XAFS Detector Requirements

STEVE HEALD,
PNCC Cat at APS

What is needed for XAFS?

S/N requirements

Possibilities with "ideal" detector

Current Detectors

X-ray Raman measurements

Summary

Measuring XAFS

$$\chi(k) = \frac{\mu(k) - \mu_0(k)}{\mu_0(k)} = \sum_j \frac{N_j}{kR_j^2} A_j(k) p_j(\mathbf{e}) \sin\left[2kR_j + \psi_j(k)\right]$$

Need to measure μ to high accuracy

Direct measurement impractical for dilute elements

Measure fluorescence or electron yield:

$$\mu'(E) = \frac{I_f}{I_0} \propto \frac{\mu(E)\sin\theta}{\mu_T(E)/\sin\theta + \mu_T(E_f)/\sin\varphi}$$

is proportional to μ(E) when $\mu(E) \ll \mu_T(E)$

Many XAFS applications involve dilute (thin) samples

Surface studies/catalysis

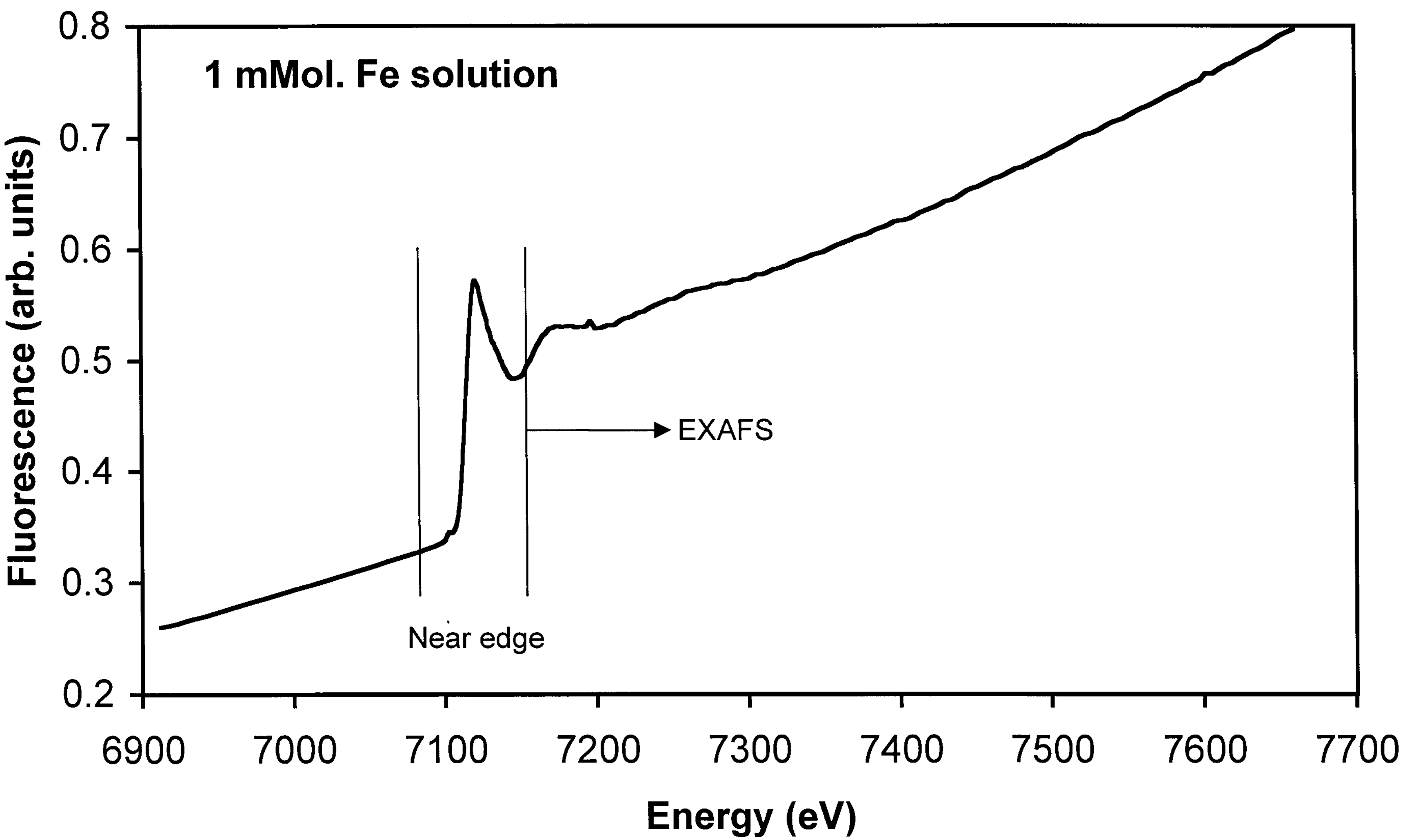
Biological systems

- Concentrated proteins in millimolar range
- Would like to measure more biologically relevant concentrations

Environmental systems

- Typical concentrations ppm and micromolar

Doping in semiconductors


1 mMol. Fe solution
Near edge
EXAFS
Fluorescence (arb. units)
0.8
0.7
0.6
0.5
0.4
0.3
0.2
6900
7000
7100
7200
7300
7400
7500
7600
7700
Energy (eV)

S/N requirements

3 measurement regimes:

- Detection of element (imaging)
  - S/N > 10
  - 10^4 data points
- Near edge measurements
  - S/N > 100
  - 50-100 data points
- Extended fine structure (EXAFS)
  - S/N > 1000
  - 100-300 data points

Performance of Ideal Detector

High flux beam provides > 10^{12} ph/sec

For EXAFS need > 10^6 signal counts/pt

Fluorescence yield 20-50%

If the absorption from the element of interest is about 10^{-6} of the total, a spectrum can be acquired in a few seconds/pt.

Practical limitations

Can't collect 4π

Good goal is 25% of 4π

Fluorescence absorbed in sample

Negligible for surface or thin sample

Maybe factor of 5 for thick sample

Radiation Damage

10^{-6} absorption still feasible in 1-2 hrs.

Example for Fe

10^{-6} absorption gives $3x10^{13}$ atoms/cm^2

small fraction of monolayer

in solution:

0.4 ppm by weight

6 micromolar

in Silicate mineral:

5 ppm by weight

Current Detectors

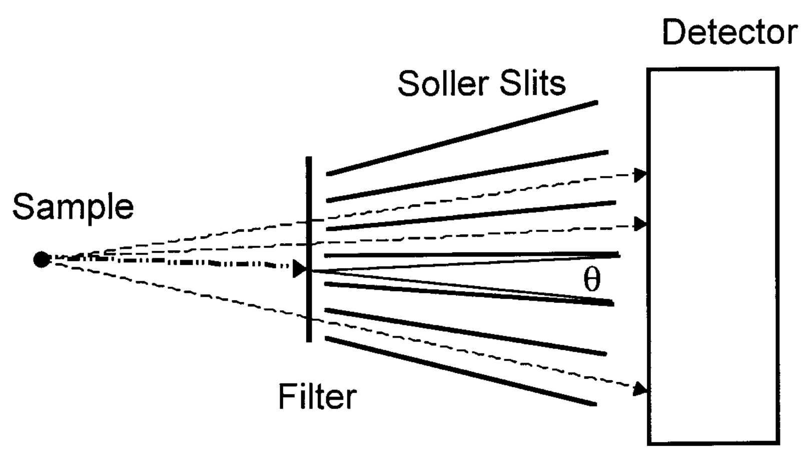
Effective count rate:

$$N_e = N_f \Big/ \sqrt{1 + N_b / N_f}$$

Note: background scattering can be 1% of total absorption

N_b can exceed 10^8

Filter-Slits:



Large solid angle

Unlimited count rate

Moderate reduction in background

Near practical limits

Current Detectors - cont.

Multi-element solid state:

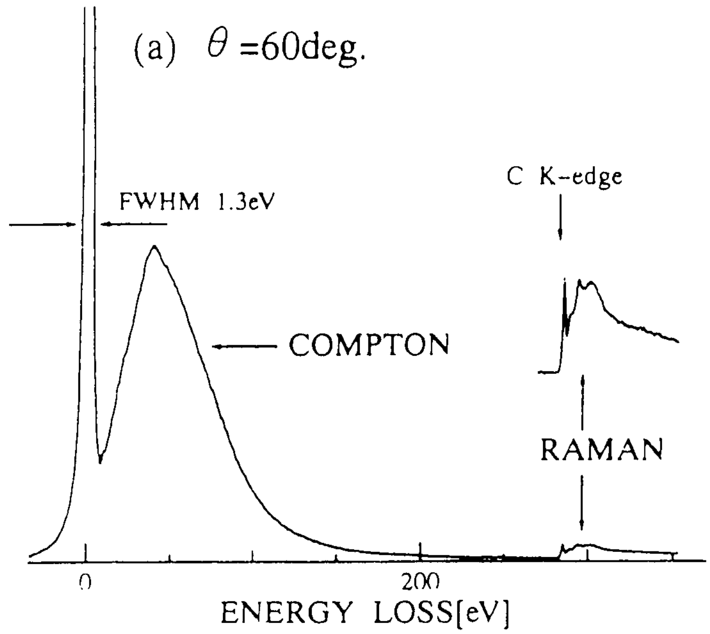
- Resolution (fwhm) 200-300 eV
- Individual element limited to few x 10^5
- Standard arrays limited to about 30 elements

Diffraction based detectors

- Rowland circle, log-spiral (Bragg and Laue), multilayers
- Can have excellent resolution (background discrimination)
- Unlimited count rates

X-ray Raman

When qr<<1 gives XAFS information:



(Udagawa, et al. (1997). J. de Phys. IV, Colloque C2, 347-352)

Allows hard x-ray probe of low energy edges:

simplifies measuring low-Z edges in solutions and wet samples, materials under pressure, radioactive samples, and materials incompatible with vacuum

Detectors for XRS

Scattering cross-section low
→signals similar to fluor. example

Detector resolution determines spectrum resolution → need 1-2 eV

Generally Rowland circle based diffraction

Cryogenic detectors? (currently 5 eV)
Need large arrays to increase count rate

Conclusions

Further development of both solid-state arrays and diffraction-based detector warranted

Solid state arrays:

→Need to handle $>10^8$ hz

→Preferable to keep resolution close to 200 eV

Diffraction based detectors:

→Need to increase efficiency

→Should strive for better resolution than solid state detectors

→If above met, best bet for extreme diluteness

X-ray Raman

→ 1-2 eV resolution