Towards single molecule shape determination with laser generated soft x-rays

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Talk

- Towards Ultra-fast x-ray single molecule studies
- Single molecule shape
- Development of a High Harmonic Source
- Initial Scattering Studies
- Future Experiments
Current ways to find protein structure

- X-ray crystallography
  - Needs a crystal
  - Crystal may influence structure
- Cryo-electron microscopy
  - 2D crystal, but can be small
- NMR
  - No crystals, but size limitations
Avoiding the crystal problem....
Many groups looking at this for work with FELs.

- **single** molecule
- Crystal

Huge advantages, huge problems!

- No need to crystallize
- No averaging
- Damage to molecule from X-rays
- Signal / noise issues
Molecular Cluster → Shape → Structure

X-ray scattering

X-ray diffraction of crystals

Molecular dynamics simulation
Small Angle Solution X-Ray Scattering
Using Molecular Shape to Characterise Protein Complexes

The molecular envelope of the 2:1 complex formed between Mo and Fe component proteins of nitrogenase, derived from solution x-ray scattering.

Docking Model of the complex using the crystal structures of the individual proteins: not in agreement with the molecular envelope.

The significant structural changes predicted using solution x-ray scattering are confirmed by the subsequent crystal structure of the complex.

http://srs.dl.ac.uk/mbg/saxstech.html
Synchrotron & FEL technology does not fit in the laboratory

“Sure, it’s an eyesore, but we get better time than anyone else.”

But recent developments may change this
Soft x-rays

- Wavelength of a few nm
- Ideal for probe nm shape of protein complexes, biological machines
- Nanomaterials
- Soft x-rays can be manipulated quite readily
- Absorption is a problem
Damage limitation

- Conventional damage threshold: 200 ph/Å²

Damage process
- inelastic scattering of electrons out of molecule
- Coulomb repulsion of remainder
- Timescale? fs

HHG - the simple model

- Electron tunnels out of atom as field increases
- Electron accelerates in laser field as free particle
- Electrons which come back to the atom can recombine and emit an energetic photon
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\[ E = h\nu = I_p + 3U_p \]
Observed spectrum mainly due to Phase Matching

The theoretical cutoff is not reached

With modified capillaries we can reach in to the water window
Practical aspects of HHG

- Capillary tube holds Ar gas at low pressure (also Ne, N₂ and N₂O)
- Need very high laser powers, Peak intensity $\sim 10^{15} \text{ W/cm}^2$ & Peak E-field $\sim 100 \text{ GV/m}$
- Laser focused into capillary, guided along bore
- X-rays generated as a coherent beam along capillary
X-ray throughput for high harmonic generation

- Ultrafast amplified laser:
  - 4mJ, 20fs, 1kHz, 800nm

- X-ray photons:
  - 10^7 X-ray photons, detection 50%
  - <30th harmonic=27nm, 10^-5 efficiency

- Aperture:
  - 10nm
  - 10^10 X-ray photons

- 1% transmission

- Argon 50 Torr, 150μm capillary, 3cm

- CCD:
  - 10nm aperture
  - 1% scattering

Original estimates
Square Grid Diffraction

- Record x-ray diffraction by filter support grid.
- 340µm square apertures, 18µm bars.
- 50cm source to grid, 100cm grid to camera.
- Observe spatial variation of diffraction patterns.
- Can we extract x-ray spectrum?
Characterize and to control the wavelength and spatial profile of the x-ray beam.
Taper mounted inside a holding capillary

50 µm
Tapered Capillary Focussing

- Grazing incidence reflection.
- Parabolic or elliptical profile.
- Not a true focus but x-ray beam is intensified by a factor of
- Study individual objects or small part of larger objects.
200 nm

2D lattice of 200 nm latex spheres

It is the gaps that transmit the x-rays
Scattering close to the direct beam

Camera-taper distance 10.2 cm, direct beam

Camera-sample distance: 10 cm, sample X: 5.8 mm

Direct beam
Scattering image showing the location of the CCD image.
Scattering with diffraction circles for the different harmonics superimposed
Scanning X-ray nanoprobe

- SNOM like system, but not in the near field for the x-rays
- X-ray focusing – parabolic tapered capillary
- ultrafast laser system
- Capillary-based X-ray generation

Metallized particles

Scanning substrate

CCD
Capillary-based X-ray generation

ultrafast laser system

Electrospray or laser desorption

Fluorescence

X-ray focusing – parabolic tapered capillary

Capillary-based X-ray generation

CCD
Enable NEXAFS/XANES

Pressure tuning, &
tune by using the
Dazzler to change the
fundamental
dispersion altering
Absorption

Scattering
Non-linear x-ray spectroscopy

- Focussed fs beam of attosecond pulse train
- Very high peak power
- Non-linear spectroscopy and microscopy should be possible
- Extend the range of resonances that can be probed using our wavelength range

Data from: www-cxro.lbl.gov
Detectors

- Need highly efficient detector
- Xray photon counting
- Single pulse
- 3D detector
- Use conventional and innovative designs
  - Nanoscale lithography?
Yb fibre CPA system

Ti:sapphire replacement to provide a more compact source requiring less maintenance

On track for 30fs, 0.1mJ/pulse, with high average power (100's Watts)
HHG vs Other Sources

- Tabletop source
- Short pulse duration
- Well defined time structure
- Good coherence
- Relatively inexpensive
- BUT
- Lower energy
- Lower flux
Nanoscale X-Ray Basic Technology Group

School of Chemistry
School of Physics
ORC
CCLRC-RAL
Credits:

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**Places**
School of Chemistry
School of Physics & Astronomy
Optoelectronics Research Centre
CCLRC RAL