Landscape of Damage Tolerance

Ionisation and subsequent sample explosion causes diffraction intensities to change

Agreement factor:

$$R = \frac{\sqrt{I(t)} - \sqrt{I_o}}{\sqrt{I_o}}$$

Initial LCLS parameters

Tolerable damage (single exposures)

Landscape of Damage Tolerance

Agreement factor:
Predicted scattering from a single RUBISCO molecule \( (R_{\text{electronic}} = 15\%) \):

- 10 fs, \( 5 \times 10^{12} \)
- 50 fs, \( 8 \times 10^{11} \)
- 100 fs, \( 3 \times 10^{11} \)

- 562kDa

\( 10 \text{ fs} \quad 5 \times 10^{13} \)
\( 5 \text{ fs} \quad 1 \times 10^{13} \)
\( 1 \text{ fs} \quad 5 \times 10^{13} \)
Nanocrystal of lysozyme

1 LYSOZYME

5x5x5 LYSOZYMES
Angular reconstitution and averaging (cryo-EM photographs of the large ribosomal subunit)

Courtesy of M. van Heel, London (Phillips CM300 FEG, liquid helium)
**Calculated Limits of Resolution with \( R_{\text{electronic}} = 15\% \)**

<table>
<thead>
<tr>
<th>Pulse duration (FWHM)</th>
<th>10 fs</th>
<th>50 fs</th>
<th>100 fs</th>
<th>230 fs</th>
</tr>
</thead>
<tbody>
<tr>
<td>Photons/pulse (100 nm spot)</td>
<td>(5 \times 10^{12})</td>
<td>(8 \times 10^{11})</td>
<td>(3 \times 10^{11})</td>
<td>(5 \times 10^{10})</td>
</tr>
<tr>
<td>((R = 15%))</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

- **Single lysozyme molecule**
  - MW: 19,806
  - MW: 26 Å, 30 Å, >30 Å, >30 Å

- **3x3x3 cluster of lysozymes**
  - Total MW: 535,000
  - MW: <2.0 Å, 3.0 Å, 6.5 Å, 12 Å

- **Single RUBISCO molecule**
  - MW: 562,000
  - MW: 2.6 Å, 4.0 Å, 20 Å, 30 Å

- **Single viral capsid (TBSV)**
  - MW: ~3,000,000
  - MW: <2.0 Å, <2.0 Å, <2.0 Å, 2.4 Å

**Single virus particles look very promising**
Reconstruction of the Shapes of Gold Nanocrystals Using Coherent X-Ray Diffraction

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(Received 15 May 2001; published 19 October 2001)

FIG. 1 (color). Coherent x-ray diffraction pattern of the immediate vicinity of the (11T) Bragg reflection of a 1 μm gold nanocrystal. A beamstop blocks the center. The color contour levels are logarithmically spaced.
FIG. 2 (color). Stages of reconstruction of the diffraction data. 
(a) Coherent x-ray diffraction pattern surrounding the specular 
(111) Bragg reflection of a 1 μm gold nanocrystal, measured 
without a beamstop. (b) Symmetrized data. (c) Data filtered 
by multiplication by a circular Gaussian function. (d)–(f) Cal-
culated diffraction patterns obtained by the inversion algorithm;
the three examples used different random numbers for the initial 
phases at each pixel. The color contour levels have the same 
logarithmic spacing in all panels.

FIG. 3 (color). Reconstructed real-space projected images of 
the gold nanocrystals displayed on the same scale. (a),(b) SEM 
images of larger Au particles. (c) Size of the “support” con-
straint used in the inversion routines. (d)–(f) Real-space im-
ages obtained by inversion of the data in Fig. 2(c); the Fourier 
transforms of these images are the diffraction patterns shown in 
Figs. 2(d)–2(f).
Use of coherent X-ray diffraction to map strain fields in nanocrystals

I.K. Robinson\textsuperscript{*}, I.A. Vartanyants

Fig. 1. Simulated diffraction pattern of the octahedral crystal shown in the upper panel. The 3D shape is projected onto the plane of the page, Fourier transformed in 2D and plotted as a contour map in the lower panel. This pattern is repeated around every reciprocal lattice point of the crystal’s diffraction pattern.
Nanoscale Dynamics in Condensed Matter

Nano (1-100nm) scale of great importance in condensed matter
Dynamics very challenging over entire 1-10^{-15} sec range

- **Simple Liquids** – Transition from the hydrodynamic to the kinetic regime.
- **Complex Liquids** – Effect of the local structure on the collective dynamics.
- **Polymers** – Entanglement and reptative dynamics.
- **Glasses** – Vibrational and relaxational modes in the mesoscopic space-time region.
- **Dynamic Critical Phenomena** – Order fluctuations in alloys, liquid crystals, etc.
- **Quasicrystals** – Nature of phason and phonon dynamics.
- **Surfaces** – Dynamics of adatoms, islands, and steps during growth and etching.
- **Ferroelectrics** – Order-disorder vs. displacive nature; correlations and size effects.

Rate $\sim Q^2$
- e.g. composition change by diffusion

Rate indep. of $Q$:
- e.g. deformation by viscous flow
Scattering Techniques for Equilibrium Dynamics

**X-Ray Photon Correlation Spectroscopy**

*Probe thermal fluctuations:*

**X-Ray Transient Grating Spectroscopy**

*Excite and probe fluctuations:*

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**Graphs:**
- **X-Ray Photon Correlation Spectroscopy**
- **X-Ray Transient Grating Spectroscopy**

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A perfect crystal X-ray analyser with 1.5 meV energy resolution

C. Masciovecchio\textsuperscript{a}, U. Bergmann\textsuperscript{a}, M. Krisch\textsuperscript{a}, G. Ruocco\textsuperscript{b}, F. Sette\textsuperscript{a,\ast}, R. Verbeni\textsuperscript{a}

\begin{center}
\includegraphics[width=\textwidth]{figure.png}
\end{center}

\begin{align*}
\text{Si} & (11 \ 11 \ 11) \\
\text{fwhm} & 1.5 + 0.2 \text{ meV}
\end{align*}

\begin{center}
\text{Intensity (counts/s)} \\
\text{Energy (meV)}
\end{center}
Collective Dynamics in Water by High Energy Resolution Inelastic X-Ray Scattering

F. Sette, G. Ruocco, M. Krisch, U. Bergmann, C. Masciovecchio, V. Mazzacurati, G. Signorelli, and R. Verbeni

1European Synchrotron Radiation Facility, B.P. 220 F-38043 Grenoble Cedex, France
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(Received 12 April 1995)

FIG. 3. Dispersion relation in water as obtained from the fit. The solid line indicates the best linear fit up to 10 nm⁻¹, and the slope corresponds to the indicated speed of sound.
In **milliseconds - seconds** range:
Uses high *average* brilliance

transversely coherent X-ray beam from LCLS

\[ g_2(\Delta t) = \frac{\langle I(t) I(t + \Delta t) \rangle}{\langle I \rangle^2} \]

\[ \tau^{-1}(Q) = \text{Rate}(Q) \]

“movie” of speckle recorded by CCD

\[ I(Q, t) \]
XPCS using a split pulse

In **picoseconds - nanoseconds** range:
Uses high *peak* brilliance

transversely coherent X-ray pulse from LCLS

variable delay

**10 ps \( \Leftrightarrow 3\) mm**

sum of speckle patterns from prompt and delayed pulses recorded on CCD

\[ I(Q, \Delta t) \]

Contrast as \( f(\text{delay time}) \)

\[ \tau \]

\( \Delta t \)