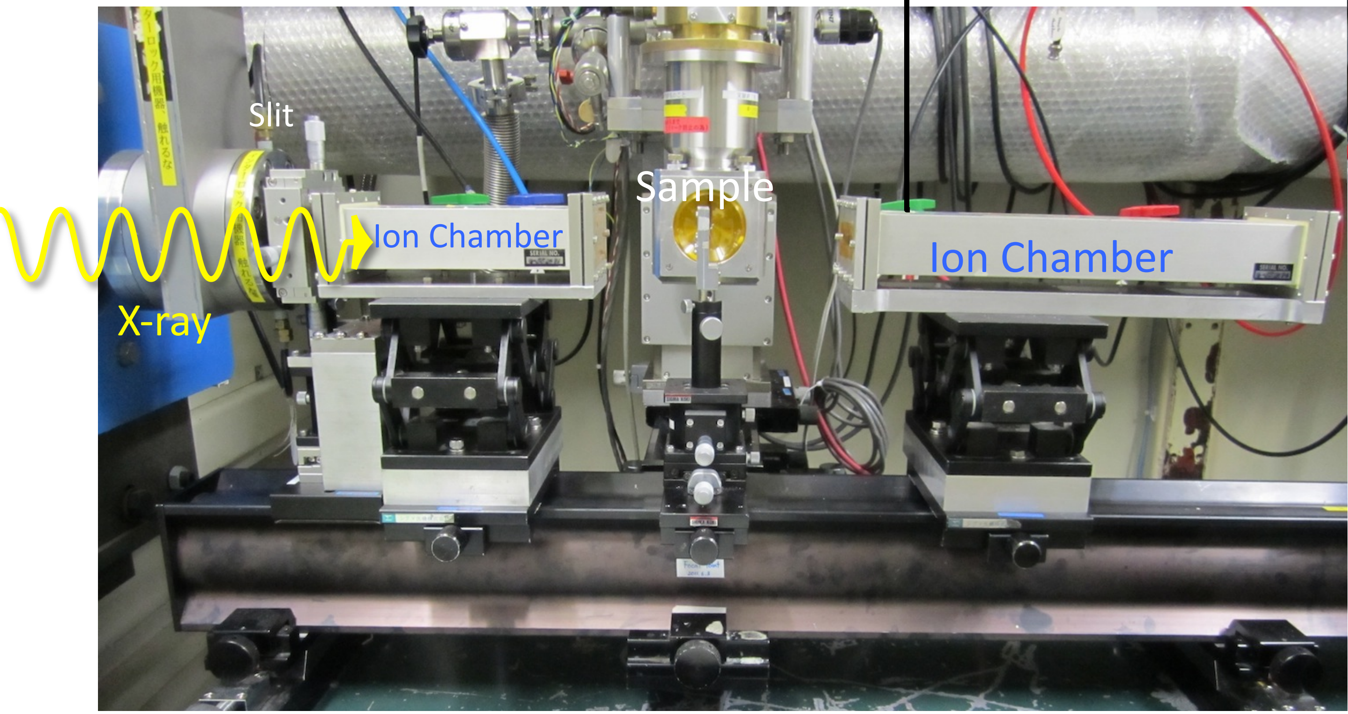
$$i \approx 8.5 \times 10^{-8}\ \mathrm{A}$$

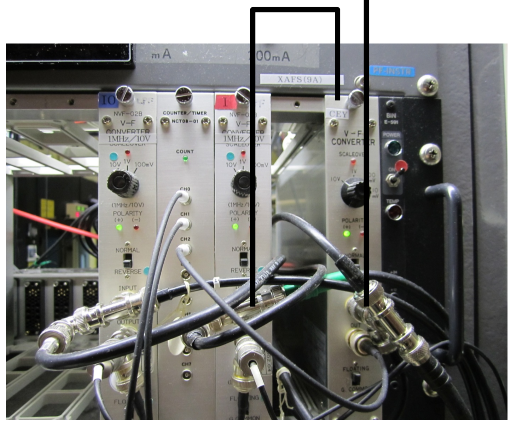
$$i = \alpha E e N / W$$

α ：検出効率（0.2）
E ：光子エネルギー（8000 eV）
e ：電荷素量（1.6 x 10^{-19} C）
N ：入射光子数（10^{10} photons/s）
W ：窒素ガスのイオン化エネルギー（30 eV）

Setup of transmission mode XAFS

Absorption $$\mu t(\lambda) = \ln\left(\frac{I_0(\lambda)}{I(\lambda)}\right)$$

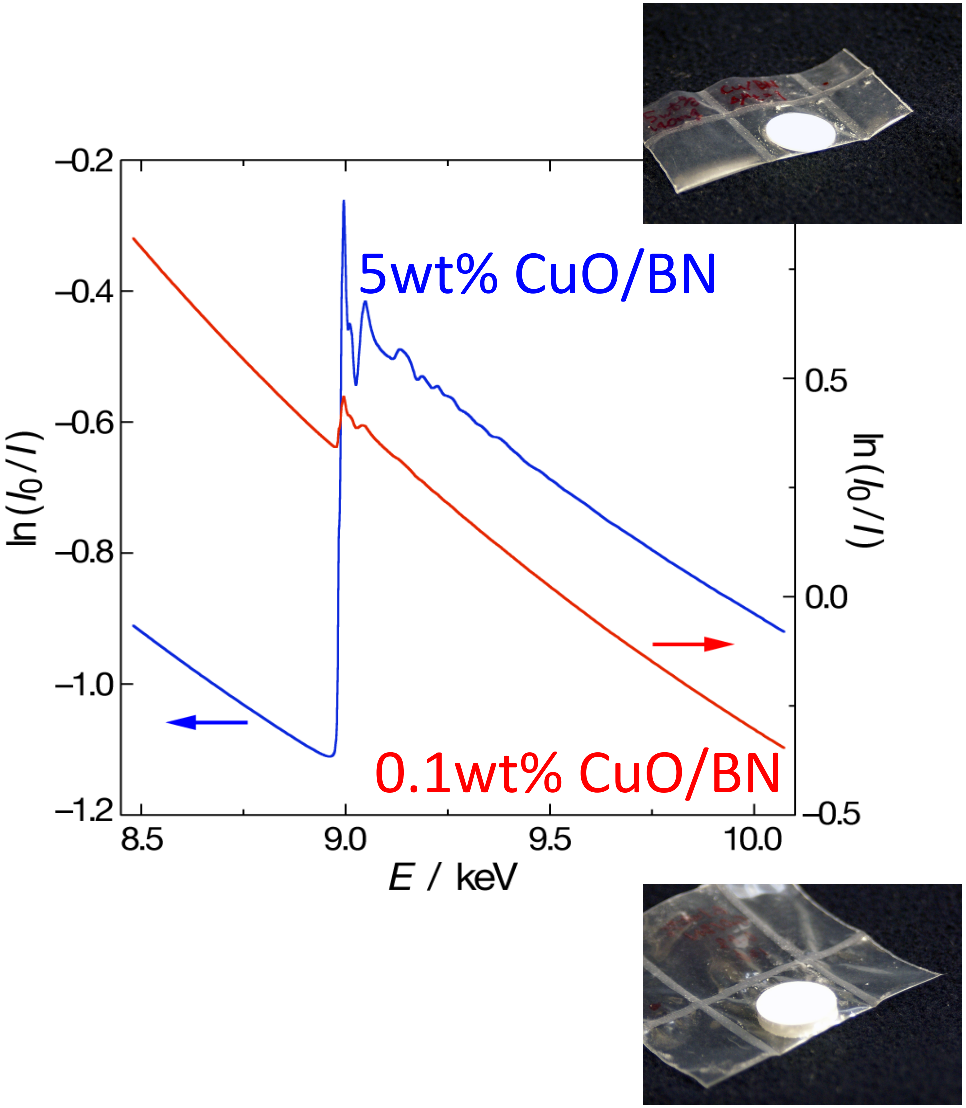


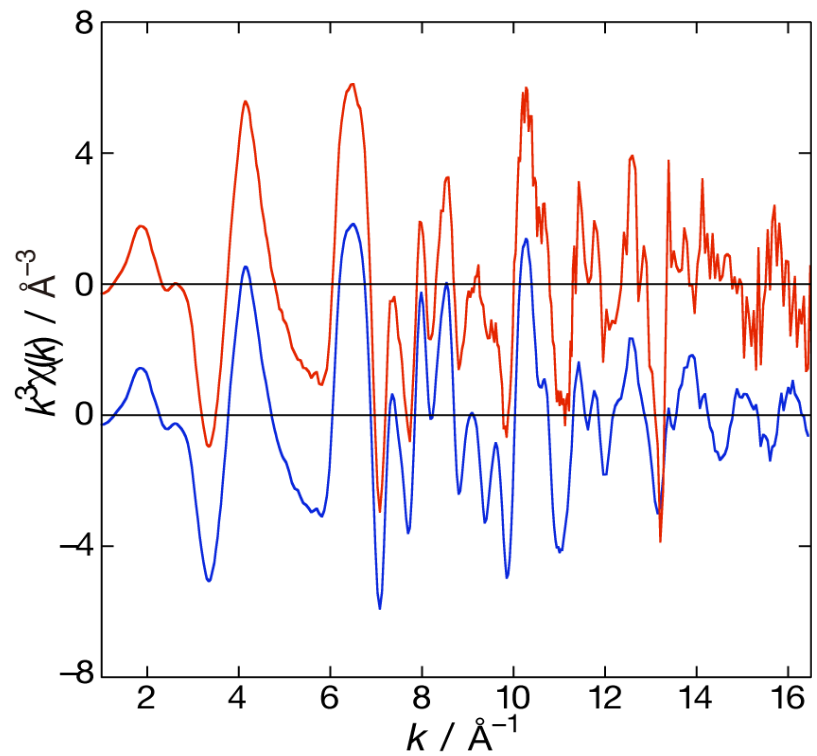


Ion Chamber → Amp → V-F Converter → Counter

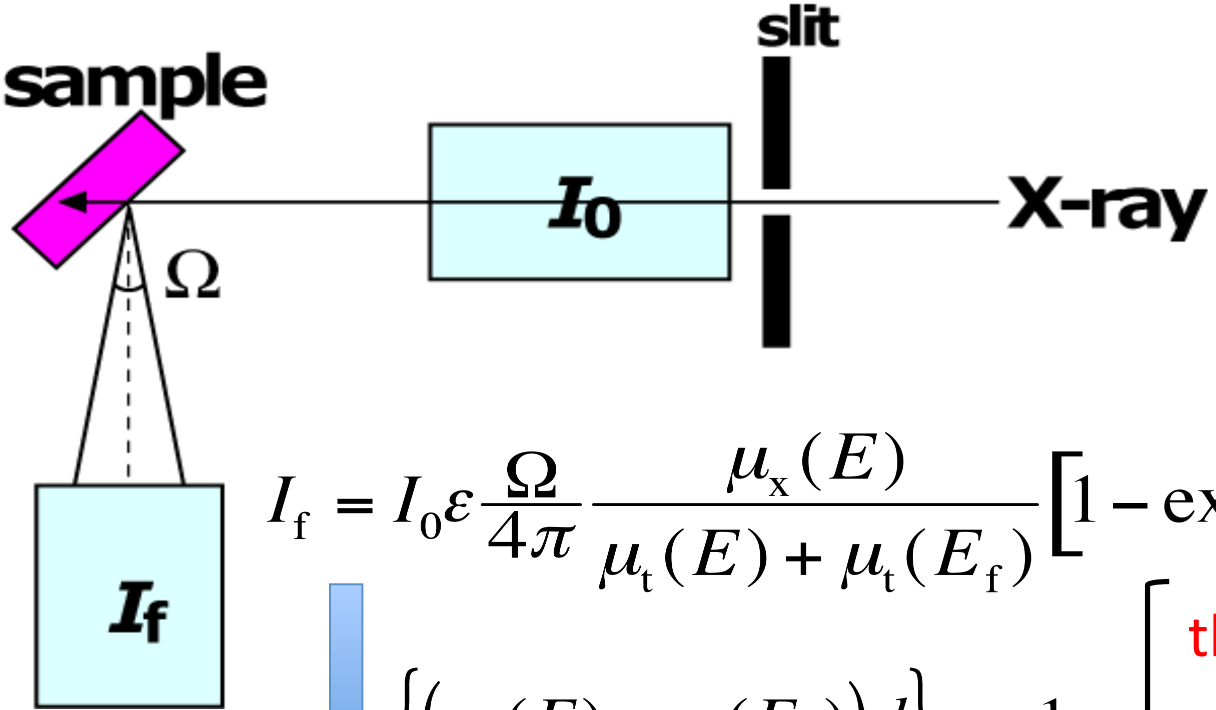
Current prop. to x-ray intensity — Cur. => Volt. — Volt. => Frequency

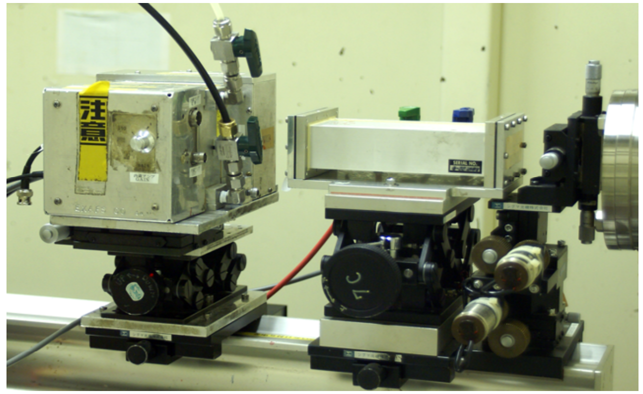
Transmission mode XAFS spectra





Fluorescence mode XAFS





$$I_\mathrm{f} = I_0 \varepsilon \frac{\Omega}{4\pi} \frac{\mu_\mathrm{x}(E)}{\mu_\mathrm{t}(E) + \mu_\mathrm{t}(E_\mathrm{f})} \left[1 - \exp\left\{ -\left(\mu_\mathrm{t}(E) + \mu_\mathrm{t}(E_\mathrm{f}) \right) d \right\} \right]$$

$$\left\{ \left(\mu_\mathrm{t}(E) + \mu_\mathrm{t}(E_\mathrm{f}) \right) d \right\} << 1$$

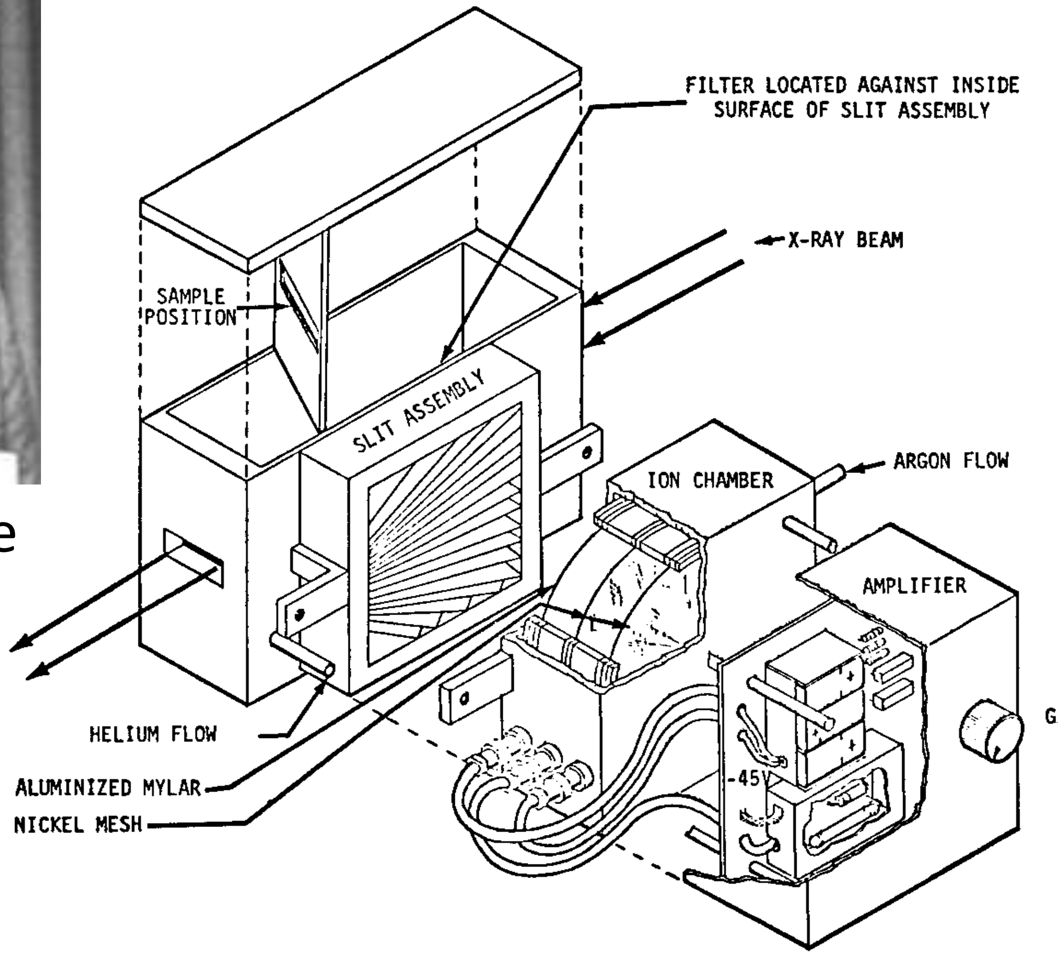
- thick but dilute
  (ex. 0.01 M aq.)
- concentrated but thin
  (ex. 1000 Å film)

$$I_\mathrm{f} = I_0 \varepsilon \frac{\Omega}{4\pi} \mu_\mathrm{x}(E) d$$

$$\therefore \frac{I_\mathrm{f}}{I_0} \propto \mu_\mathrm{x}(E)$$

Ion chamber for Fluo. XAFS: Lytle Detector

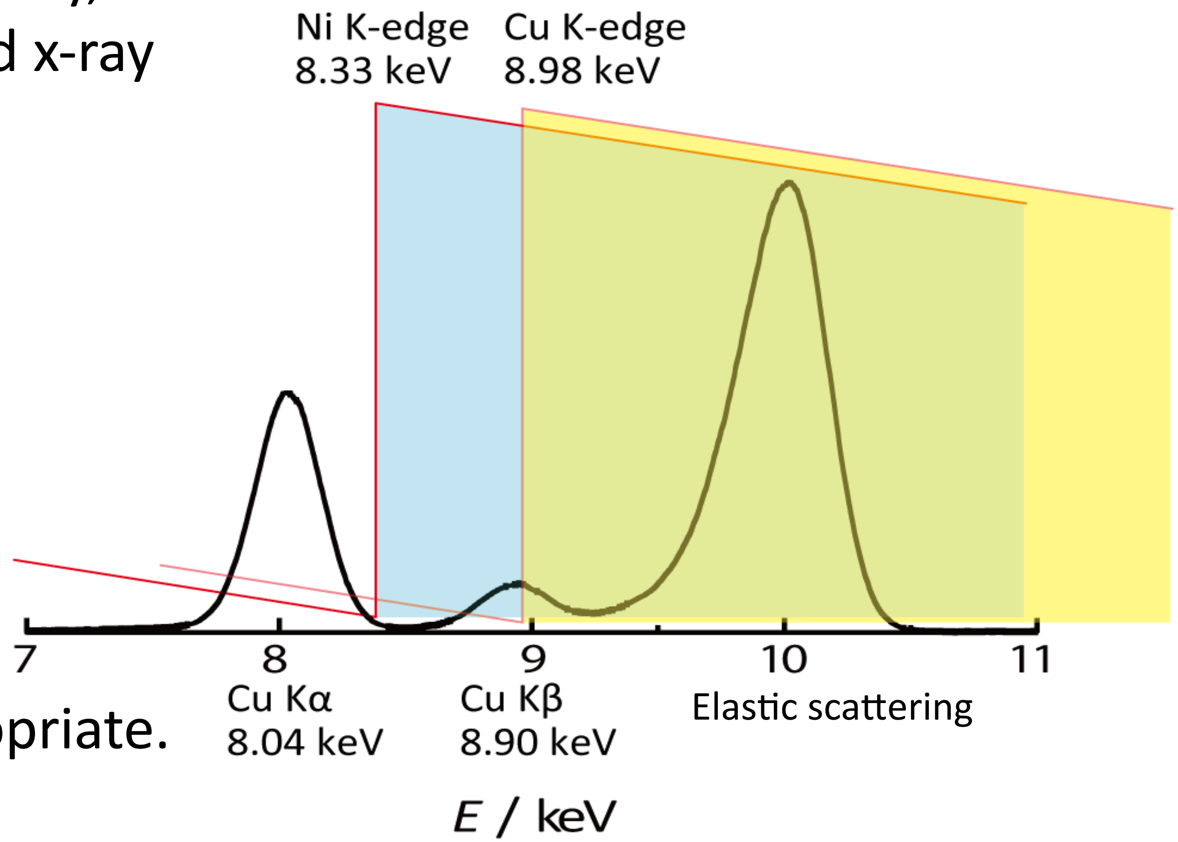
Dr. Farrel W. Lytle



Not expensive, large solid angle, home made possible

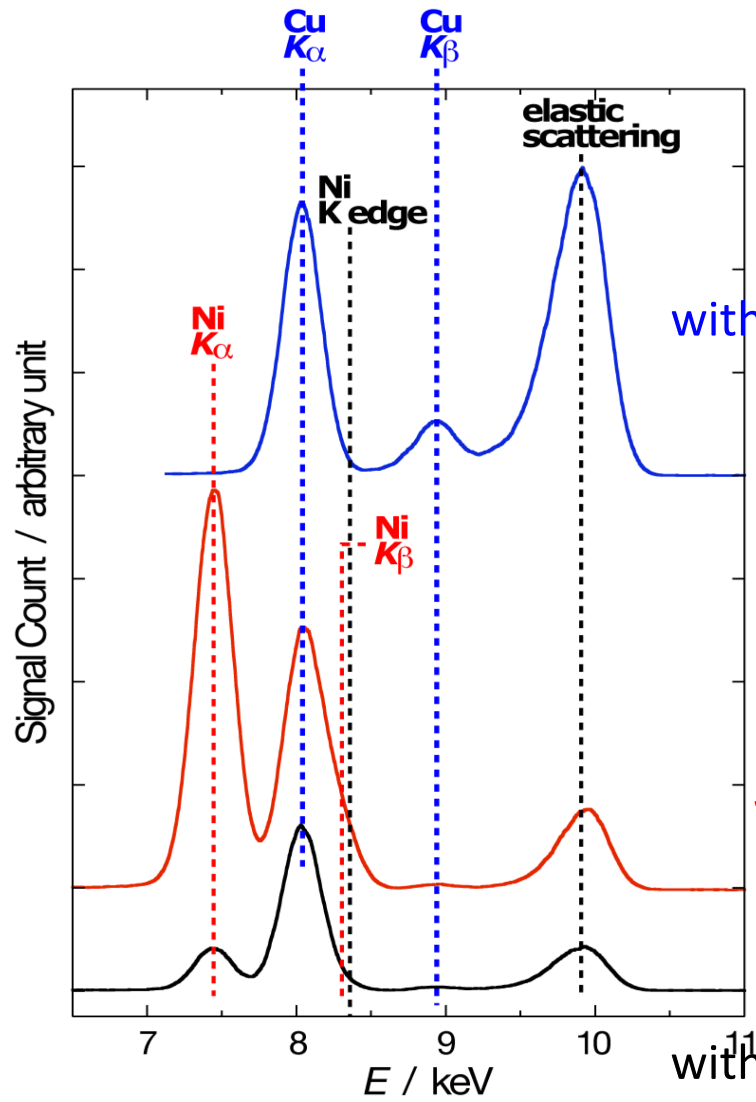
Function of the filter

Transparent for Fluorescent x-ray,
absorbing elastically scattered x-ray



A ”Z-1” filter is mostly appropriate.

Function of Filter & Soller slit of Lytle detector

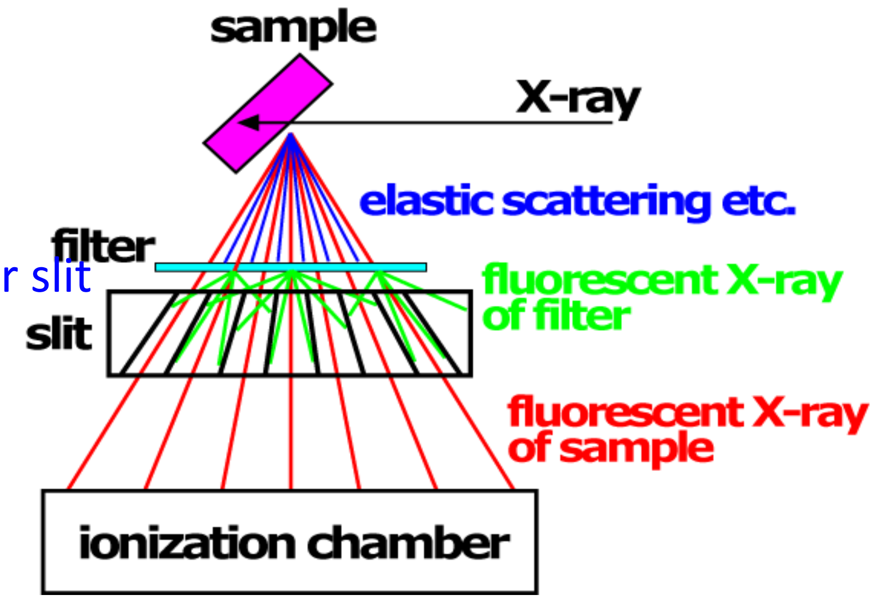


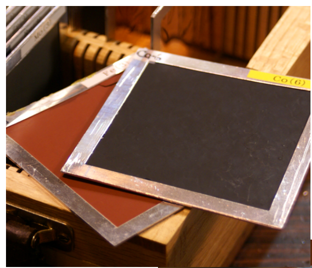
without filter or soller slit

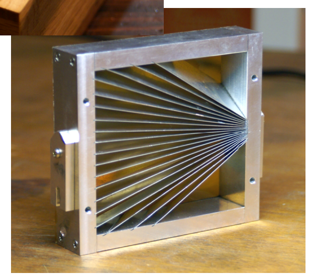
with Ni filter (μt=6)
but without soller slit

with Ni filter (μt=6) & soller slit +

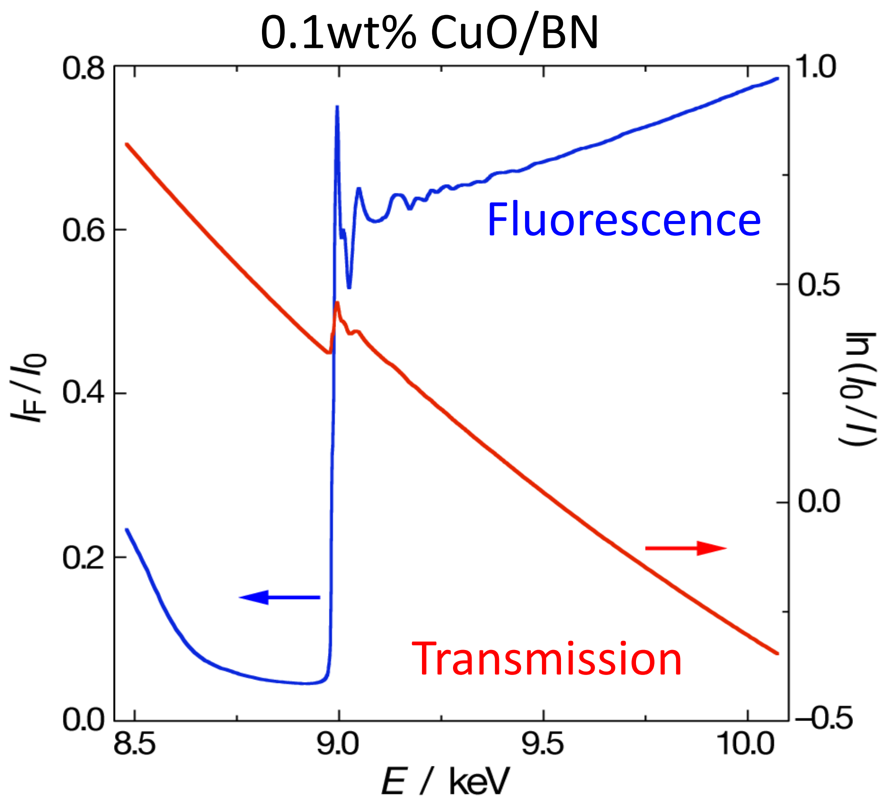
Sample: 2 mM CuSO4 aq.

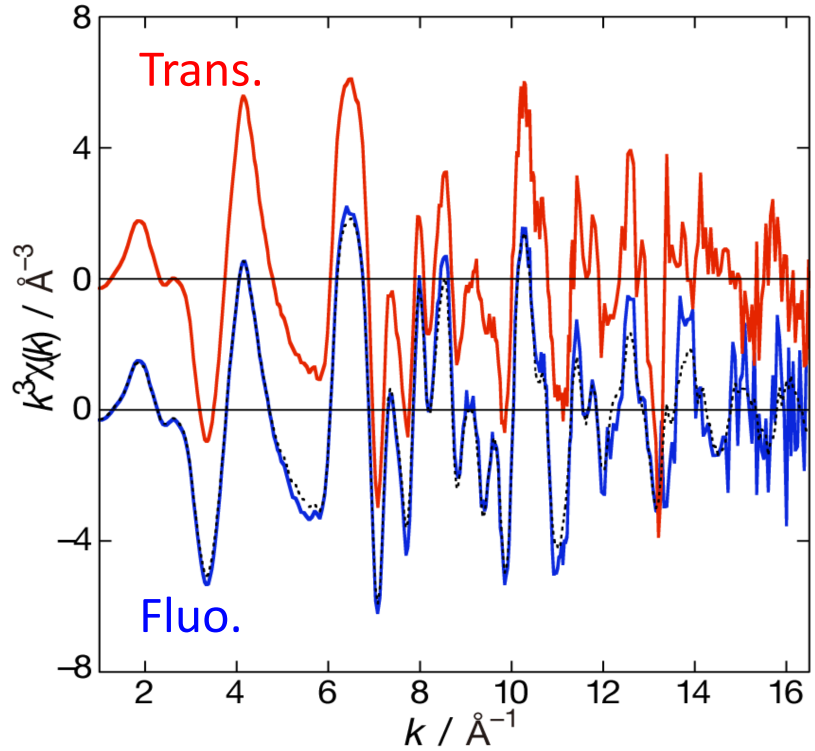






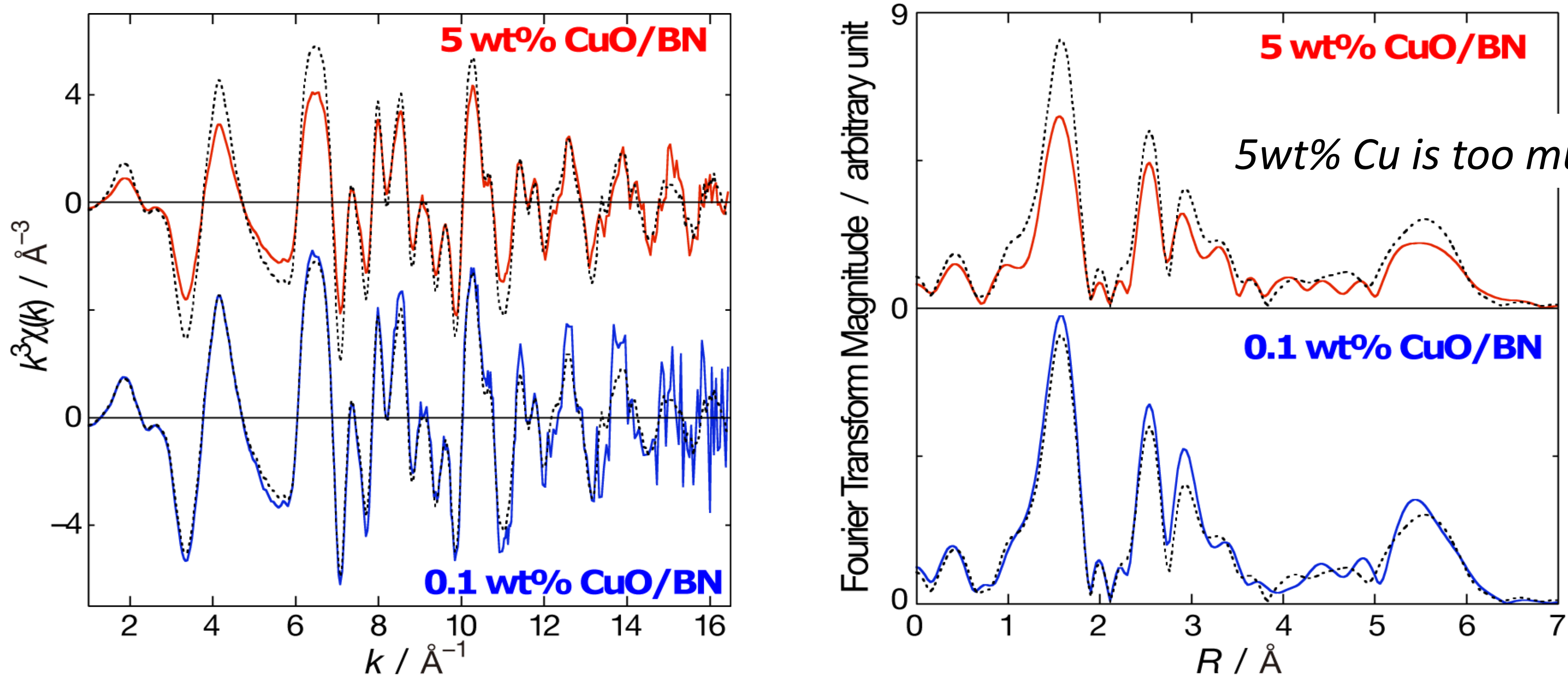
Trans. mode & Fluo. mode





Suitable sample for Fluo. mode XAFS

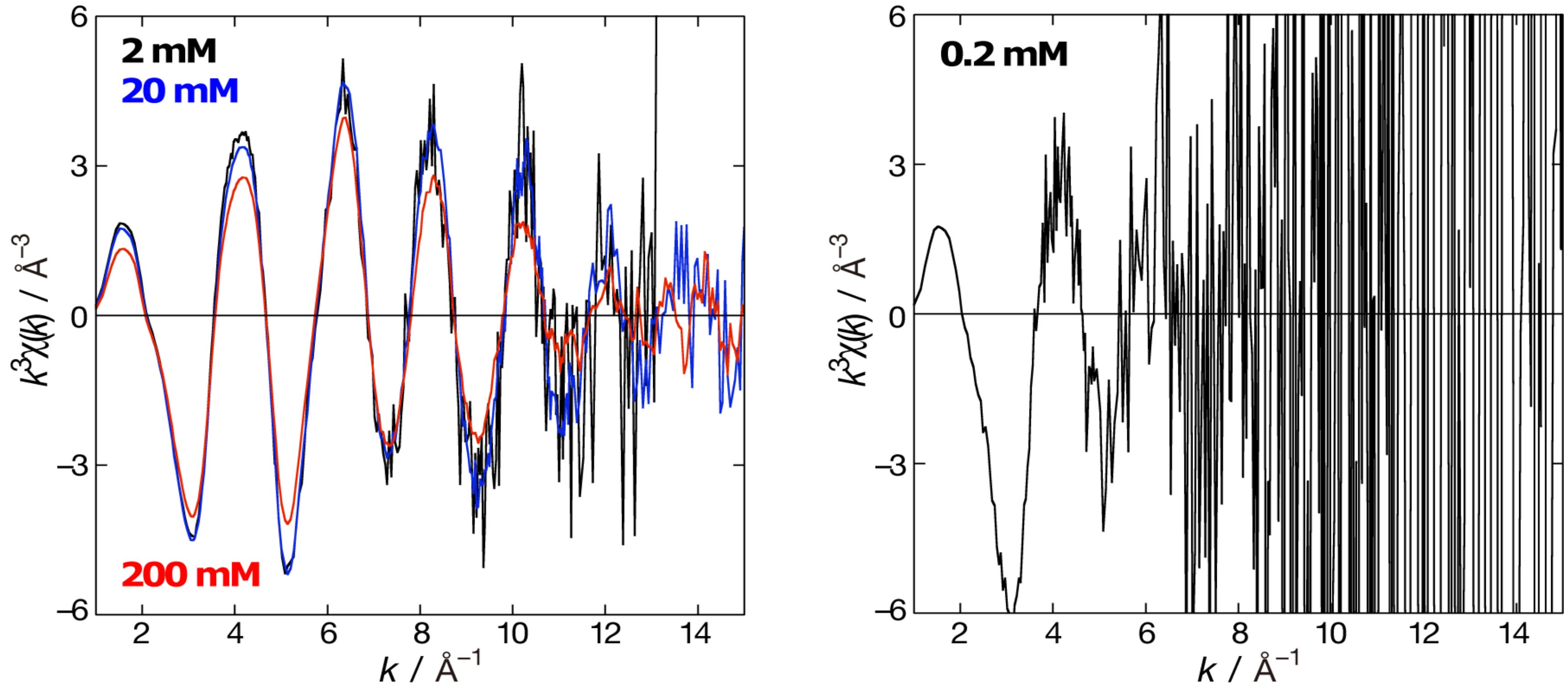
dotted line: trans mode XAFS for 5wt% sample



Samples for Fluo. mode XAFS must be...

- thick but **dilute**: ex. 0.01 M (10 mM) aq.
- concentrated but **thin**: ex. 1000 Å thin film

Suitable sample condition for Fluo. mode XAFS

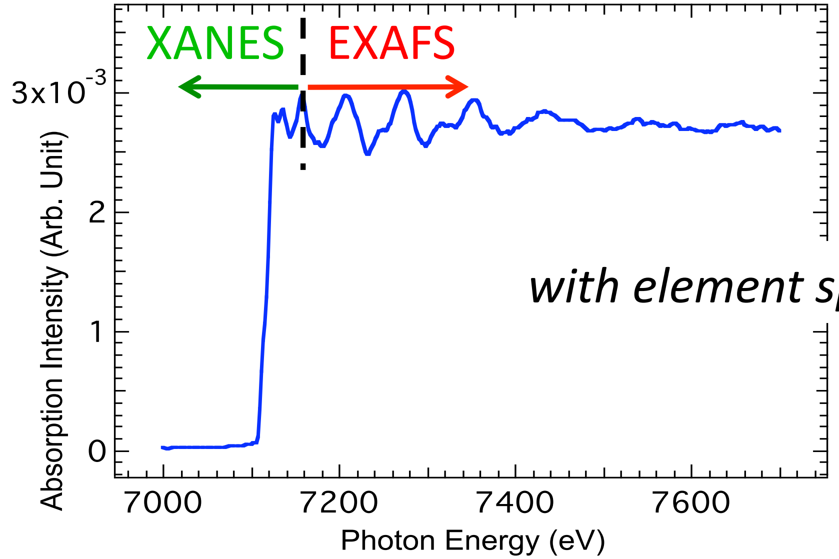


for $CuSO_4$ solution

dencity	0.2 mM	2 mM	20 mM	200 mM
weight percent	0.0013 wt%	0.013 wt%	0.13 wt%	1.3 wt%
atomic percent	0.00036 at%	0.0036 at%	0.036 at%	0.36 at%

Take-home massage

<u>XAFS : XANES + EXAFS</u>



with element specificity

- XANES gives us...
  - Valence state
  - Symmetry

<u>The ruler is de Broglie wave of electron!!</u>

- EXAFS gives us...
  - Bond length
    - **A local structure** is given.
    - **Crystallinity, or long range order is not required**.
  - Coordination number (CN)
    - Simply, the number of atoms around the atom.
    - CN enables us to estimate sizes of nano clusters.