EXAFS Spectroscopy

What is EXAFS?
- EXAFS = Extended X-ray Absorption Fine Structure, a technique for determining atomic structure
- EXAFS oscillations are due to quantum interference between the photoelectron waves from X-ray emission and those backscattered from nearby atoms
- EXAFS gives numbers, elements, distances of neighboring atoms without the need for a crystalline sample
- Currently, EXAFS requires a synchrotron radiation light source with a tunable monochromatic beam

Laboratory EXAFS Spectroscopy
- A commercial laboratory EXAFS instrument would be a major advance, opening up the technique
- EXAFS gives numbers, elements, distances of neighboring atoms without the need for a crystalline sample
- EXAFS = Extended X-ray Absorption Fine Structure, a technique for determining atomic structure

Resolution Requirements for EXAFS
- Gaussian broadening of experimental EXAFS spectra decaes peak amplitudes in Fourier transform
- Conclusion: ~20 eV FWHM is OK, <15 eV is ideal

Statistics Requirements for EXAFS
- Adding Poissonian noise to 15 eV broadened EXAFS spectra degrades spatial resolution
- Estimate 50 mM Fe can be measured to k = 17 Å⁻¹ in a few hours – assuming 100 counts/eV bandwidth
- Conclusion: Acquisition time of ~3-10 hours for a 50 mM sample requires 400,000 counts at 4 keV bandwidth

Comparison of Different Technologies

<table>
<thead>
<tr>
<th>Detector</th>
<th>Resolution</th>
<th>Speed/Pixel</th>
<th>Stability</th>
<th>Energy Range</th>
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</thead>
<tbody>
<tr>
<td>Ge, Si</td>
<td>~100-200 eV</td>
<td>~1000 counts/s</td>
<td>Good</td>
<td>~MeV</td>
</tr>
<tr>
<td>Crystals</td>
<td>~1 eV</td>
<td>Scanning</td>
<td>Difficult</td>
<td>~100 keV</td>
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<tr>
<td>TESs, MMCs</td>
<td>~2 eV</td>
<td>~10 counts/s</td>
<td>Good</td>
<td>~100 keV</td>
</tr>
<tr>
<td>STJs</td>
<td>~15 eV</td>
<td>~1000 counts/s</td>
<td>Good</td>
<td>~1 keV</td>
</tr>
</tbody>
</table>

Conclusions
- STJ detectors offer the best prospects for a practical commercial laboratory EXAFS spectrometer
- Need to develop a 128-pixel hard X-ray STI with:
  - Energy Range: 1000 – 12,000 eV
  - Resolution: < 20 eV FWHM
  - Speed: ~ 2,000 – 5,000 counts/s per pixel

EXAFS dominated by F-F interactions. Curve fit consistent with expected cubic structure

MgF₂ EXAFS with STJs
- Publication quality EXAFS spectrum of 0.4 µm LiF film on 0.1 µm parylene in 4 hours
- EXAFS contains F-Mg and F-F interactions. Curve fit consistent with expected cubic structure