The European Synchrotron

XAFS FUNDAMENTALS, DATA REDUCTION AND ANALYSIS

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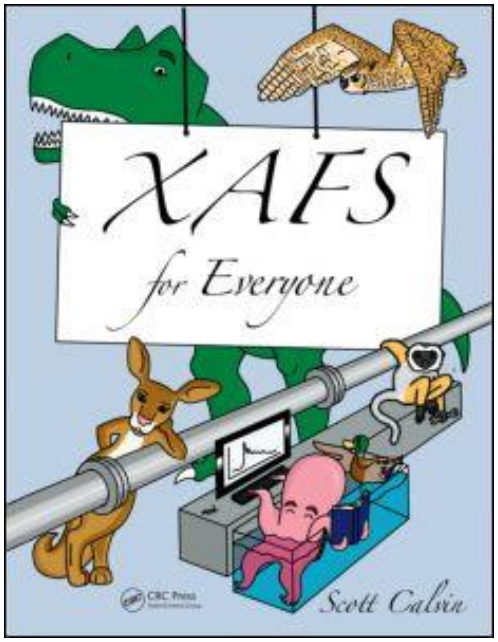
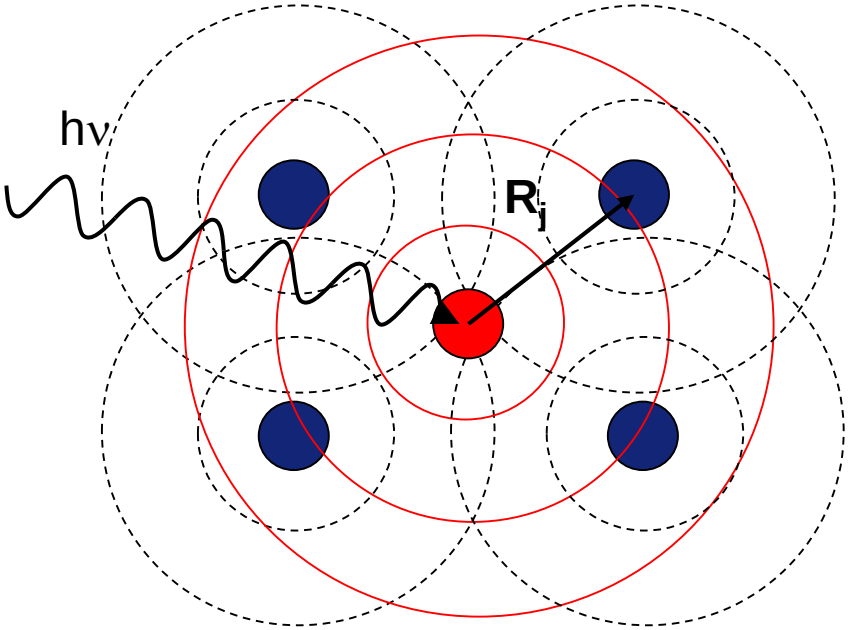
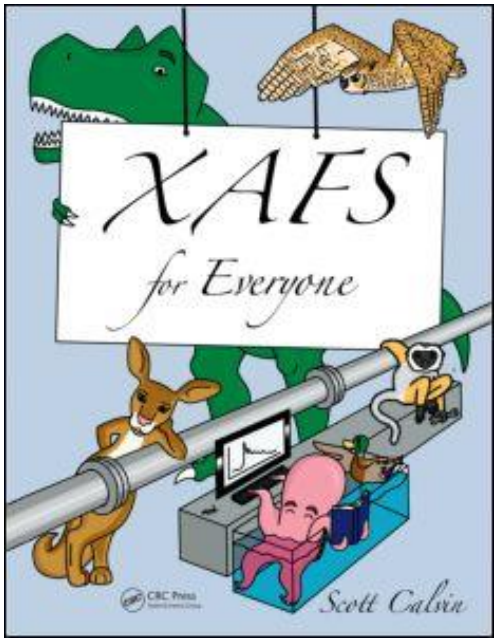
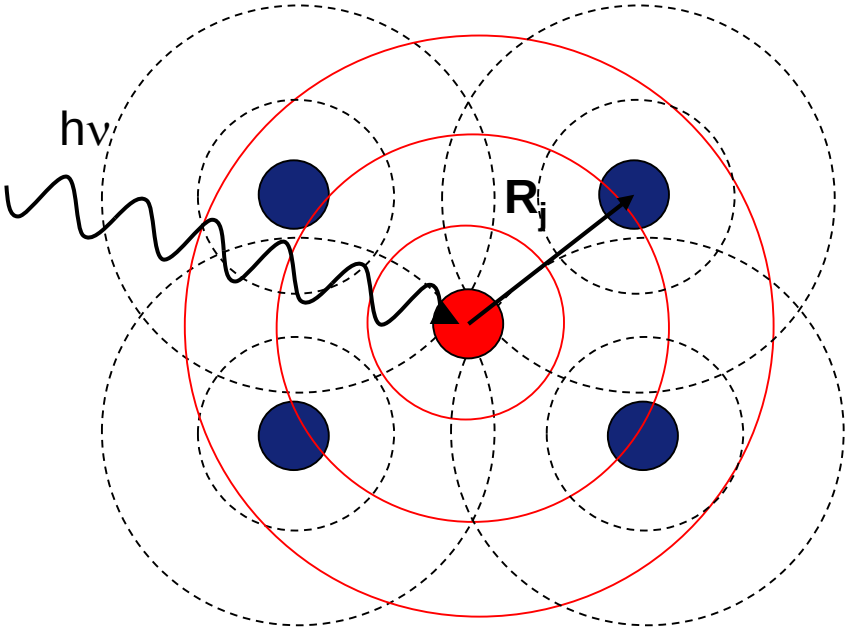




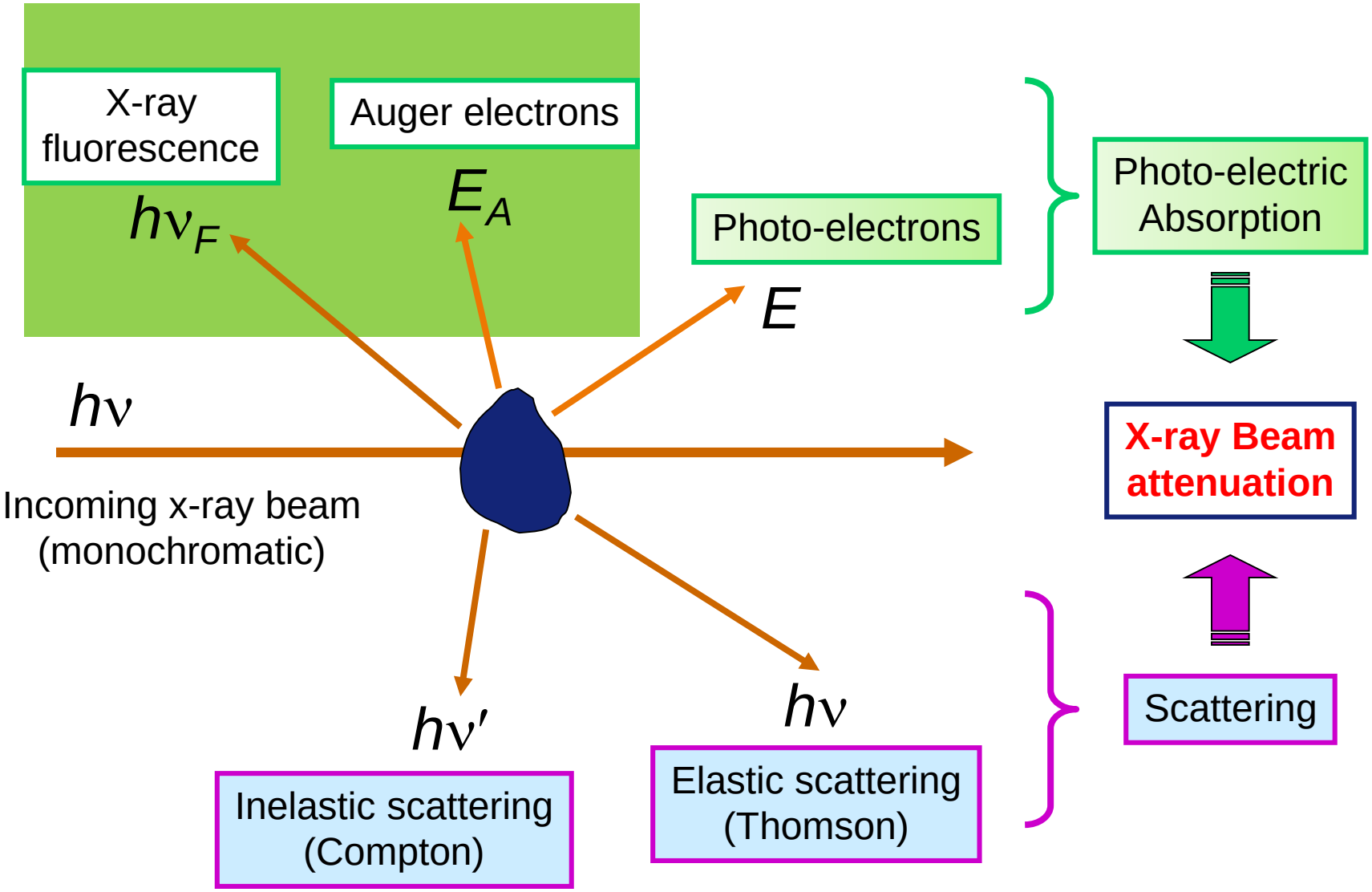
XAFS FUNDAMENTALS, DATA REDUCTION AND ANALYSIS

1. **Fundamentals of X-ray Absorption Fine Structure (XAFS)**
2. **Measurement of Cu foil at BM23**
3. **Data analysis Cu foil**
4. **Real sample preparation, CuO**
5. **Data analysis, comparison**



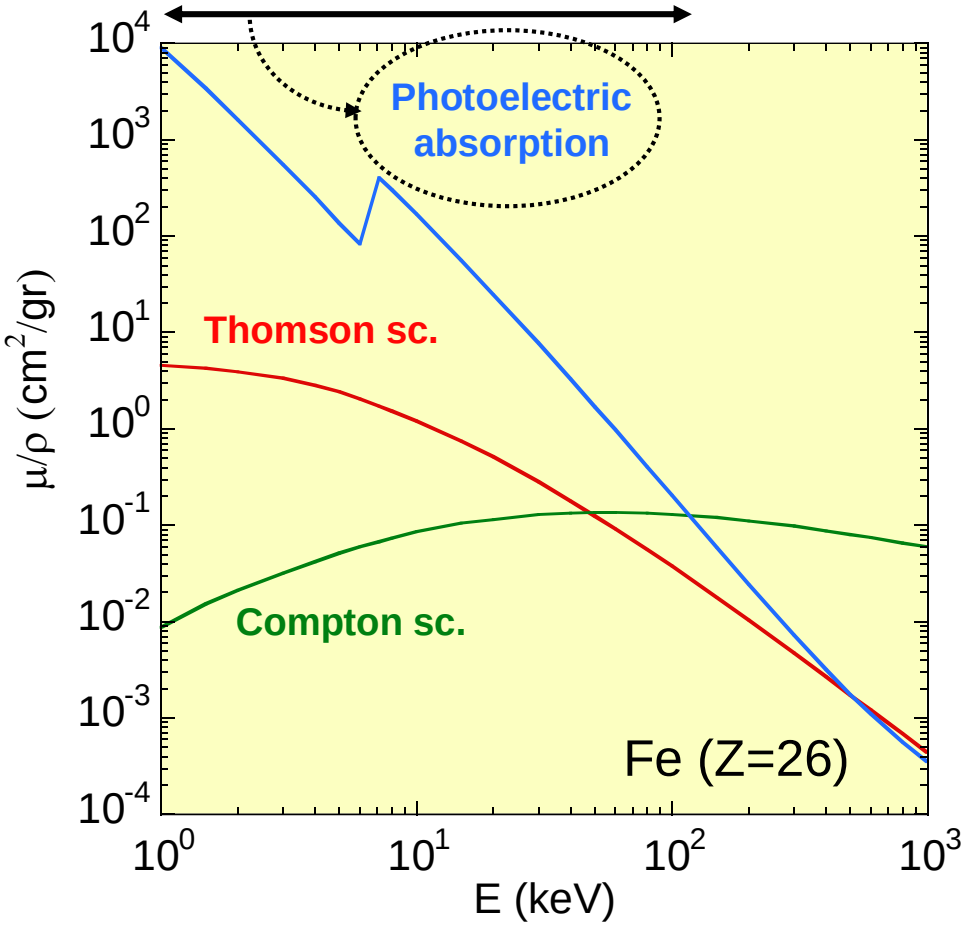


INTERACTION OF X-RAYS WITH MATTER (E< 1 MeV)



ATOMIC CROSS SECTION (E< 1 MeV)

- Quantifies the strength of the X-ray – matter interaction
- For photon energies between 1 and 30 keV the photoelectric absorption is the leading interaction with matter

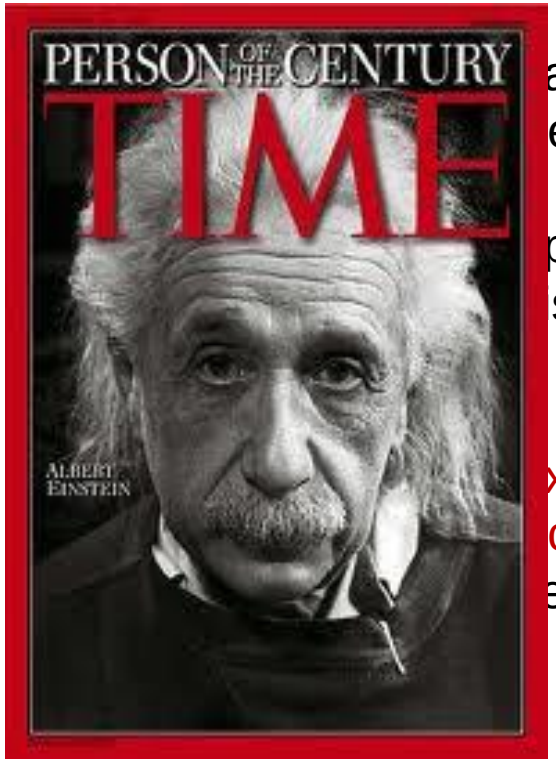


$$\mu/\rho = (N_A/A)\sigma_a$$

$$\sigma_a = \sigma_{pe} + \sigma_{coh} + \sigma_{incoh} + \sigma_{pp}$$

X-RAY ABSORPTION PROCESS: PHOTOELECTRIC EFFECT

Hard X-rays (light with energy $1 \leq E \leq 100$ keV or wavelength $0.12 \leq \lambda \leq 12$ Å) are absorbed by all matter through the photoelectric-effect:



ay has an energy
e binding energy of
(**K**=**1**s; **L**$_{I}$=**2**s; L$_{II}$,
photon is absorbed
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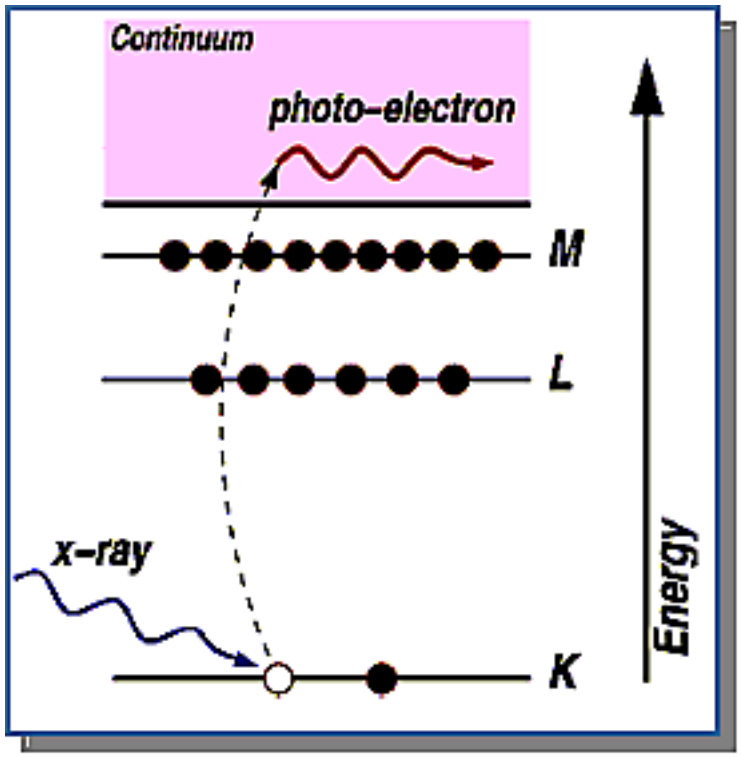
xcited state with an
core hole) and any
en to the ejected

Nobel Prize 1921



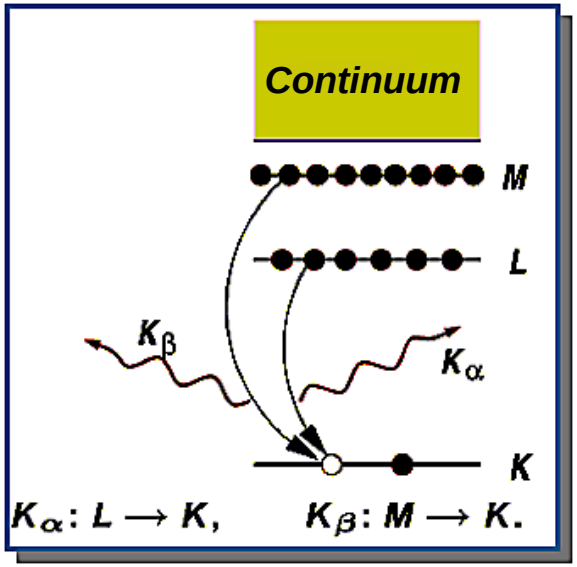
The excited core-hole will relax back to the "*ground state*" of the atom by two main mechanisms: X-ray Fluorescence, for hard x-ray regime (> 2 keV) and Auger Effect for lower energy x-ray absorption.

DE-EXCITACTION PROCESSES

When x-rays are absorbed by the photoelectric effect, the excited core-hole will relax back to a "ground state" of the atom. A higher level core electron drops into the core hole, and a *fluorescent x-ray* or *Auger electron* is emitted.

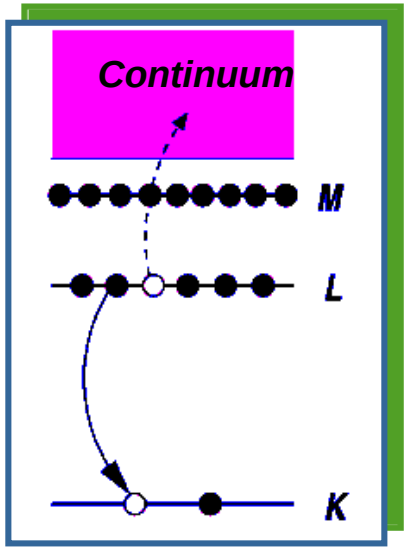
X-ray Fluorescence:

A higher energy core-level electron fills the deeper core-hole, ejecting an x-ray of energy equal to the difference of the core-levels.



Auger Effect:

A higher energy core-level electron drops into the core-hole and a second electron is emitted into the continuum from another core-level.



X-ray fluorescence and Auger emission occur at discrete energies that are characteristic of the absorbing atom.

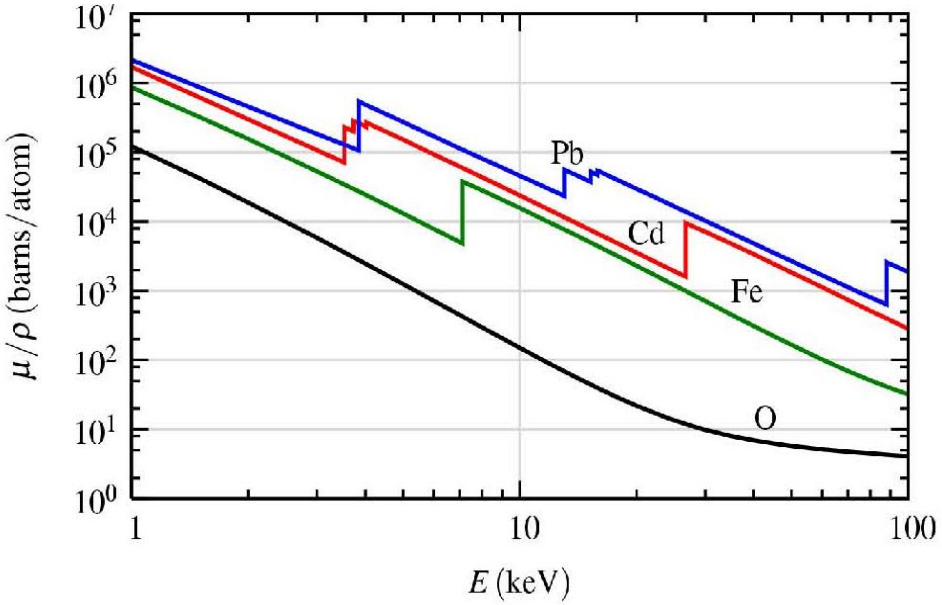
THE ABSORPTION COEFFICIENT μ

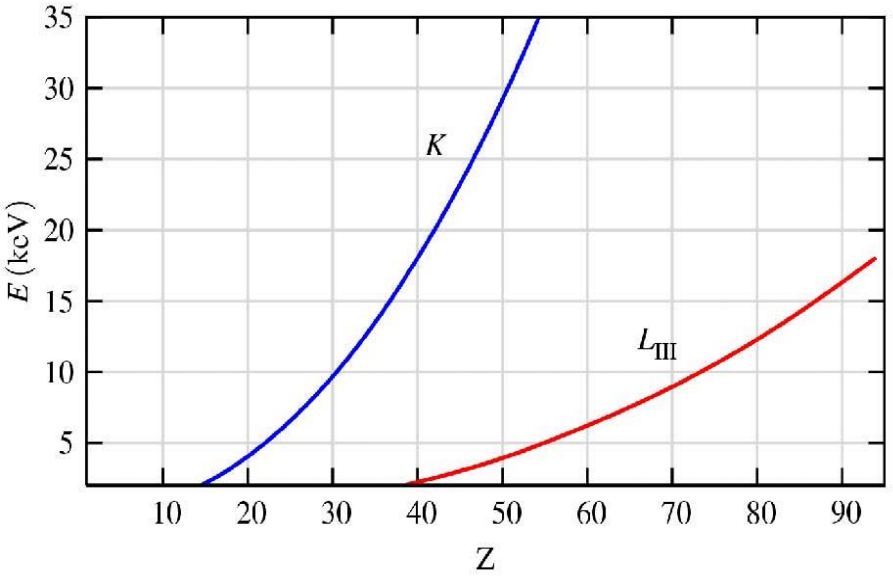
The probability that an x-ray beam passing through a material of thickness t will be absorbed is given by the ***linear absorption coefficient***, μ:

$$\mu \approx \frac{\rho Z^4}{A E^3}$$

Good contrast $\mu(E) \propto Z^4 / E^3$

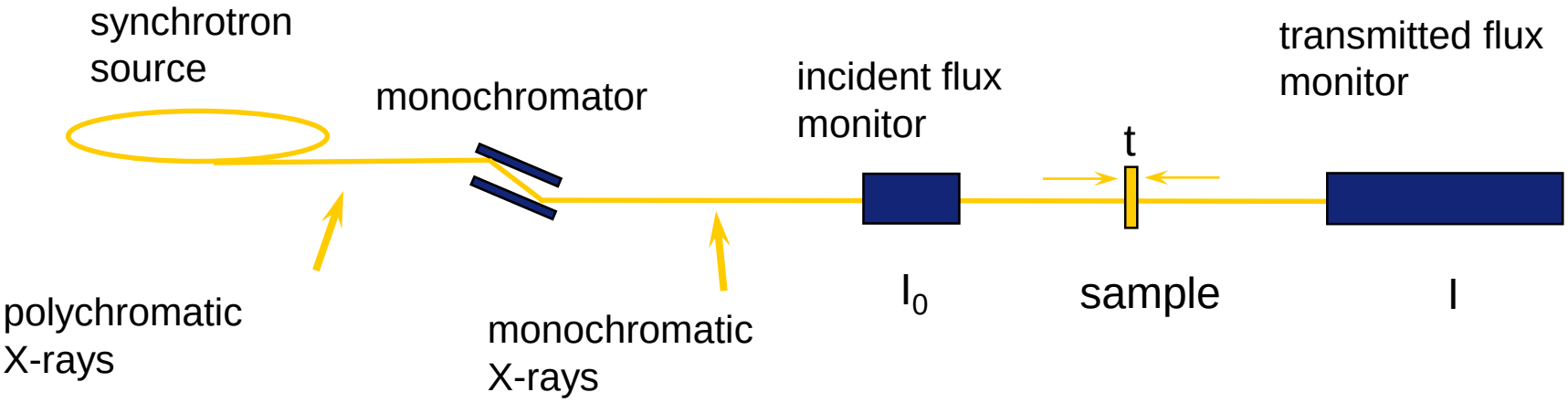
Element specific $E_K \propto Z^2$





X-RAY ABSORPTION MEASUREMENT

XAFS measures the energy dependence of **μ(E)** near and above the absorption edge of a selected element.



Transmission:

The absorption is measured directly by measuring what is transmitted through the sample:

$$I = I_0 e^{-\mu(E)t}$$

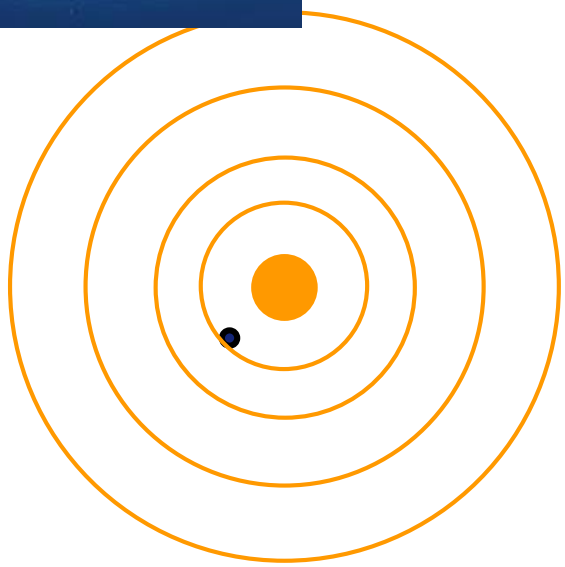
$$\mu(E)\, t = -\ln(I/I_0)$$ Beer-Lambert Law

Fluorescence:

The re-filling the deep core hole is detected. Typically the fluorescent x-ray is measured.

$$\mu(E) \sim I_F/I_0$$

XAFS: SIMPLE PHYSICAL DESCRIPTION



Isolated “bare” atom

- X-ray photon with enough energy ejects one core (photo)electron (photoelectric effect)

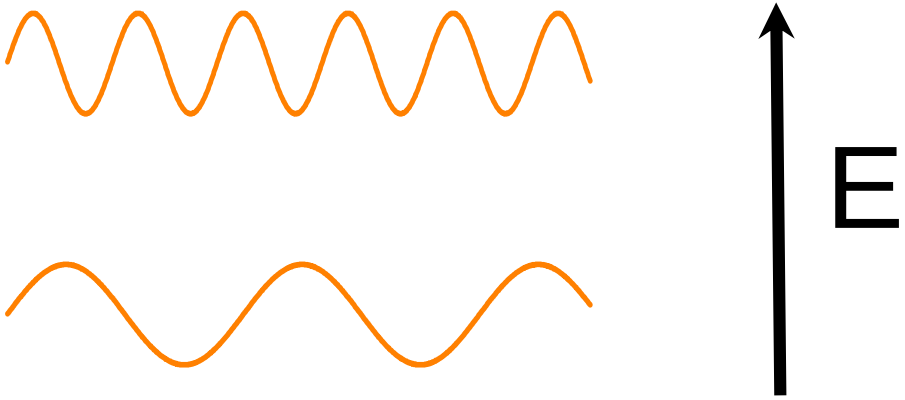
$$E_k = E_{h\nu} - E_0 = \frac{p^2}{2m} = \frac{(\hbar k)^2}{2m}$$ Kinetic energy of the p.e.

$$k = \sqrt{[2m(E_{h\nu} - E_0)/\hbar^2]}$$ wavevector of the p.e.

$$\lambda = 2\pi/k$$ wavelength of the p.e.

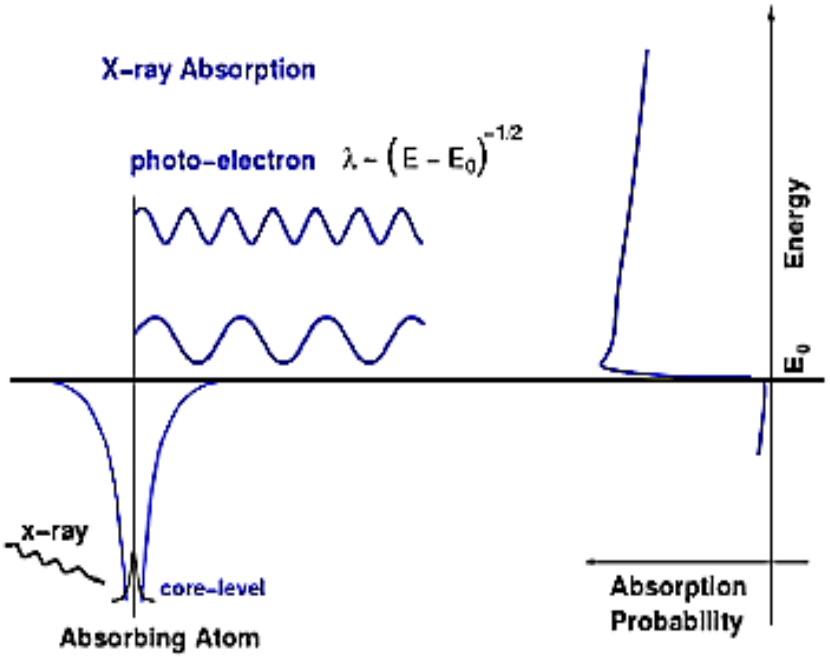
- The photoelectron can be described by a wave function approximated by a spherical wave

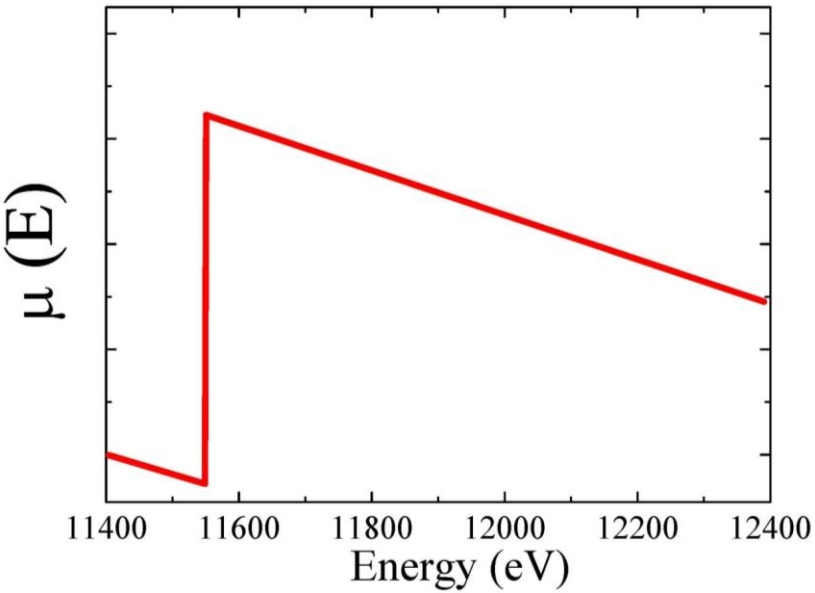
$\lambda \sim 1/(E-E_0)^{1/2}$



XAFS: SIMPLE PHYSICAL DESCRIPTION

Isolated "bare" atom



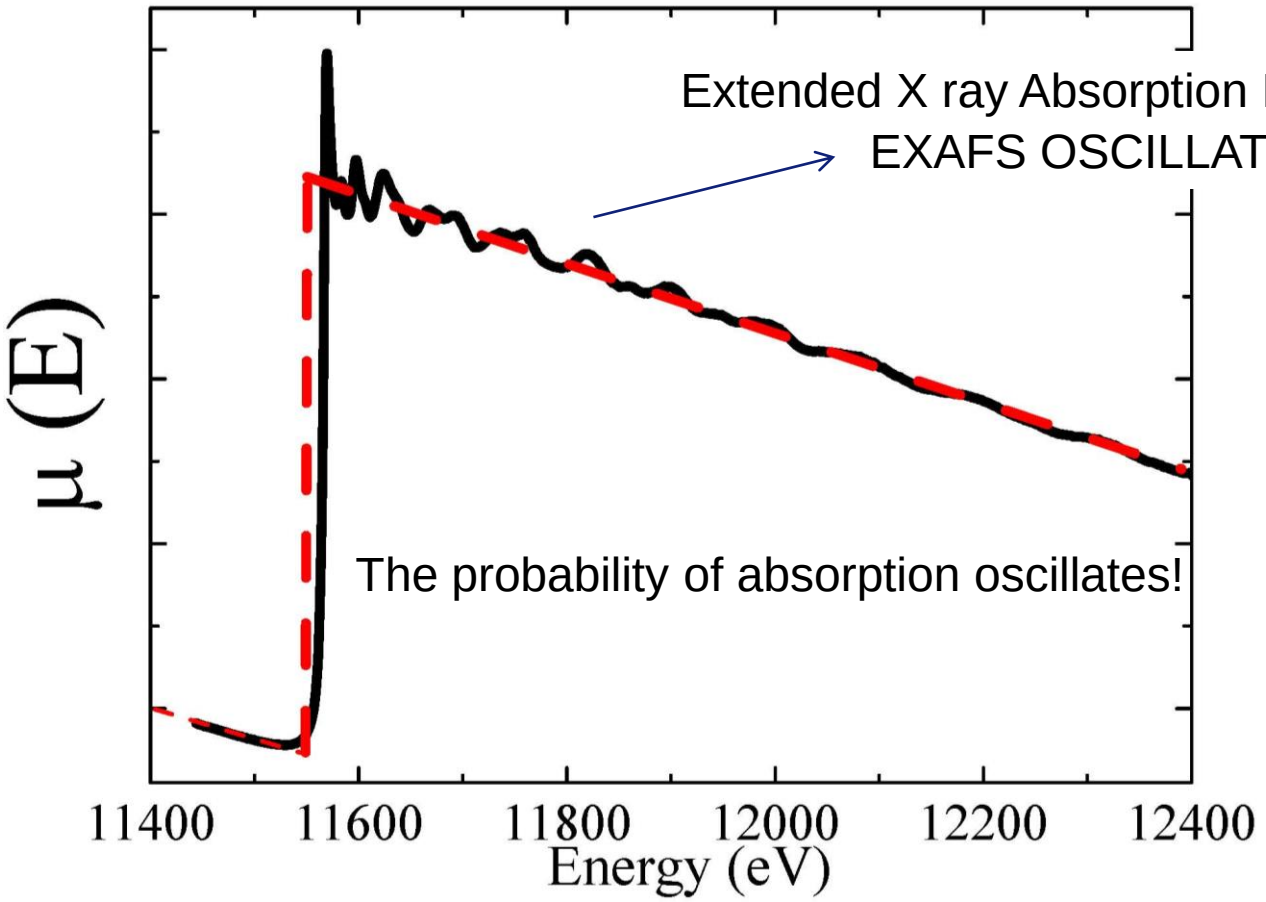


The atom absorbs an x-ray of energy E, destroying a core-electron of energy E_0 and creating a photo-electron with energy ($E-E_0$).

μ (E) has a sharp step at the core-level binding energy E_0 and is a smooth function of energy above this absorption edge.

XAFS: SIMPLE PHYSICAL DESCRIPTION

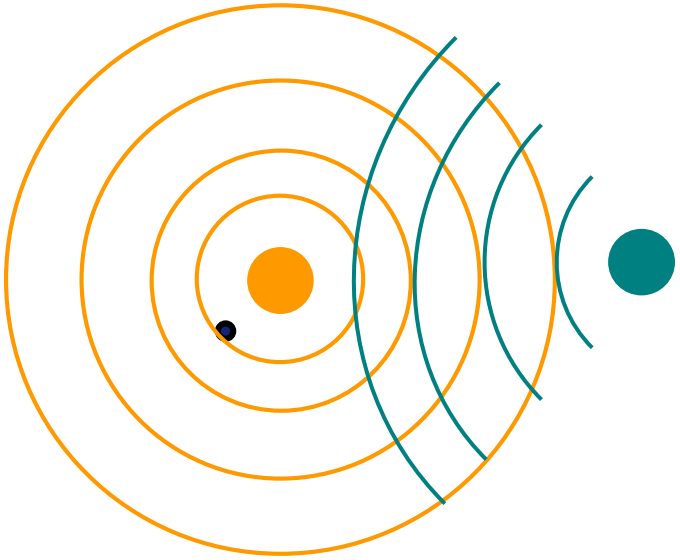
Condensed Matter



Proximity of neighboring atoms strongly modulates the absorption coefficient

EXAFS QUALITATIVELY: CONDENSED MATTER

Diatomic molecule



- The photoelectron can scatter from a neighbouring atom giving rise to an incoming spherical wave coming back to the absorbing atom
- The outgoing and ingoing waves may interfere.

The ejected photo-electron propagates, can scatter from a neighbouring atom and returns to the absorbing atom.

Interference between out-going and back-scattered photo-electron waves at the core site give rises to **modulation** of the absorption coefficient.

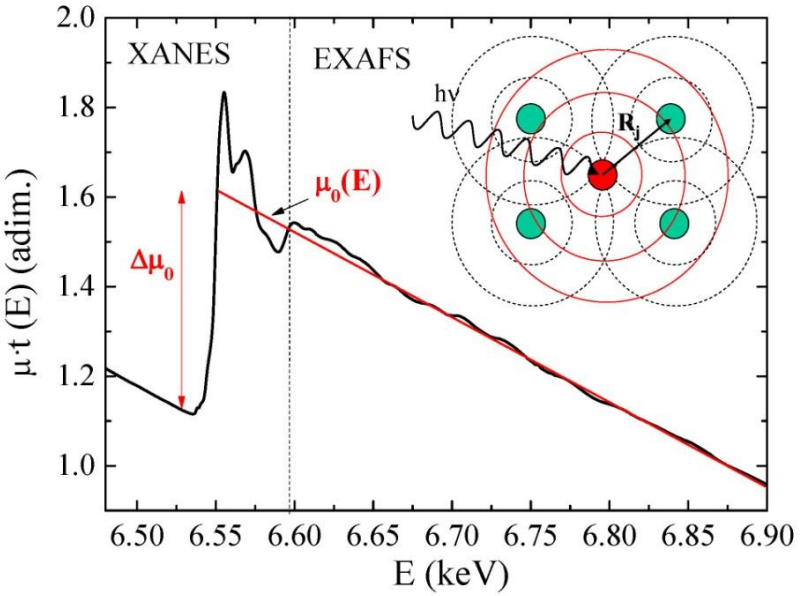
EXAFS DEFINITION

What? Oscillatory behaviour of the of the X-ray absorption as a function of photon energy beyond an absorption edge

When? Non isolated atoms

Why? Proximity of neighboring atoms strongly modulates the absorption coefficient

The EXAFS oscillations are an interference effect of the photo-electron with itself, due to the presence of neighboring atoms.

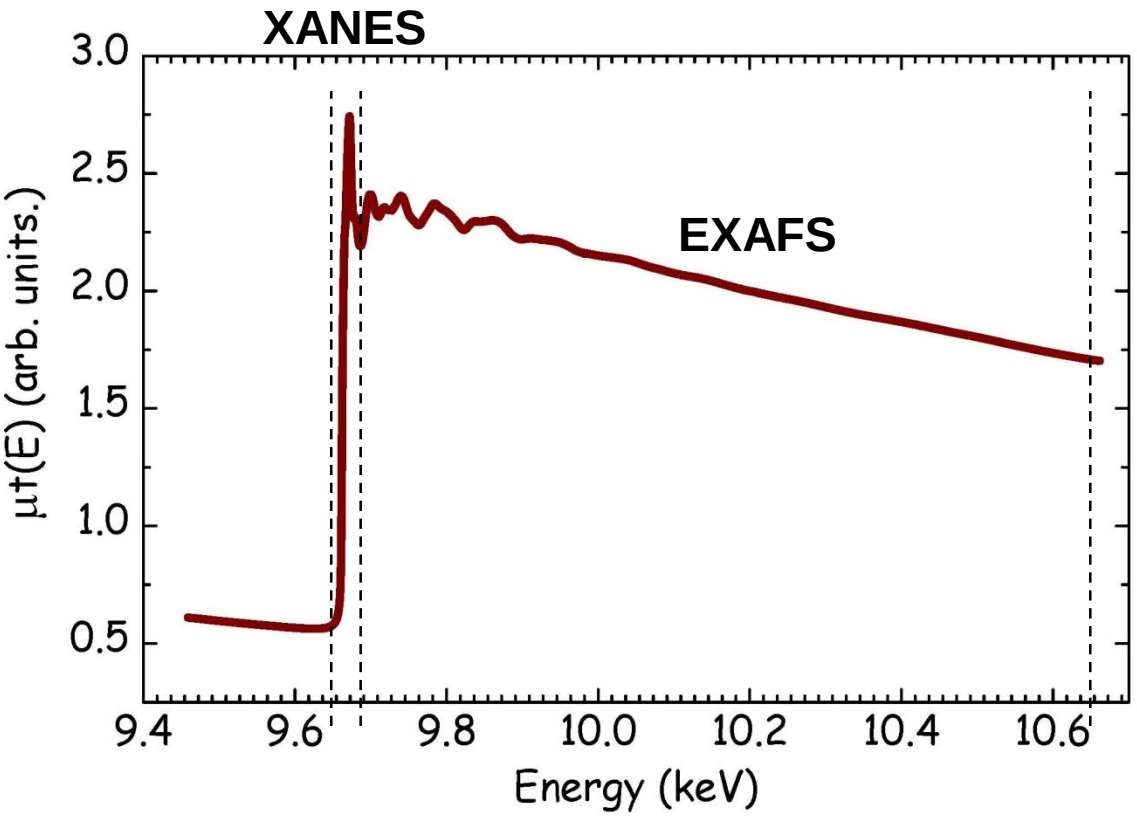


EXAFS oscillations:

$$\chi(E) = \frac{\mu(E) - \mu_0(E)}{\Delta\mu_0(E_0)}$$

- $\mu_0(E)$ smooth "bare atom" background
- $\Delta\mu_0(E_0)$ edge step or jump

XAFS NOMENCLATURE: XANES AND EXAFS



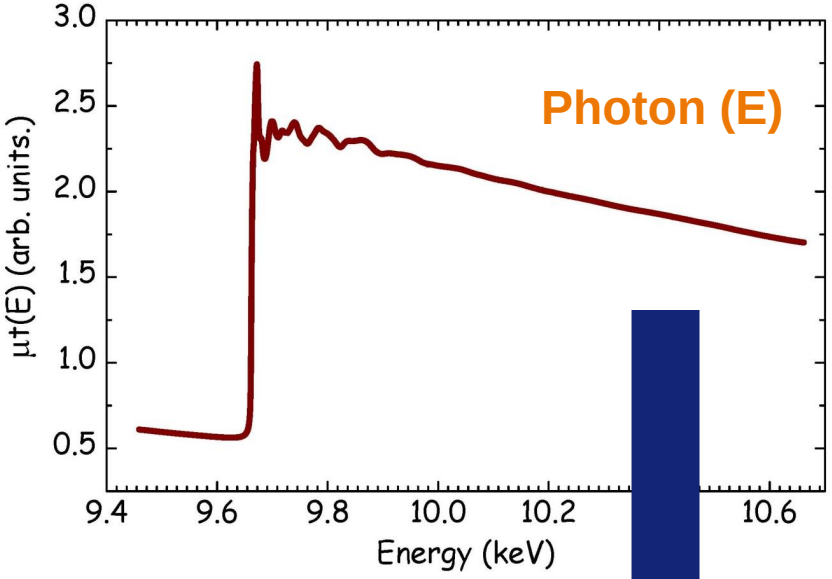
X-ray
Absorption
Near
Edge
Structure

up to ~ 60 eV
above the edge

Extended
X-ray
Absorption
Fine
Structure

from ~ 80 eV
to 1200 eV
above the edge

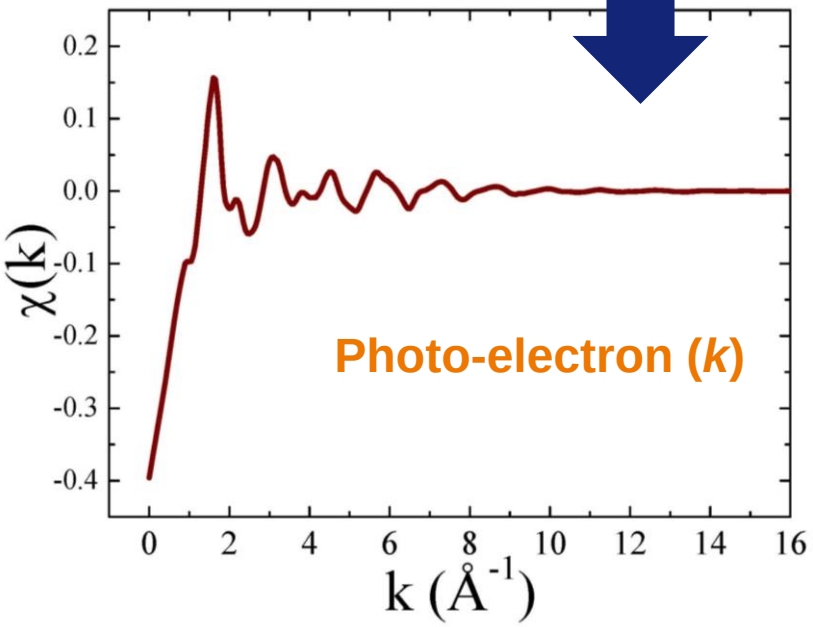
EXAFS OSCILLATIONS, χ(k)

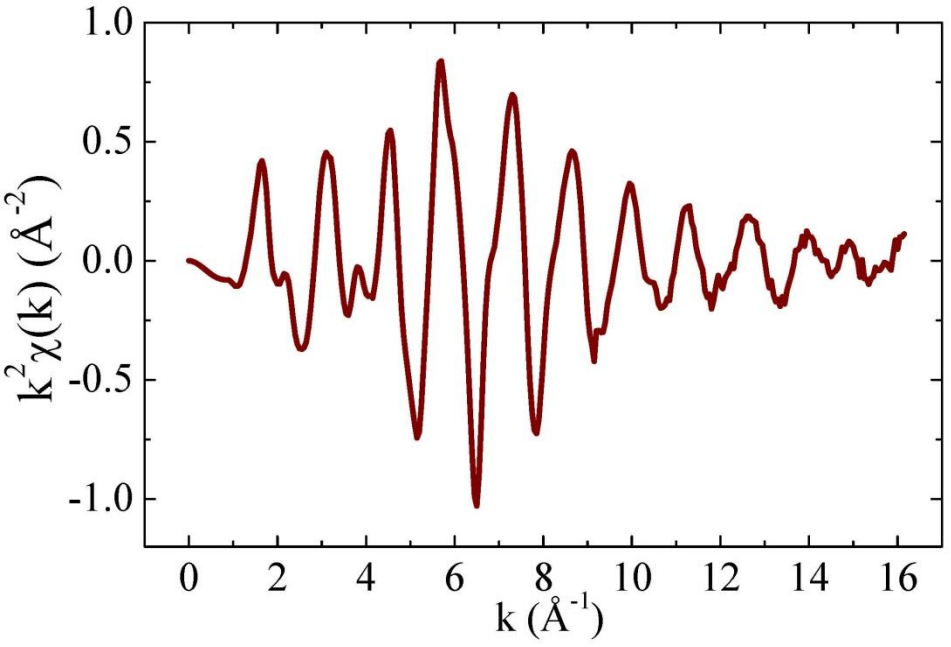


EXAFS depends on the wave nature of the photo-electron

$$\sqrt{\frac{2m(E-E_0)}{\hbar^2}} = k = \frac{2\pi}{\lambda}$$

k^2 or k^3 weighted
↓
Oscillations at high-k





EXAFS: PHYSICAL DESCRIPTION

Fermi´s Golden Rule describes μ(ω) as a transition between two quantum states :

$$\mu(\omega) \propto \sum_f W_{if}\, \delta(E_i - E_f + \hbar\omega)$$

Energy conservation

Transition probability $W_{if} \propto \left| \langle \psi_i | H | \psi_f \rangle \right|^2$

Approximations!

Weak interaction

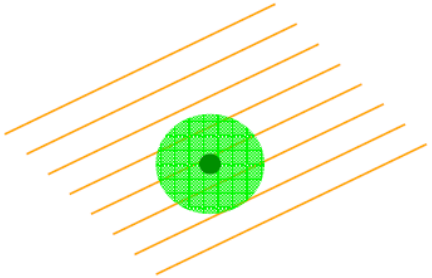
1st order perturbation

$|\psi_i\rangle$ Initial state: core-electron (x-ray photon)

$|\psi_f\rangle$ Final state: photo-electron (core hole)

$$|\psi_f\rangle = |\psi_f^0\rangle + |\Delta\psi_f\rangle$$

Electric dipole H

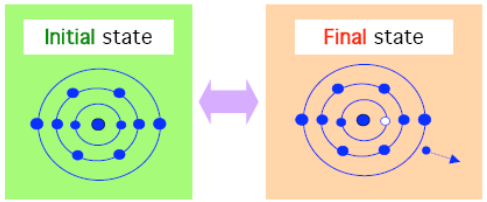


$$H \propto \vec{\varepsilon} \cdot \vec{r}$$

x-ray polarization electron position

One-electron

1 core electron excited
N-1 passive electron relaxed



$$|\Psi^{N-1}\psi\rangle = |\Psi^{N-1}\rangle|\psi\rangle$$

photoelectron ≠ passive e⁻

EXAFS: PHYSICAL DESCRIPTION

$$W_{if} \propto \left| \langle \psi_i | H | \psi_f \rangle \right|^2$$ Fermi Golden Rule

1 active electron

$$\mu(\omega) \propto \sum_f \left| \langle \psi_i | \vec{\varepsilon} \cdot \vec{r} | \psi_f \rangle \right|^2 \delta(E_i - E_f + \hbar\omega) \left| \langle \Psi_i^{N-1} | \Psi_f^{N-1} \rangle \right|^2$$

Dipole interaction

$$|\psi_f\rangle = |\psi_f^0\rangle + |\Delta\psi_f\rangle$$

Structural information

$$S_0^2 \approx 0.6 - 1$$

N-1 electrons relaxation

$$\chi(k) = \frac{\mu - \mu_0}{\mu_0} = \frac{2\,\mathrm{Re}\int d\vec{r}\,(\psi_i \vec{\varepsilon}\cdot\vec{r}\,\psi_f^{0\,*})(\psi_i^* \vec{\varepsilon}\cdot\vec{r}\,\Delta\psi_f)}{\int d\vec{r}\left|\psi_i^* \vec{\varepsilon}\cdot\vec{r}\,\psi_f^0\right|^2} \propto 2\,\mathrm{Re}(\psi_{scatt}(0))$$

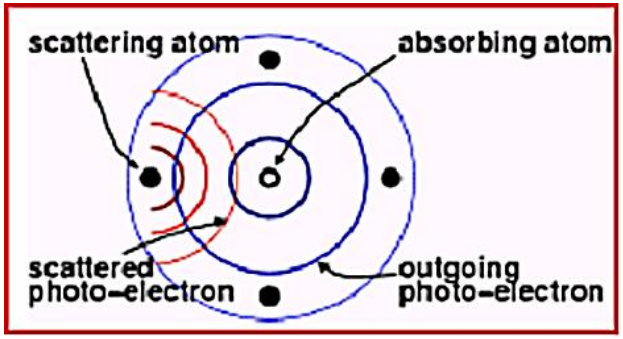
Wave-function of the scattered photo-electron at the absorbing atom

The region where $\psi_i \neq 0$ represents simultaneously the source and the detector for the photoelectron that probes the local structure around the absorber atom

EXAFS: PHYSICAL DESCRIPTION

We can build a simple model for χ from the photo-electron for a two-atomic system:

1. Leaving from the absorbing atom
2. Scattering from the neighbour atom
3. Returning to the absorbing atom



The outgoing photo-electron wave-function →

Spherical wave: $\psi(k,r) = \frac{e^{ikr}}{kr}$ + a neighbour atom at a distance R

$$\chi(k) \propto 2\,\mathrm{Re}(\psi(k,r=0)) = 2\,\mathrm{Re}(i\frac{e^{ik\mathrm{R}}}{2k\mathrm{R}}[\,f(k,\pi)e^{i\delta(k)}\,]\frac{e^{ik\mathrm{R}}}{\mathrm{R}})$$

$$\chi(k) = \frac{f(k,\pi)}{kR^2} sin(2kR + \delta(k))$$

Back & forth path

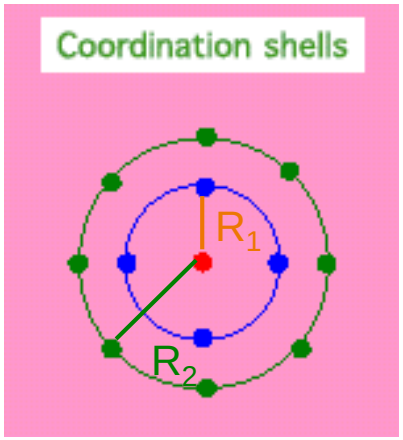
Spherical wave attenuation

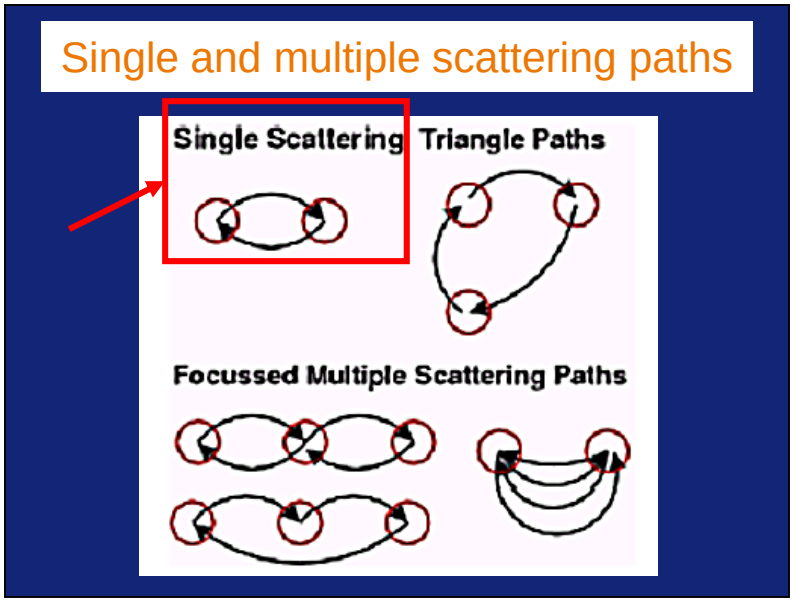
Back-scattering amplitude

phase-shift →

"Neighbour atom"

THE EXAFS EQUATION: MANY ATOMIC SYSTEM





Multiple-scattering paths are most important when the scattering angle is > 150 º

$$\chi(k) = \sum_j \frac{S_0^2 N_j f_j(k,\pi) e^{-2R_j/\lambda(k)} e^{-2k^2\sigma_j^2}}{kR_j^2} \sin(2kR_j + \delta_j(k))$$

Amplitude reduction term

Intrinsic losses on the EXAFS spectrum

Photo-electron mean-free path (including core-hole lifetime)

Thermal and static mean-square disorder in R

THE EXAFS EQUATION PARAMETERS

$$\chi(k) = \sum_j \frac{S_0^2 N_j f_j(k,\pi) e^{-2R_j/\lambda(k)} e^{-2k^2\sigma_j^2}}{kR_j^2} \sin(2kR_j + \delta_j(k))$$

- Parameters we need to calculate

$f(k)$ scattering amplitude

$\delta_j(k)$ phase-shift

} scattering properties of the atoms neighboring the photoabsorber (depend on the atomic number)

- Parameters to fit

R Distance to the neighbouring atom

N Coordination number of the neighbouring atom

σ^2 Disorder in the neighbour distance

THE EXAFS EQUATION PARAMETERS

$$\chi(k) = \sum_j \frac{S_0^2 N_j f_j(k,\pi) e^{-2R_j/\lambda(k)} e^{-2k^2\sigma_j^2}}{kR_j^2} \sin(2kR_j + \delta_j(k))$$

R

Distance to the neighbouring atom.

Or **half path length**, is the average distance between the absorbing and scattering atoms (single scattering path).

N

Coordination number of the neighbouring atom.

Or **degeneracy** of the path, is the identical number of distinct ways, per absorbing atom, that the scattering defined by the path can take place.

σ^2

Disorder in the neighbour distance.

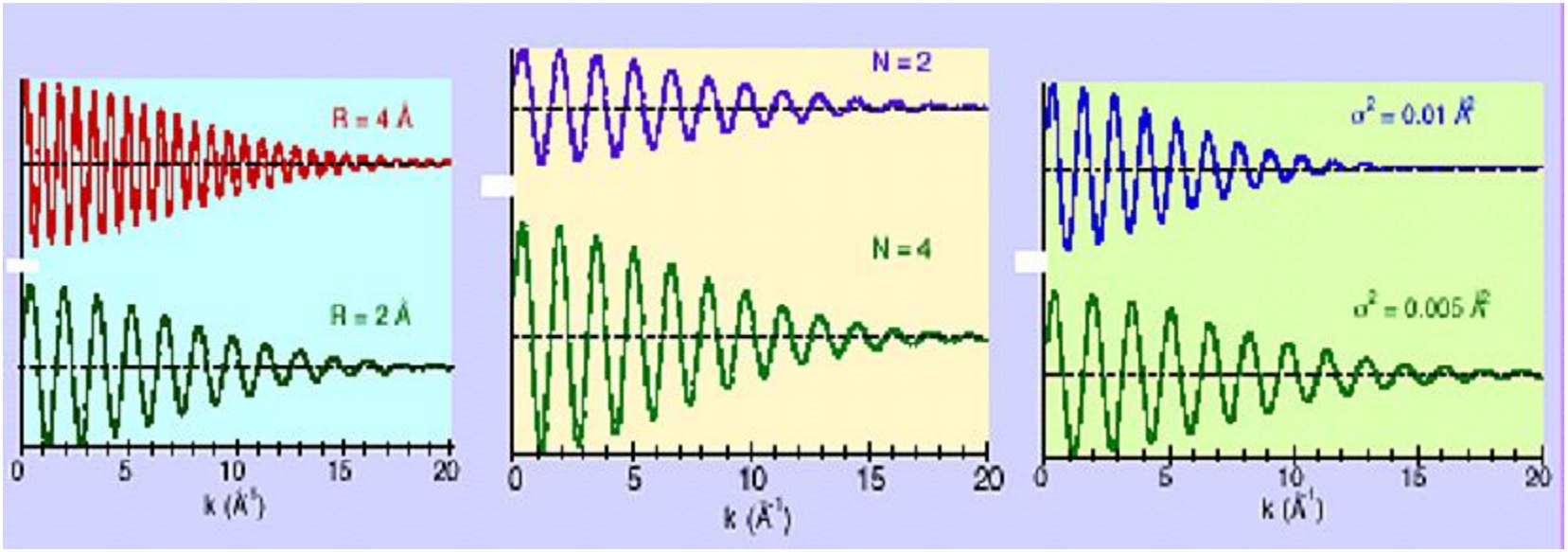
Or **Mean Square Relative Displacement** is the variance in the half path length, that is, the square of the standard deviation of the half path length: $\sigma^2 = \langle (r - r_m)^2 \rangle$.

Static and/or thermal disorder.

EXAFS takes place on a time scale much shorter than that of atomic motion, so the measurement serves as an instantaneous snapshot of the atomic configuration

EXAFS: A STRUCTURAL PROBE

If we know the scattering properties of the neighbouring atoms: $f(k)$ and $\delta(k)$, and the mean-free path $\lambda(k)$, we can determine:



Frequency → Interatomic distance R

The larger R, the smaller the spacing

Amplitude → Coordinaction number N

The amplitude of the path scales with the degeneracy.

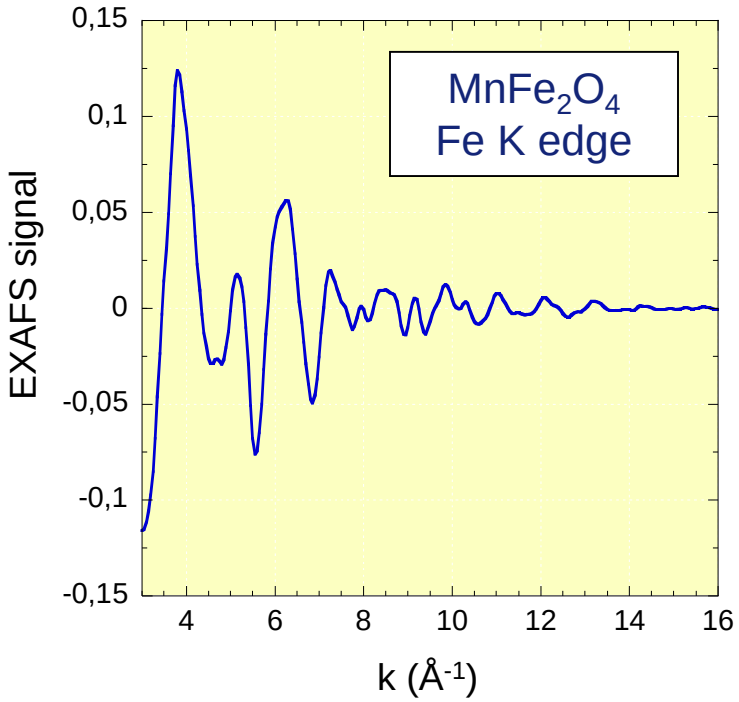
Damping → Debye-Waller factor σ^2 (disorder)

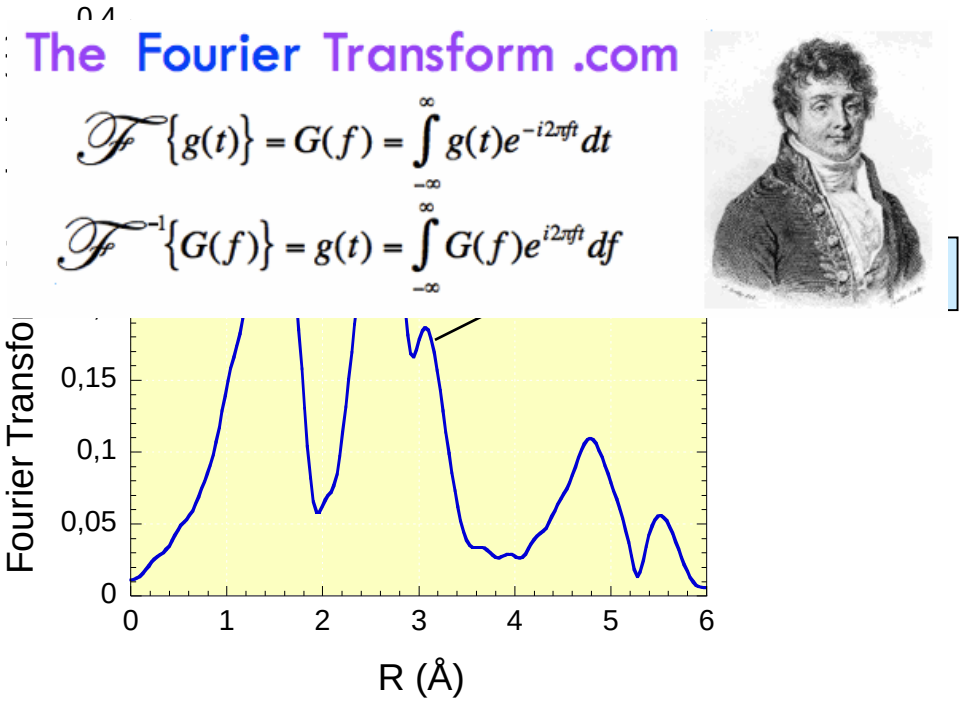
Increasing MSRD decreases the amplitude

EXAFS: A STRUCTURAL PROBE

- Multiple terms in the EXAFS equation may be significant, each of them being a modulated sinusoid → need to decompose a function into constituent sine waves

- **Fourier transformation** can be used to descompose a frequency-space signal into its different constituent frequencies. The Fourier transform of an EXAFS spectrum gives a pseudo-radial distribution function.

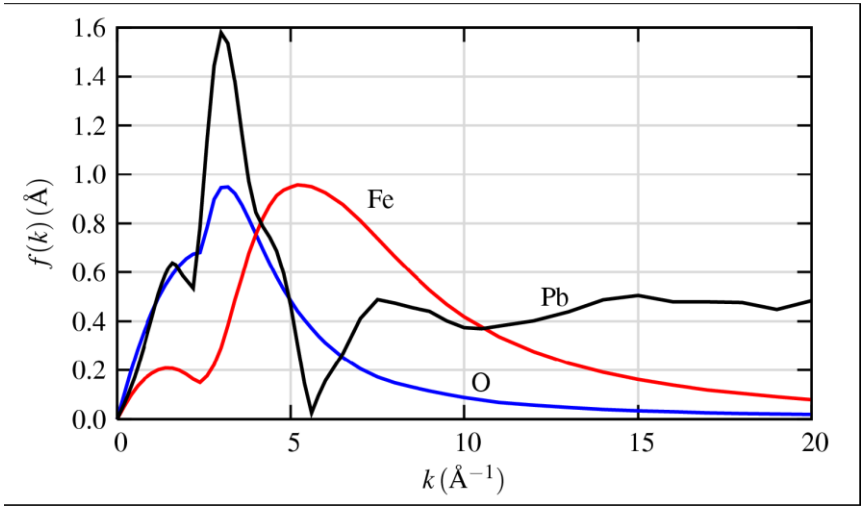




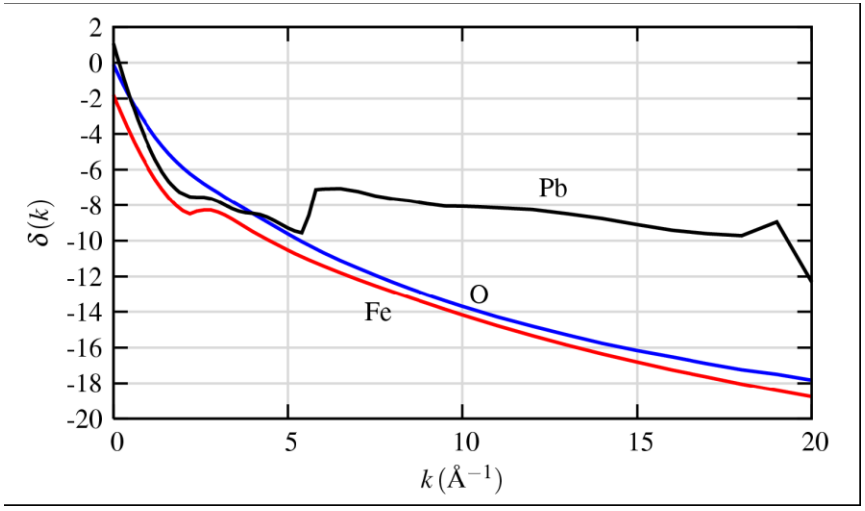
FT distances are shifted by ~ -0.5 Å

EXAFS: SELECTIVITY OF ATOMIC SPECIES

The scattering amplitude *f* (*k*) and phase shift δ (*k*) depend on the atomic number *Z*



The scattering amplitude *f (k)* peaks at different k values and extends to higher-k for heavier elements. For very heavy elements, there is structure in *f (k)*.



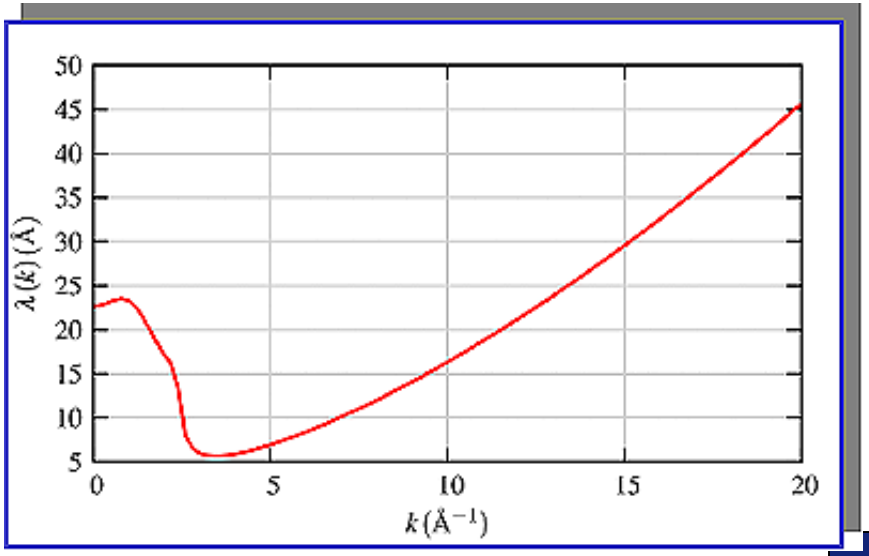
The phase shift δ(k) shows sharp changes for very heavy elements.

These scattering functions can be accurately calculated (say with the programs FEFF, GNXAS, etc.), and used in the EXAFS modeling.

EXAFS: A SHORT RANGE ORDER PROBE

The photo-electron mean-free path $\lambda(k)$ limites how far the photo-electron can go:

- Inelastic scattering
- Core-hole finite life-time



The mean-free path λ depends on k

λ < 25 Å for the EXAFS k-range

The term $\frac{e^{-2R_j/\lambda(k)}}{R_j^2}$ makes EXAFS a local atomic probe,

typically within 10 Å from the absorber

EXAFS ACCURACY

- Distances ±0.01Å The absorber–scatter distance can be measured quite accurately from the frequency of the sinusoidal oscillations.
- Coordination numbers
  Debye-Waller factors ± 20-25% High correlation between them ↔ less accurate

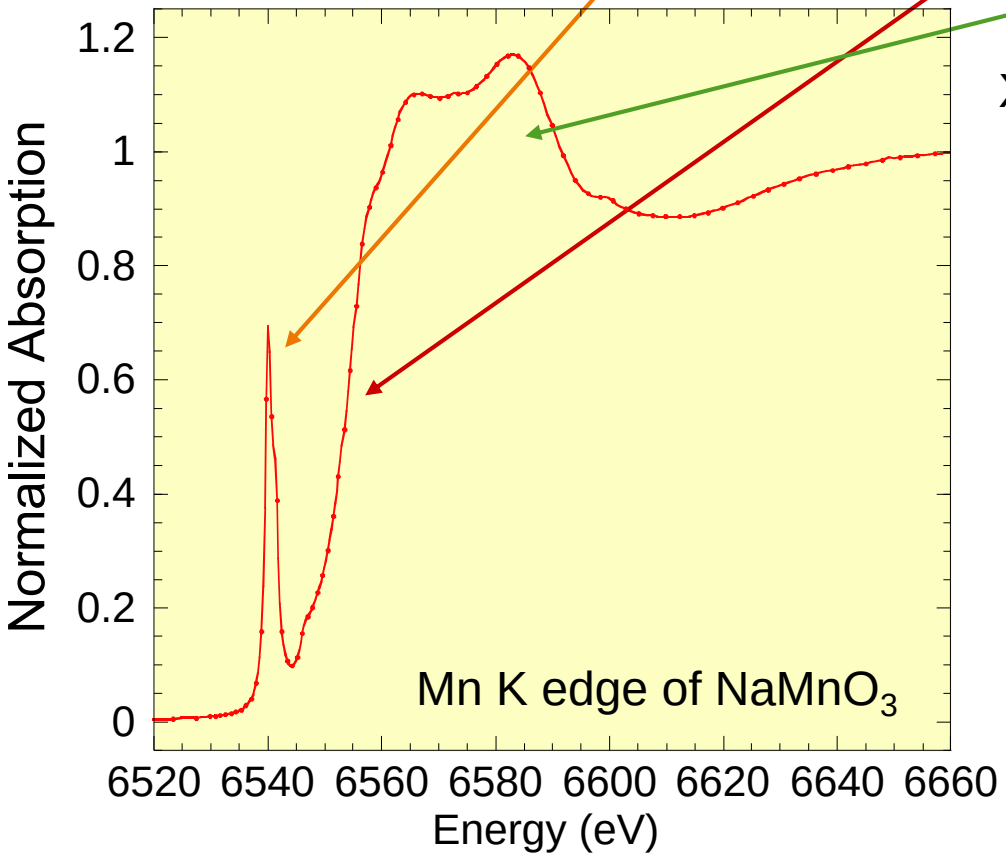
- Scattering Atom Z ± 1 (Z=6-17)
  Z ± 3 (Z=20-35)

Elements that are next to each other in the periodic table has barely distinguishable photoelectron scattering characteristics. Thus, C,N and O are impossible to distinguish and metal scattered can only be placed in the proper row of the periodic table

XANES REGION

What is XANES ?

XANES = Pre-edge + Edge + XANES



XANES is extremely sensitive to the chemistry of the absorbing atom:

- Formal oxidation state
- Coordination environment

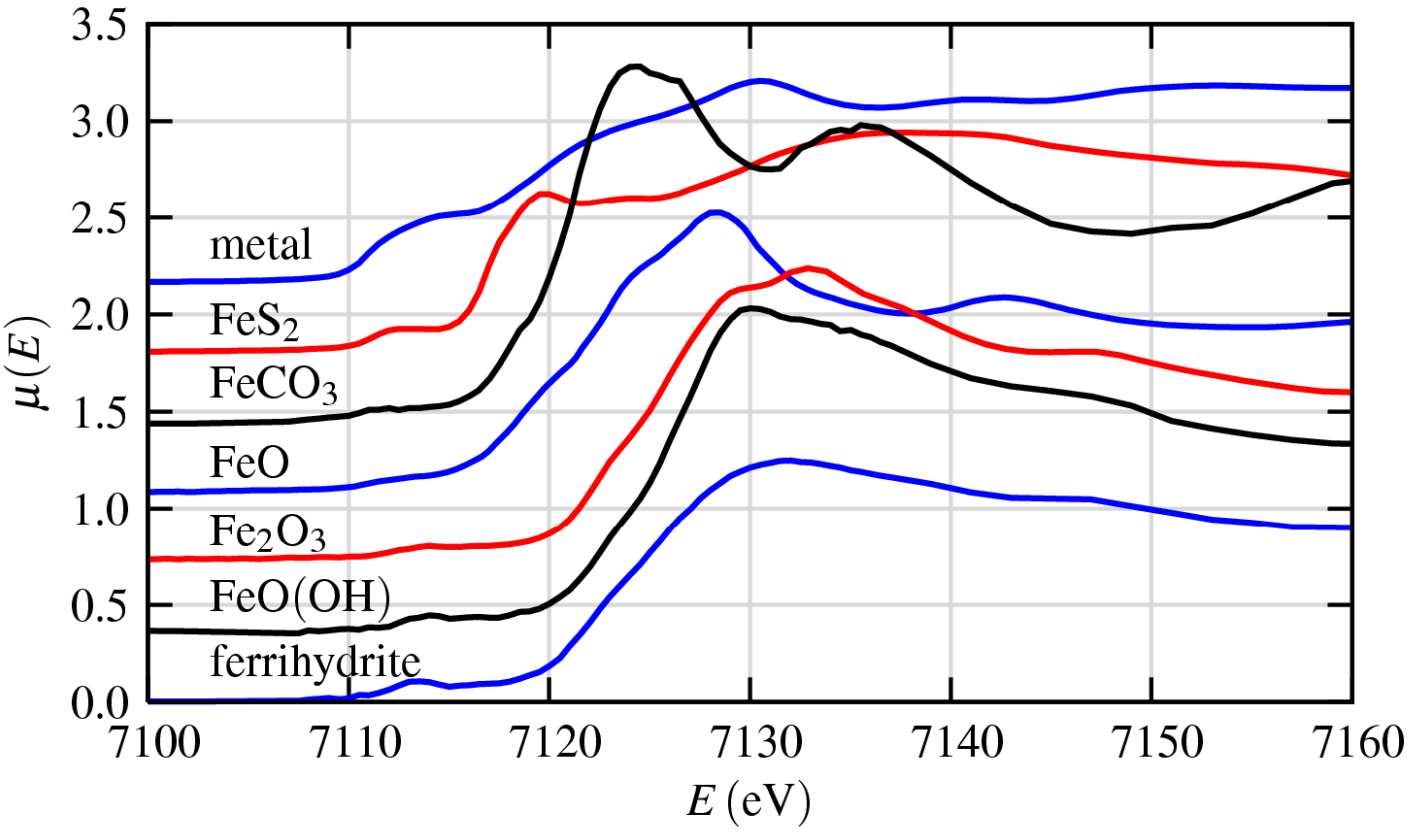
XANES probes the angular momentum of the unoccupied electronic states.

$$\Delta\ell = \pm 1$$
$$\Delta s = 0$$
$$\Delta j = \pm 1, 0$$
$$\Delta m = 0$$

WHY ARE WE INTERESTED IN XANES REGION?

Region	Transition	Information Content
Pre-edge	Electronic transitions to empty bound states (transition probability controlled by dipolar selection rules). e.g. 1s→3d, 1s→4p (1st transition series metals)	Local coordination environment around the absorbing atom. Dependence on the oxidation state and bonding.
Edge	Defines ionization threshold to continuum states.	Dependence on the oxidation state "Chemical shift": main edge (binding energy) shifts to higher energy with increasing oxidation state.
XANES	Feautures dominated by multiple-scattering resonances of the photoelectrons ejected at low $E_{kinetic}$.	Atomic positions of neighbours: Interatomic distances and bond angles.

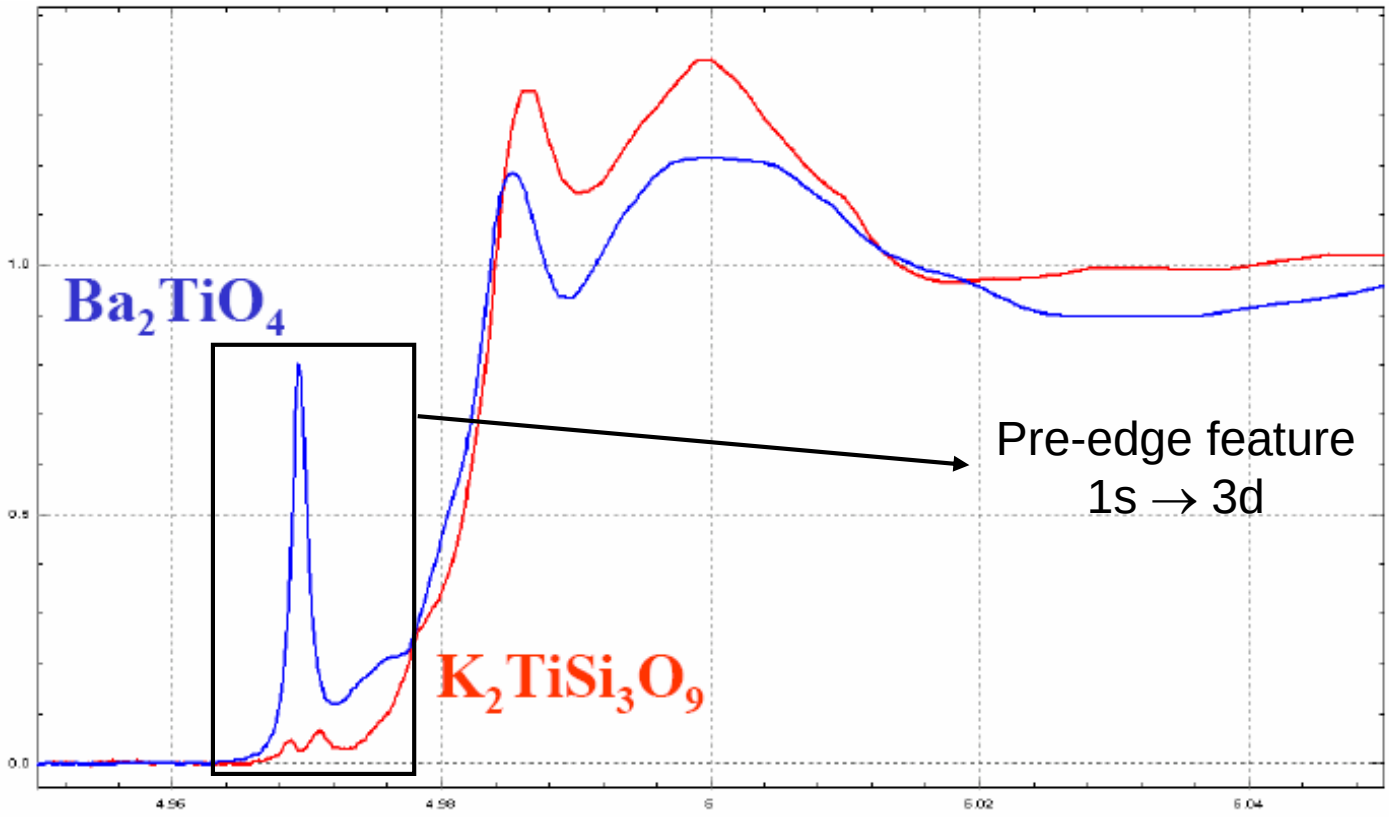
EDGE POSITION: OXIDATION STATE



XANES can be used simply as a fingerprint of phases and oxidation state.

XANES Analysis can be as simple as making linear combinations of “known” spectra to get compositional fraction of these components.

XANES ANALYSIS: LOCAL COORDINATION ENVIROMENT



Both Ti^{4+}

Ba_2TiO_4

$K_2TiSi_3O_9$

Ti K-edge XANES is highly dependent on the local coordination:
(1) Tetrahedral *vs*. Octahedral
(2) Different neighbors shells beyond the first O-shell

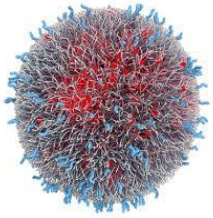
WHAT CAN XAS BE MEASURED ON?

... just about almost anything and with most elements of the periodic table

Art: Cultural Heritage

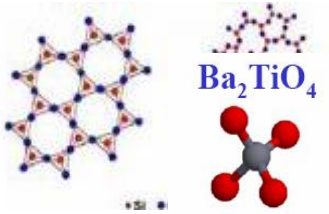
of s
p

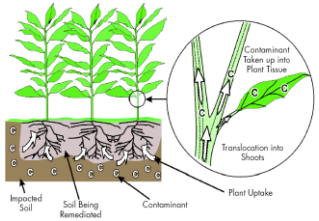
?



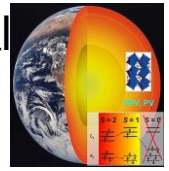
Biology

Material Science





Enviromental
Science
Geology



Chemistry
Catalysis

Physics

Local probe!

APPLICATIONS: CATALYSIS

Reproduce real catalytic reaction conditions (car exhaust pipe) to develop new catalytic

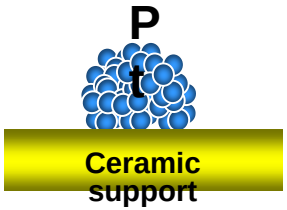
Controls 80 % world's chemical manufacturing processes

Active site : Pt, Rh, Pd

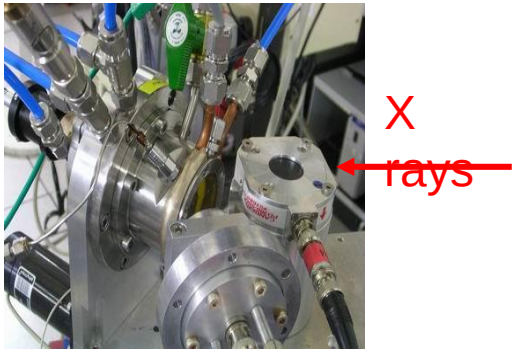
Support : alumina, etc.

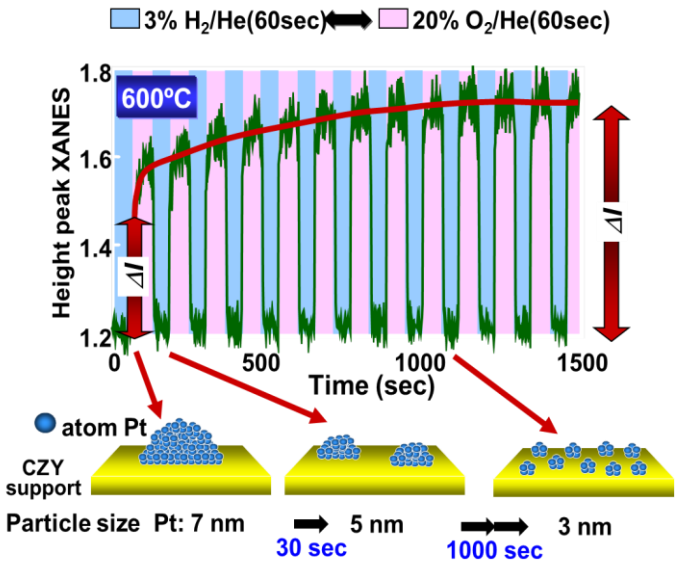
Additives : CeO_2, CeO_2-ZrO_2, alkalin… etc.

Three-way-catalysts

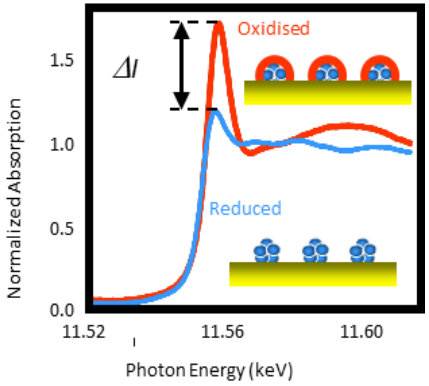


Reproduce T and mixture of gases for real driving conditions





Dynamic and *in situ* study via X ray Absorption in Fluorescence

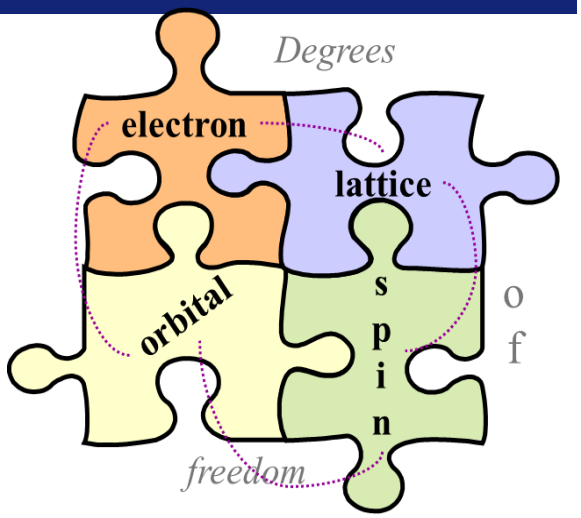


Experiment performed by TOYOTA.

APPLICATIONS: SOLID STATE PHYSICS

Structural changes due to phase transitions

- Temperature
- Pressure
- Magnetic Fields,…

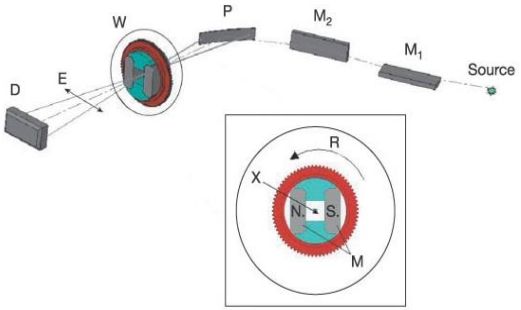


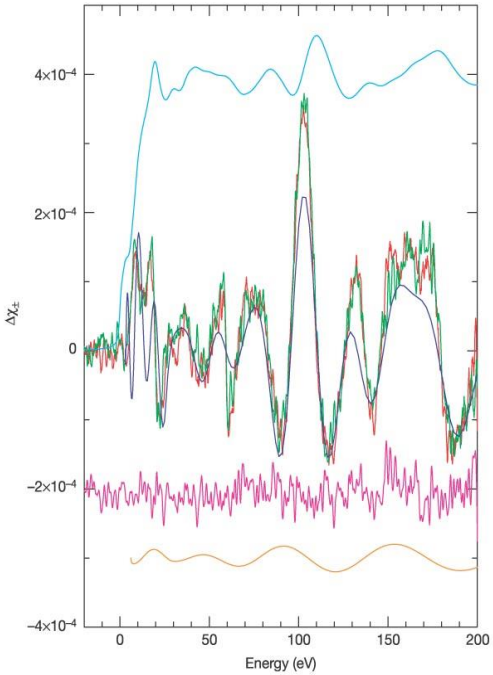
Measurement of femtometre-scale atomic displacements by X-ray absorption spectroscopy

Robert F. Pettifer[1], Olivier Mathon[2], Sakura Pascarelli[2], Michael D. Cooke[3]* & Michael R. J. Gibbs[3]

[1]Department of Physics, University of Warwick, Coventry CV4 7AL, UK
[2]European Synchrotron Radiation Facility (ESRF), BP 220, 38043 Grenoble Cedex 9, France
[3]Department of Engineering Materials, Sir Robert Hadfield Building, Mappin Street, University of Sheffield, Sheffield S1 3JD, UK

NATURE | VOL 435 | 5 MAY 2005 | www.nature.com/nature





Fe-Co thin films. Periodic strain through magnetostriction.

- Magnetostriction can be detected with EXAFS (**diff**) !
- Normal exafs accuracy 0.01- 0.001 Å
- Q-exafs→Diff-exafs sensitivity of 1 fm (0.0001 Å)

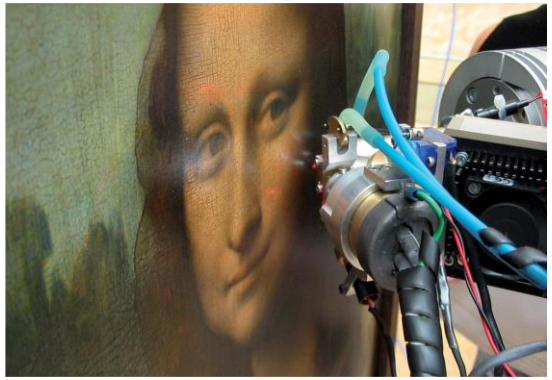
APPLICATIONS: CULTURAL HERITAGE

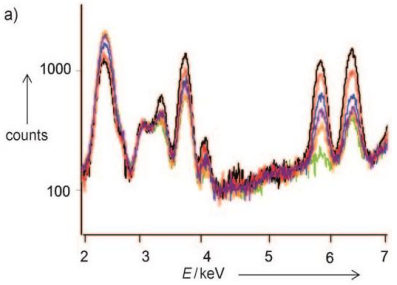
Analyzing Works of Art

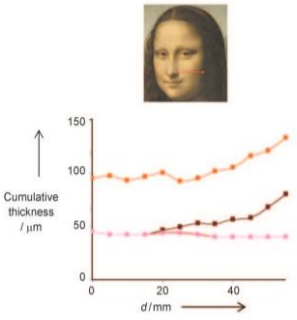
DOI: 10.1002/anie.201001116

Revealing the *sfumato* Technique of Leonardo da Vinci by X-Ray Fluorescence Spectroscopy**

Laurence de Viguerie, Philippe Walter, Eric Laval, Bruno Mottin, and V. Armando Solé*







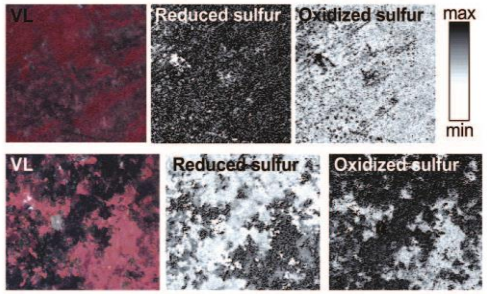
- Non-invasive
- Binder Concentration
- Pigments Inorganic composition
- Layers Thickness

- Mn, Fe pigments on the glaze
- Pb in every layer
- Glaze layers unfinished

Anal. Chem. **2006**, *78*, 7484–7492

Blackening of Pompeian Cinnabar Paintings: X-ray Microspectroscopy Analysis

Marine Cotte,*,† Jean Susini,† Nicole Metrich,‡ Alessandra Moscato,§ Corrado Gratziu,§ Antonella Bertagnini,|| and Mario Pagano||



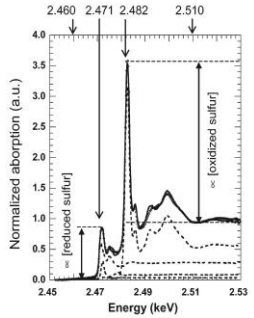
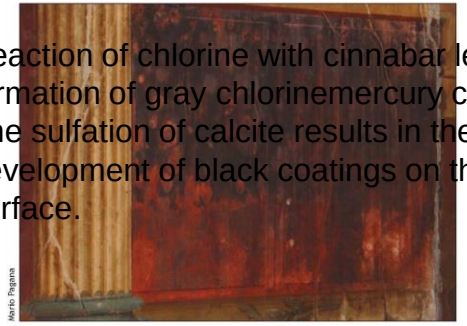


Figure 9. Computation on the μ-XANES spectra at the S K-edge: fit of the experimental data (plain) by combination of cinnabar, sulfur, corderoite, and gypsum spectra (dotted) and estimation of the reduced and oxidized sulfur concentrations by measuring the fluorescence intensity at four specific energies.

- Why do the red walls of Pompei go black?

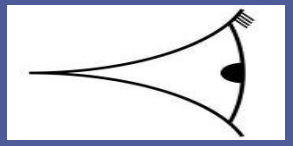
1. Reaction of chlorine with cinnabar leads to the formation of gray chlorinemercury compounds.
2. The sulfation of calcite results in the development of black coatings on the painting surface.



Turning black. A wall painted red in the remains of Pompeii.

TAKE-HOME MESSAGE

Exafs is sensitive to …



Density of electronic states

- **Local structure in non-crystalline matter**
- **Local environment of an atomic impurity in a matrix of different atomic species**
- **Study of systems whose local properties differ from the average properties**
- **Detection of very small distortions of local structure**

WHERE TO GO FROM HERE

Books and Review Articles:

Basic Principles and Applications of EXAFS
Handbook of Synchrotron Radiation, Chapter 10, pp. 995-1014, E. A. Stern and S. M. Heald, E. E. Koch, ed., North-Holland 1983

X-ray Absorption: Principles, Applications, Techniques of EXAFS, SEXAFS and XANES
in *Chemical Analysis* Vol. 92, D. C. Koningsberger and R. Prins, ed., John Wiley & sons, 1988

X-ray Absorption Fine Structure for Catalysis and Surfaces
World Scientific Series on Synchrotron Radiation Techniques and Applications Vol. 2, ed., Y. Iwasawa, 1996

X-ray absorption spectroscopy in coordination chemistry
J. E. Penner-Hahn, *Coordination Chemistry Reviews* 190-192, pp. 1101-1123, 1999

Tutorials and other Training Material:

http://xafs.org/Tutorials
http://gbxafs.iit.edu/training/tutorials.html Grant Bunker's tutorials
http://srs.dl.ac.uk/XRS/courses/ tutorial from Daresbury Lab, UK

Software resources:

http://xafs.org/Software

Analysis programs: *Atoms* + *Feff* + *iFeffit* (Theoretical XAFS calculations and fitting) – Univ. Chicago (USA)
Athena, Artemis (EXAFS Data Reduction and fitting

http://gnxas.unicam.it : *Gnxas* (Theoretical XAFS calculations and fitting) – Univ. Camerino (Italy)
http://www.esrf.fr/computing/scientific/xop/ *XOP* (DABAX data base, cross-section and lots of general x-ray Calculations, multipurpose data visualization and analysis)-M. Sanchez del Rio, and R. J. Dejus (ESRF, France)

http://srs.dl.ac.uk/XRS/index.html : *Excurv98* (Theoretical XAFS calculations and fitting) – Daresbury Lab (UK)

DATA PROCESSING AND ANALYSIS

- **Iffefit package:**

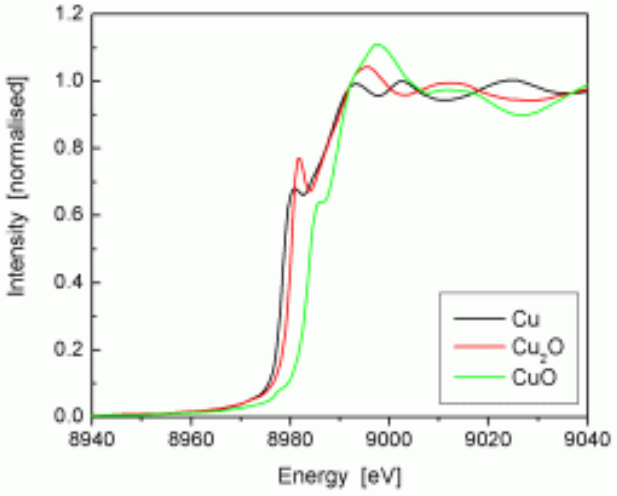
http://cars9.uchicago.edu/ifeffit/

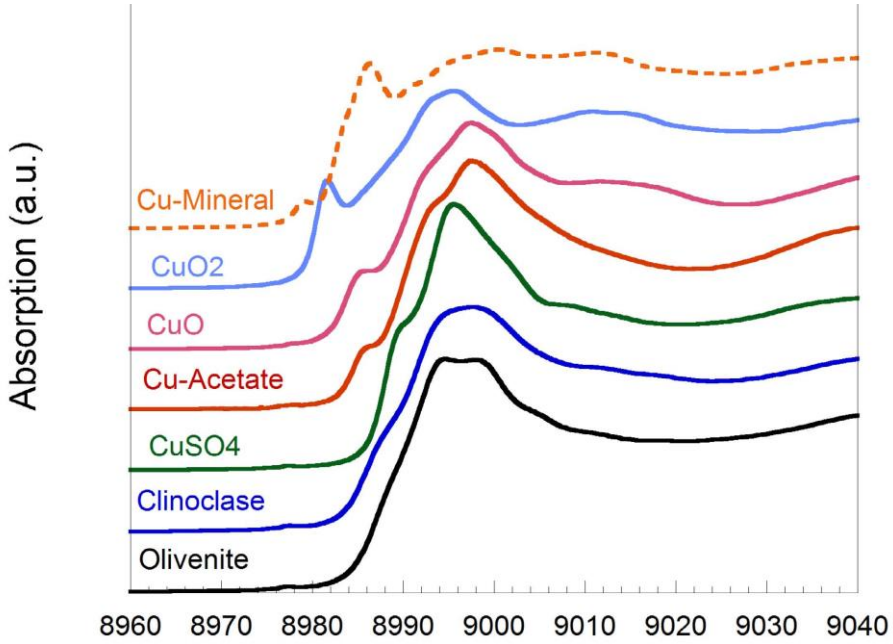
http://bruceravel.github.io/demeter/

- **Athena: data processing**

- **Artemis: data analysis using Feff**

CU FOIL AND CUO ANALYSIS: XANES





Cu foil Cu^0, $3d^{10}\ 4s^1$

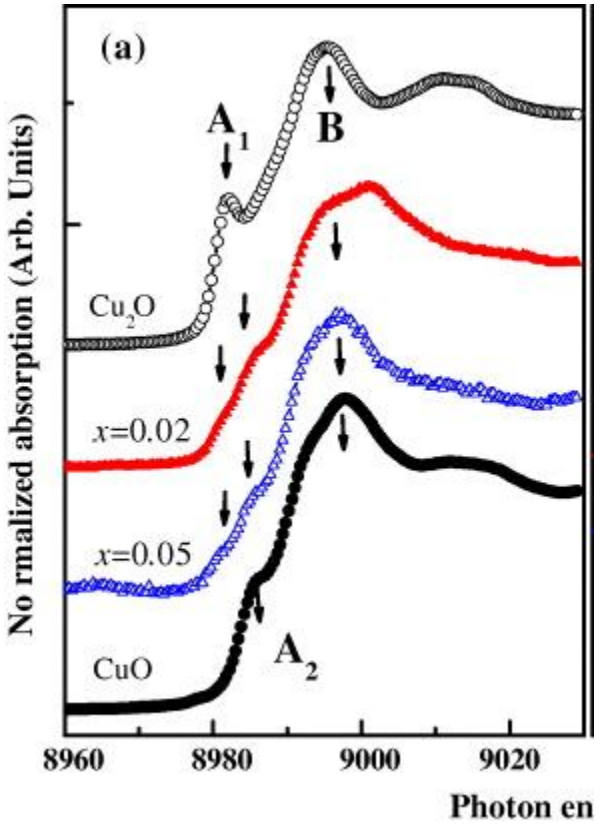
Cu_2O Cu^{1+}, $3d^9\ 4s^1$ Cu Tetrah.

CuO Cu^{2+}, $3d^8\ 4s^1$ Cu square planar

CU METAL AND CU OXIDE XAFS

Cu foil Cu^0, $3d^{10}\ 4s^1$
Cu_2O Cu^{1+}, $3d^9\ 4s^1$ Cu Tetrah.
CuO Cu^{2+}, $3d^8\ 4s^1$ Cu square planar

The pre-edge features marked A_1 and A_2, respectively, in the Cu_2O and CuO spectra represent transitions from the 1s → axial 4p state, which contain a small portion of the unoccupied 3d states as the quadruple allowed transitions and are close to the 4s state. The feature marked as B is mainly due to the transition from copper 1s to the 4p state



Cu FOIL ANALYSIS

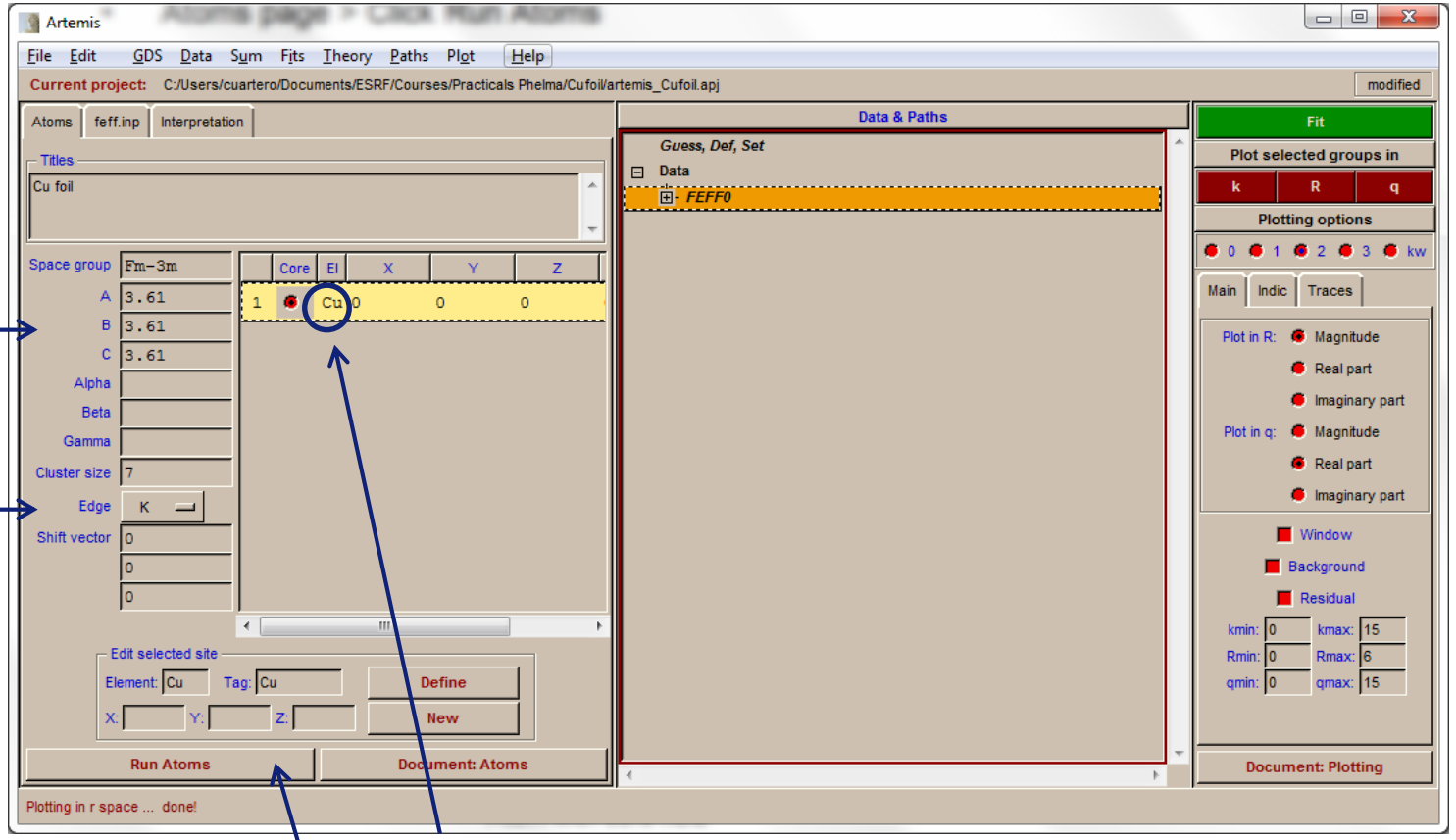
✓ Data processed, with Athena.
✓ Crystal structure (or reference crystal structure) known.
- Cu metal, FCC, Fm-3m
- CuO, monoclinic, C2/c
- Inorganic Crystal Structure data base

https://icsd.fiz-karlsruhe.de/search/basic.xhtml;jsessionid=5DC14101FB0549F273F08BC77D85DF9D

1. Create the cluster, with ATOMS.
2. Create the scattering paths, with FEFF (integrated in Atoms)
3. 1st shell analysis, with ARTEMIS.

Cu FOIL ANALYSIS: ATOMS

1. Create the cluster
   - Atoms page > Click Run Atoms



Structural info

Absorption edge

Atom with core hole

Make input (feff.inp) for theoretical calculation (FEFF)

Cu FOIL ANALYSIS: ATOMS

1. Create the cluster
   - Theory input page feff.inp > Click Run Feff

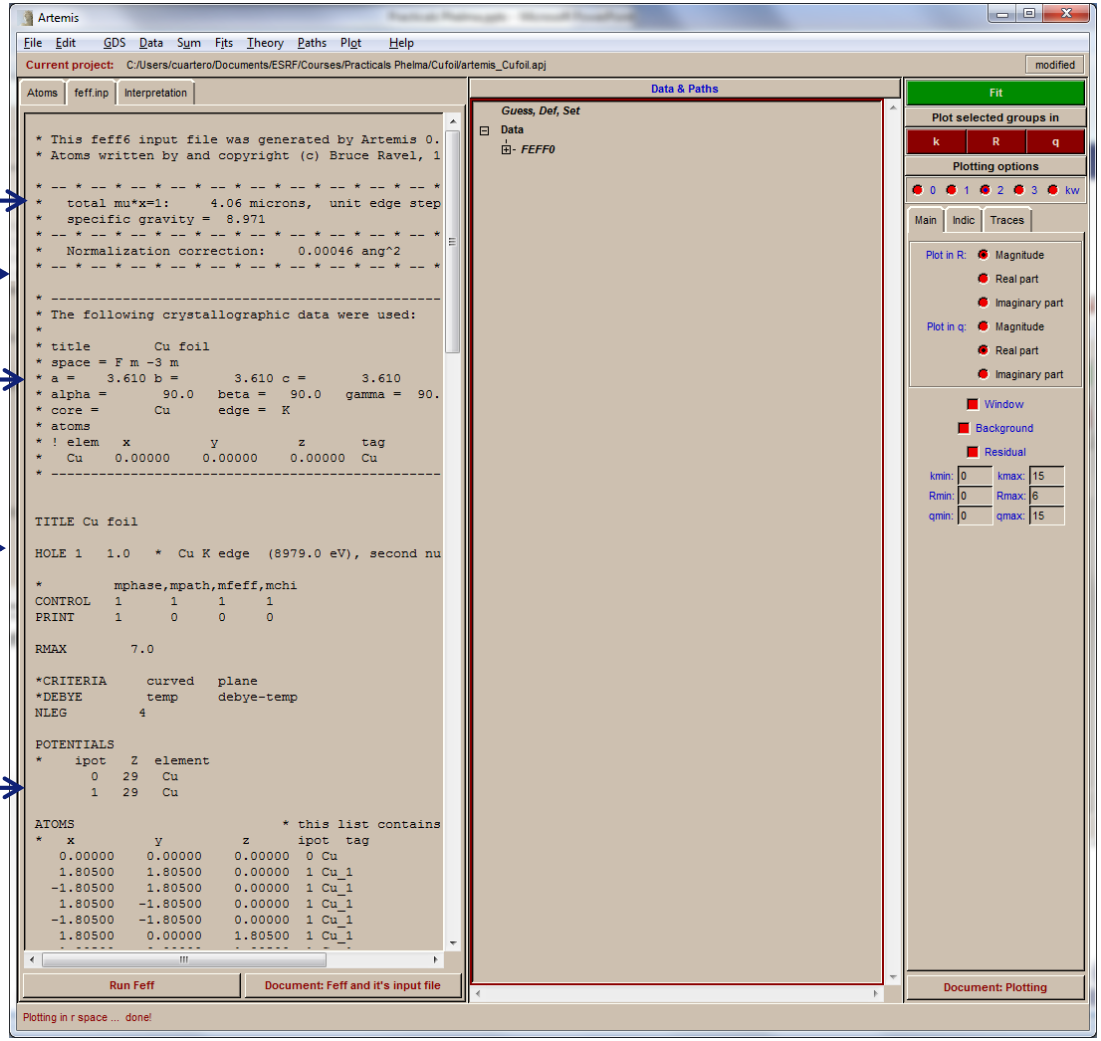
Absorption lenghts

Normalization correction

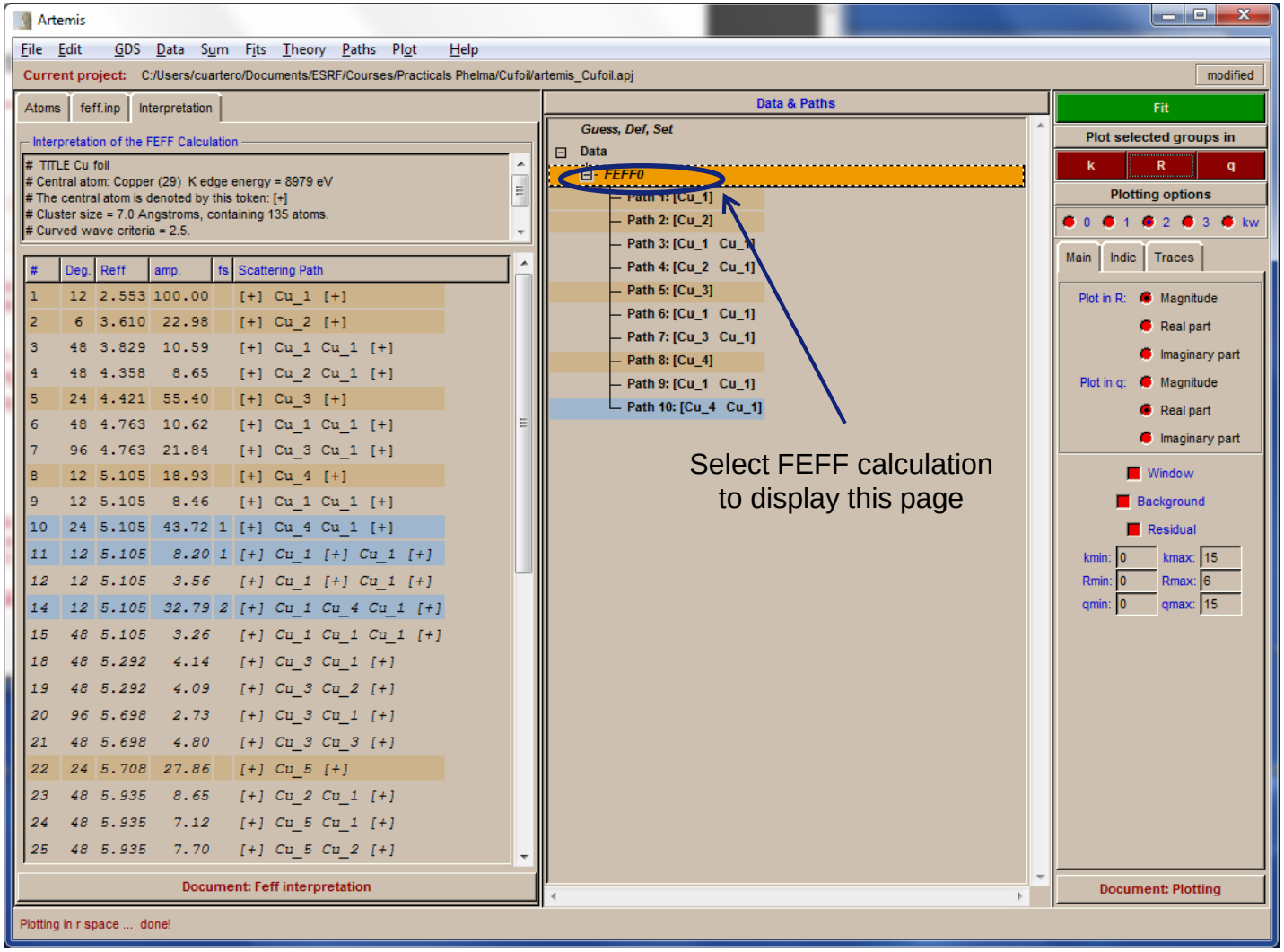
Crystallographic Info

Hole number
and S02 value

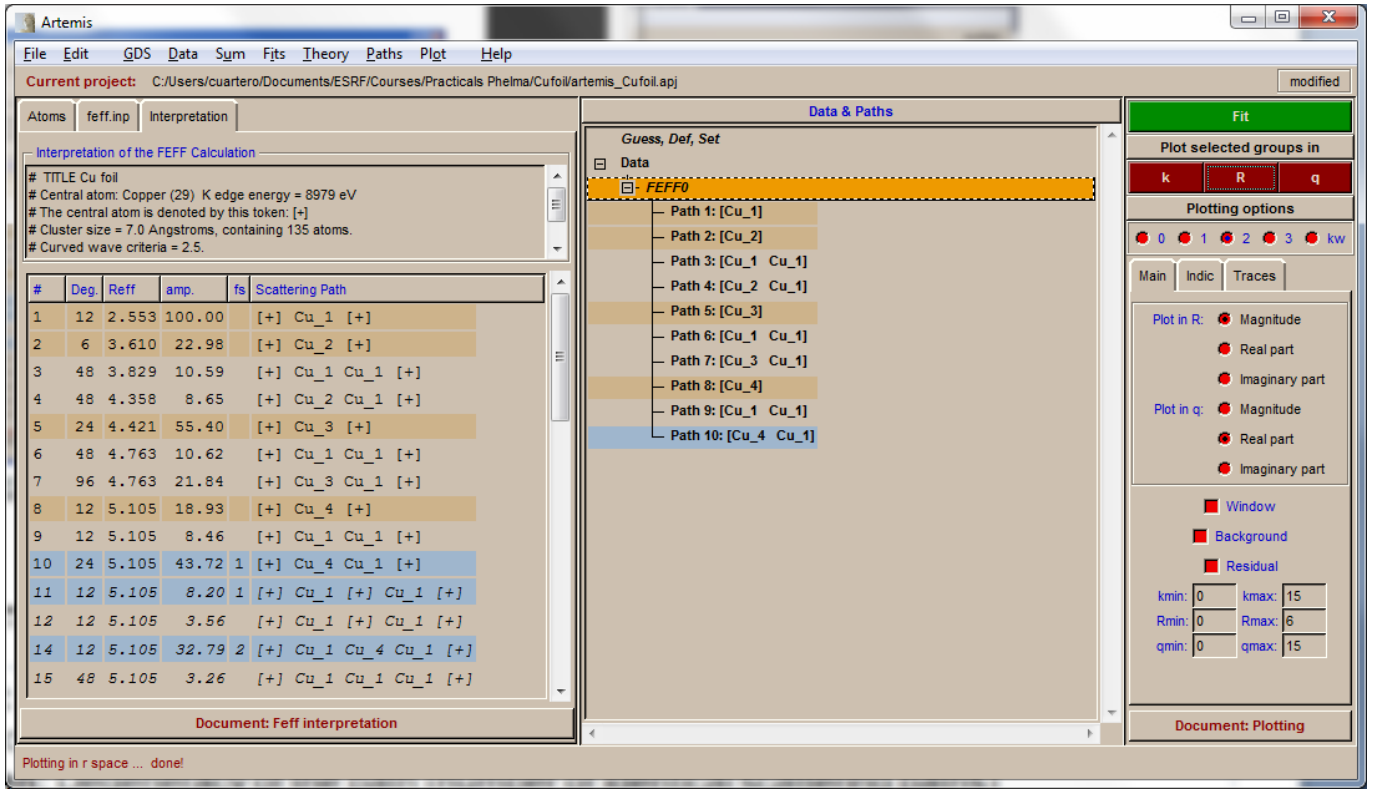
Atomic potential index list



Cu FOIL ANALYSIS: ARTEMIS



Cu FOIL ANALYSIS: ARTEMIS

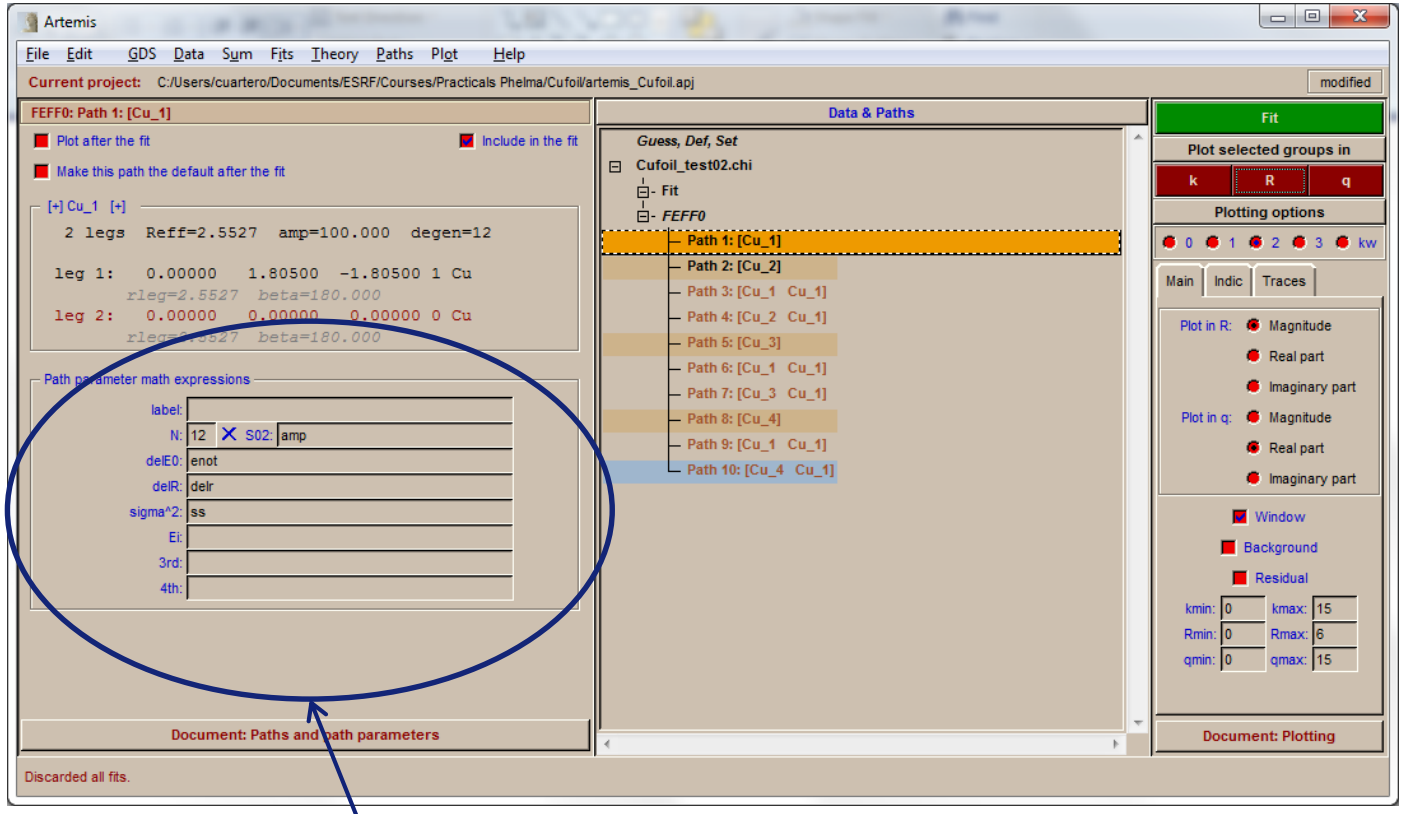


Feff paths

- **Deg:** Degeneracy of the path (number of identical scattering paths)
- **Reff:** Inital half path length (bond length for single scattering path)
- **amp:** Estimate of amplitude of path relative to first path.
- **fs:** Number of forward scattering events.
- **Scattering Path:** atoms scattering photoelectron, [+] symbol represents core atom.

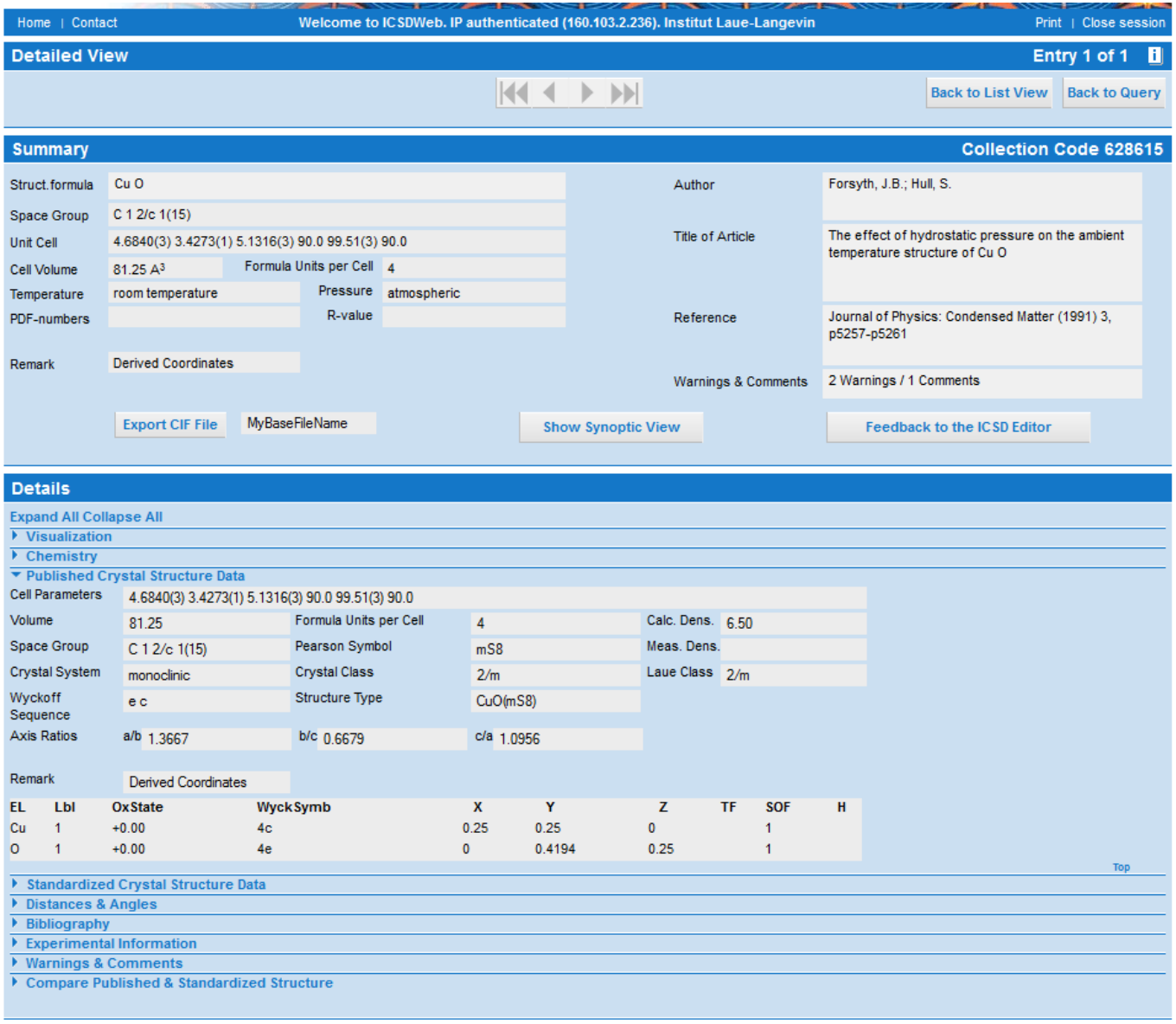
Cu FOIL ANALYSIS: ARTEMIS

Path description



Fitting parameters

CUO XTAL STRUCTURE



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Detailed View — Entry 1 of 1

Back to List View | Back to Query

Summary — Collection Code 628615

Struct. formula	Cu O	Author	Forsyth, J.B.; Hull, S.
Space Group	C 1 2/c 1(15)		
Unit Cell	4.6840(3) 3.4273(1) 5.1316(3) 90.0 99.51(3) 90.0	Title of Article	The effect of hydrostatic pressure on the ambient temperature structure of Cu O
Cell Volume	81.25 A^3	Formula Units per Cell	4
Temperature	room temperature	Pressure	atmospheric
PDF-numbers		R-value	
Reference	Journal of Physics: Condensed Matter (1991) 3, p5257-p5261		
Remark	Derived Coordinates		
Warnings & Comments	2 Warnings / 1 Comments		

Export CIF File | MyBaseFileName | Show Synoptic View | Feedback to the ICSD Editor

Details

Expand All Collapse All

- Visualization
- Chemistry
- Published Crystal Structure Data

Cell Parameters	4.6840(3) 3.4273(1) 5.1316(3) 90.0 99.51(3) 90.0				
Volume	81.25	Formula Units per Cell	4	Calc. Dens.	6.50
Space Group	C 1 2/c 1(15)	Pearson Symbol	mS8	Meas. Dens.	
Crystal System	monoclinic	Crystal Class	2/m	Laue Class	2/m
Wyckoff Sequence	e c	Structure Type	CuO(mS8)		
Axis Ratios	a/b 1.3667	b/c 0.6679	c/a 1.0956		

Remark: Derived Coordinates

EL	Lbl	OxState	WyckSymb	X	Y	Z	TF	SOF	H
Cu	1	+0.00	4c	0.25	0.25	0		1	
O	1	+0.00	4e	0	0.4194	0.25		1	

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