Atomic Form Factors and X Ray – Atom Scattering

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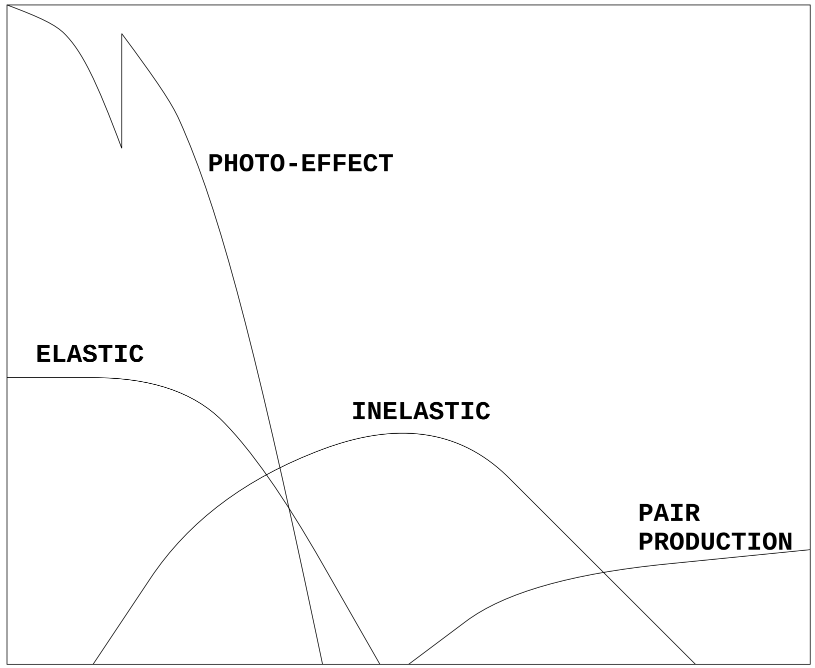
Photon-Atom Scattering

- Interested at how X ray scatter off a single atom
- The types of scattering processes include
  - Elastic (Rayleigh) Scattering
  - Inelastic (Compton) Scattering
  - Photo Effect
  - Pair Production
  - Nuclear Thomson Scattering

Theoretical Cross Section for Photon Scattering for Carbon



PHOTON ENERGY

Scattering Amplitudes

- Schrödinger Equation for a scattering process

$$[H_0 + H']\psi = E\psi$$

- Scattering Wave Function as $r \to \infty$ can be considered as an incident and scattered wave.

$$\psi(r) = \psi_i(r) + \psi_s(r)$$

$$\psi(r) = A\left[e^{ik\cdot r} + f(k,\theta,\phi)\frac{e^{ikr}}{r}\right]$$

- $f(k,\theta,\phi)$ is the scattering amplitude

- Differential Cross Section

$$\frac{d\sigma}{d\Omega} = |f(k,\theta,\phi)|^2$$

Relevance of Atomic Form Factors

- The scattering amplitude depends on the atomic form factor
- Scattering amplitude – form factor relationship depends on how atom-radiation interaction is modeled
- Atomic Form Factors are used to determine diffraction, scattering and attenuation processes of X ray interactions with matter.

Definition of Atomic Form Factors

- Total Atomic Form Factor

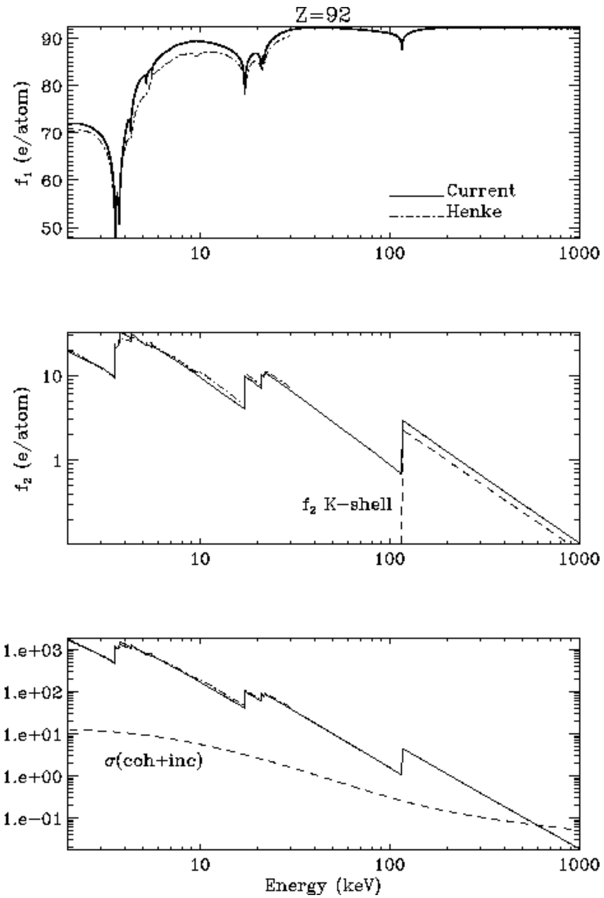
$$f = f_0 + f' + if''$$

- Away from absorption edges (for a spherically symmetric atom)

$$f_0(q) = \int e^{iqr}\rho(r)dr = 4\pi\int_0^\infty \rho(r)\frac{\sin qr}{qr}r^2dr$$

- $q = k_f - k_i = 2|k|\sin\left(\frac{\theta}{2}\right)$ is the change in the photon's momentum and θ is the scattering angle.
- $\rho(r) = \psi^*(r)\psi(r)$ is the electron density.
- The real and imaginary components f' and f'' describe the situation when the photon energy is close to one of the atom's energy levels – an absorption edge.

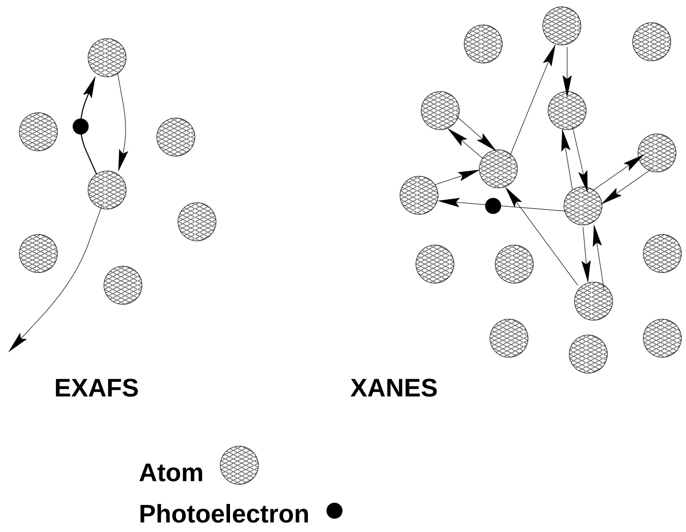
Examples of Atomic Form Factors



Scattering from Multiple Atoms

Experiments deal with many atoms, and there are a number of effects which cannot be explained by treating the atom as an isolated system.

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



Existing Theoretical And Experimental Results

- **THEORY**
  - Partially-Relativistic Quantum Mechanics
    - ∗ Hubbel, Scofield
  - Relativistic Quantum Mechanics
    - ∗ Dirac-Hartree-Fock, *S*-Matrix, Relativistic Multipole etc.
    - ∗ Cromer and Liberman, Kissel and Pratt, Creagh, Chantler
- **EXPERIMENT** – Errors of 10% –20% for best data
  - Experimental Synthesis
    - ∗ Henke, Gullikson
  - Experimental Compilation
    - ∗ Hubbel

Main Project Aims

- Develop the theory for atomic form factors for low Z atoms.
- Determine atomic form factors for low Z atoms and compare with existing theories and experimental results.
- Investigate and develop the theory of anomalous X ray resonance scattering (EXAFS, XANES, DAFS) – effects of local interactions on the atomic form factor.

Proposed Approach

- Atom – Relativistic Quantum Mechanics (Dirac)
- X Ray – Classical Radiation Field using electric dipole and/or electric quadrupole approximation
- Investigate the effect of local interactions on the atomic form factor
- Use a Dirac-Hartree-Fock computational approach to determine for multi-electron atoms the
  - Energy eigenvalues of the atom
  - Corresponding wave functions
- Use these wave functions to determine the atomic form factors for the different atoms over a range of X ray energies.
  - Angular dependent component of the atomic form factor f_0
  - Energy dependent components of the atomic form factor f' and f''