The Scientific Revolution Enabled by X-ray Free Electron Lasers

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LCLS at SLAC

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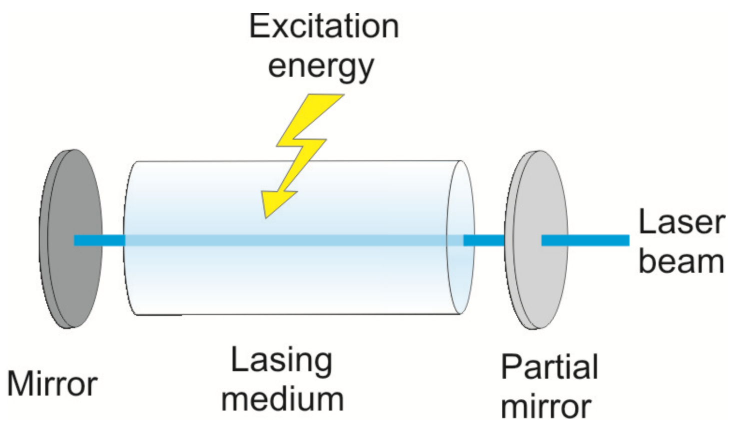
What is an x-ray free electron laser, anyway?

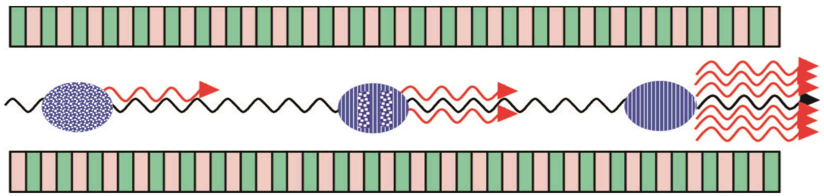
Optical versus X-Ray Laser

Optical laser



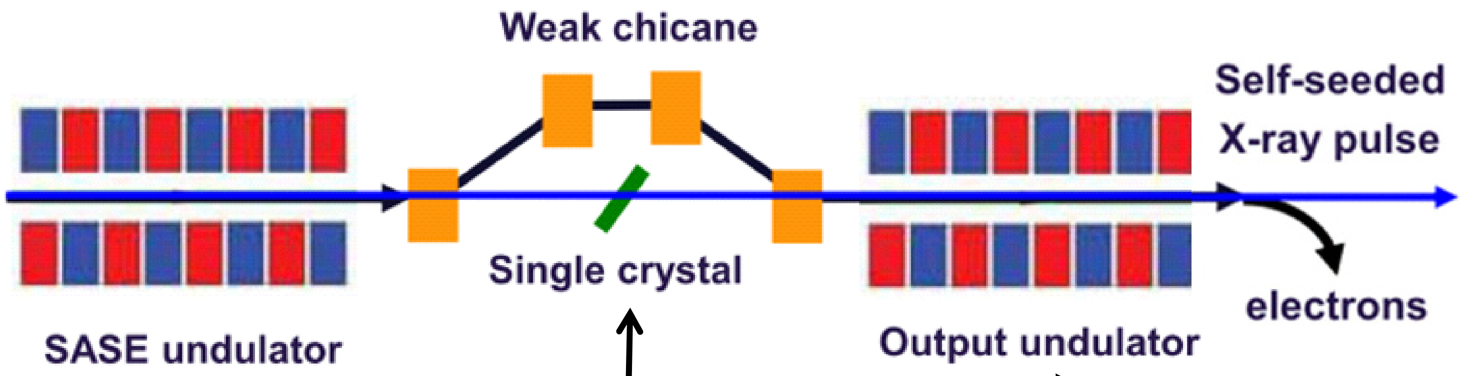
- bound electrons in atoms
  - transitions between discrete states
- amplification through stimulated emission
- fixed photon energy around 1 eV
- compact size

X-ray “free electron” laser



- free electrons in bunch
  - radiation in periodic H-field
- amplification through
  - ➢ electron ordering in its own radiation (SASE)
  - ➢ electron ordering in imposed radiation (seeding)
- tunable photon energy > 1000 eV
- very large size

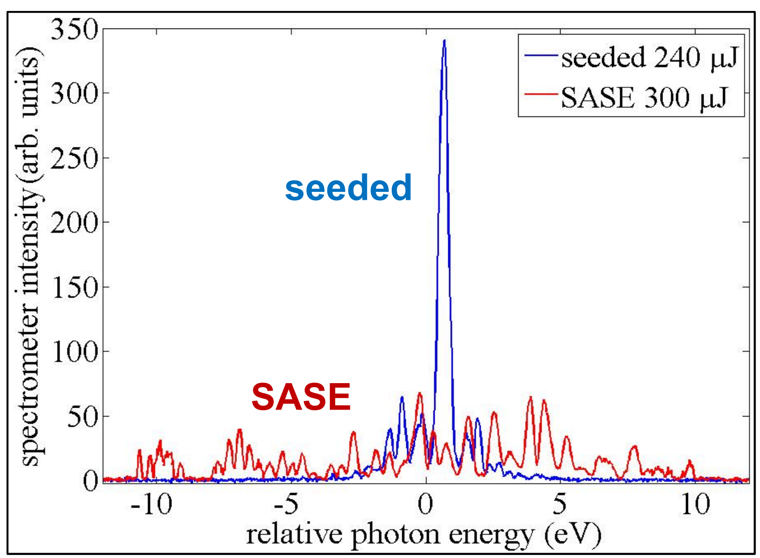
SASE versus self seeded x-ray beam



Intense x-ray source with spiky spectrum

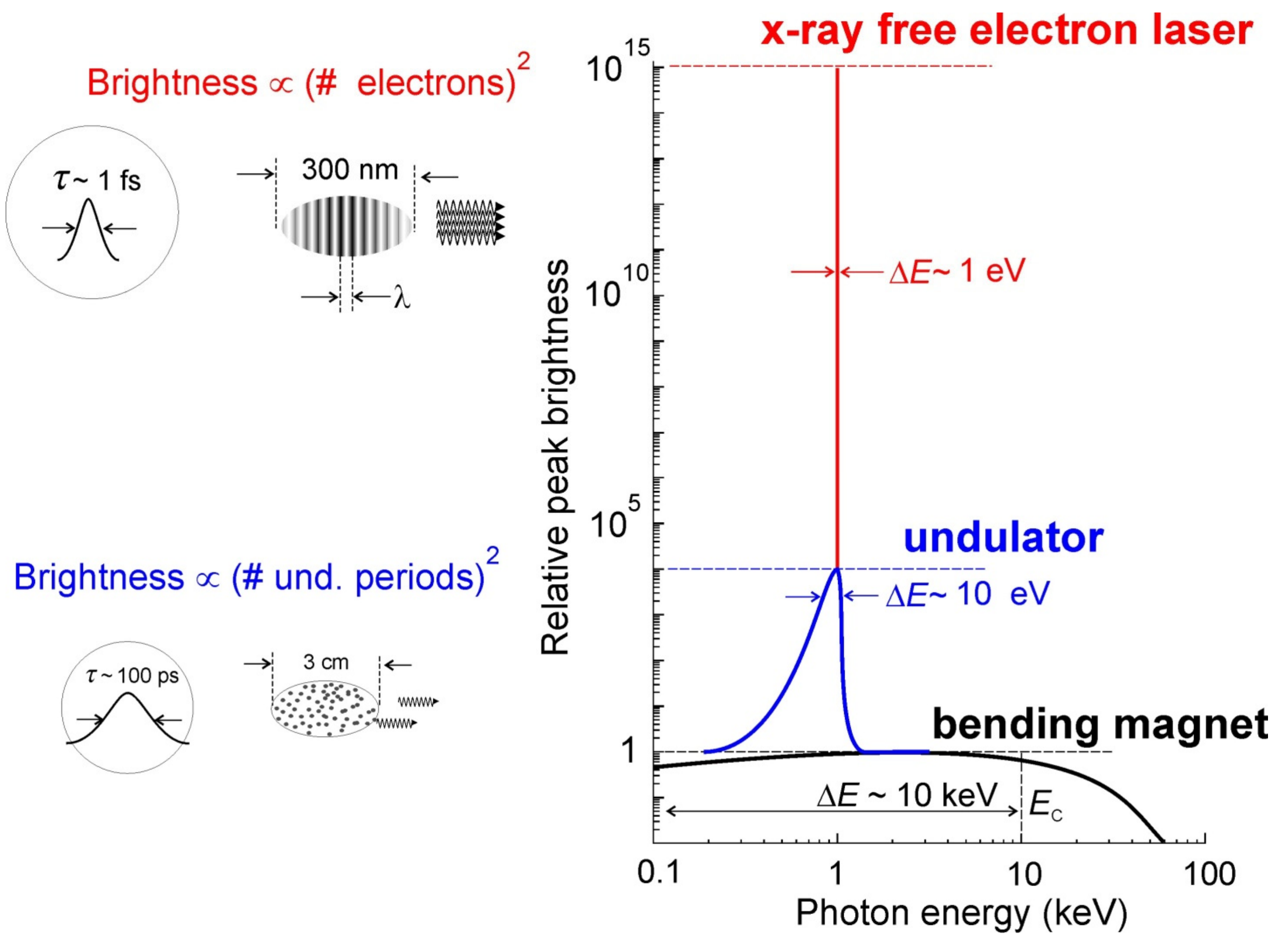
Monochromator filter creates seed with controlled spectrum

FEL amplifier (exponential intensity gain)



8.3 keV
40 pC

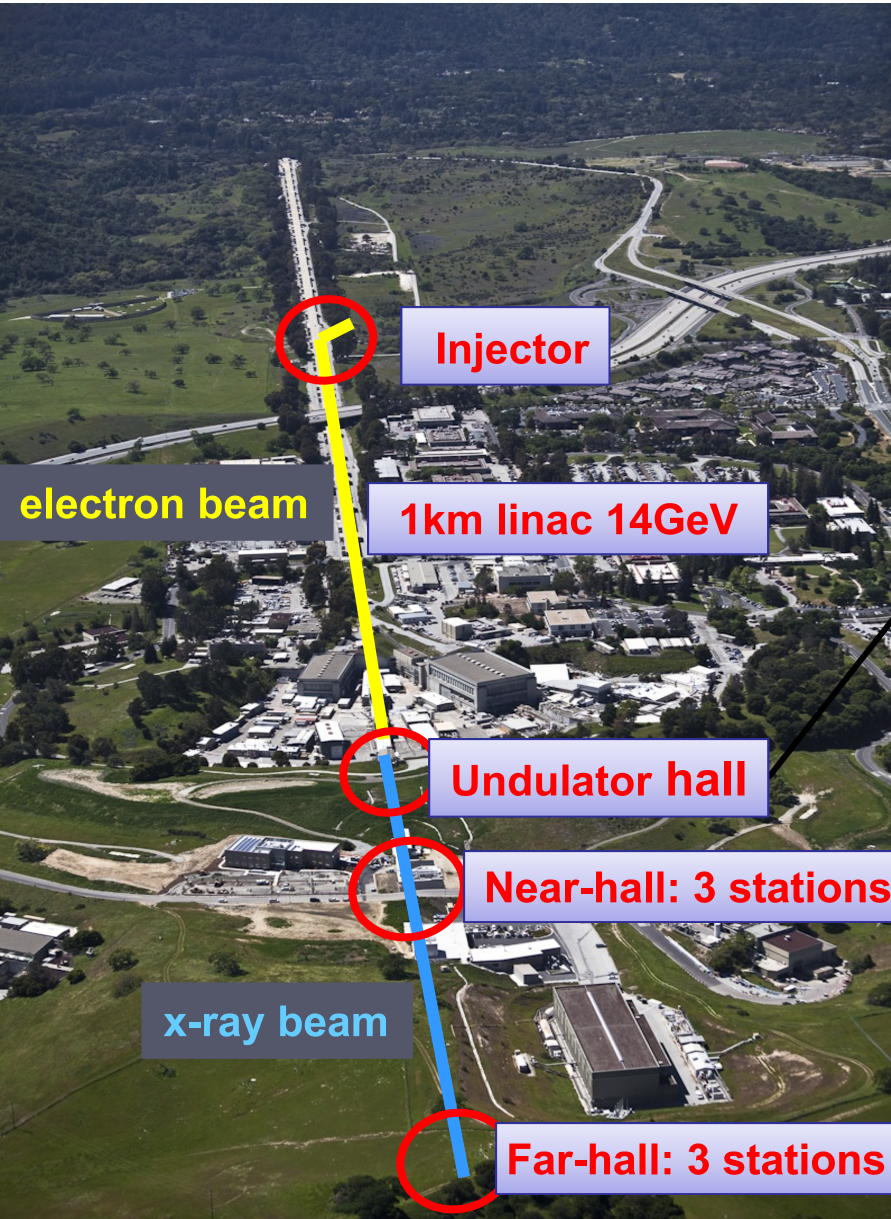
X-ray properties: storage ring versus FEL

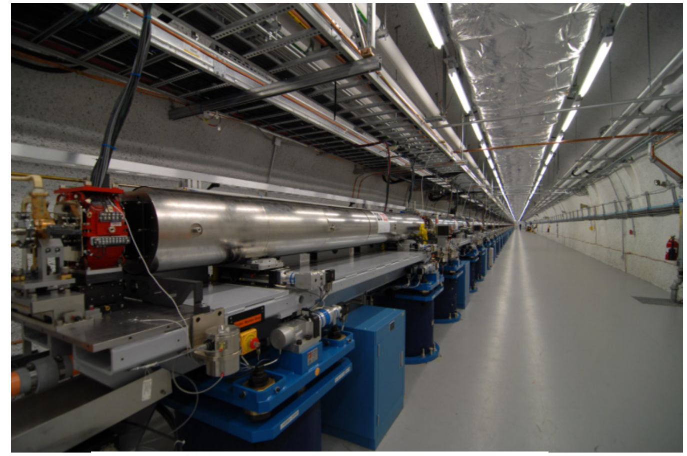


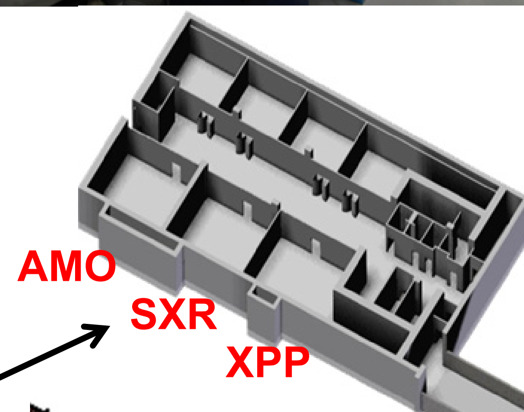
- **Assume same energy bandwidth (~ 1eV)**
- **XFEL photons in 10 fs = ring undulator photons in 1 s**
- **XFEL photons are coherent**

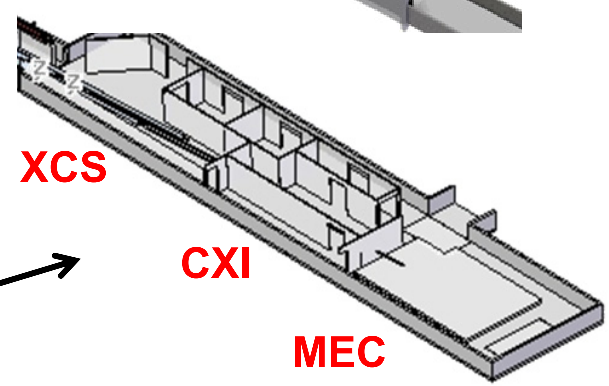
LCLS:

the world's first x-ray free electron laser

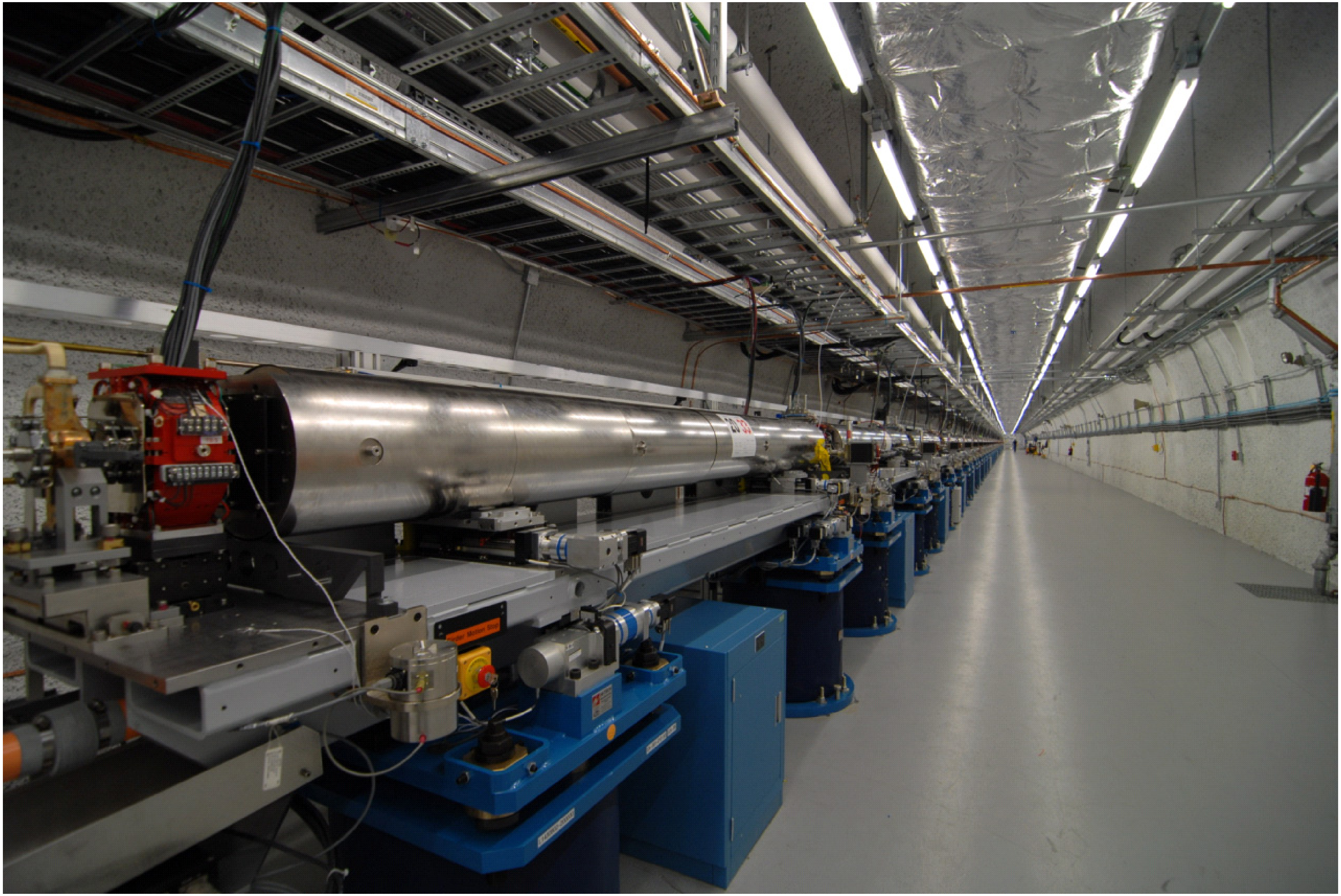








Where the x-rays are made…

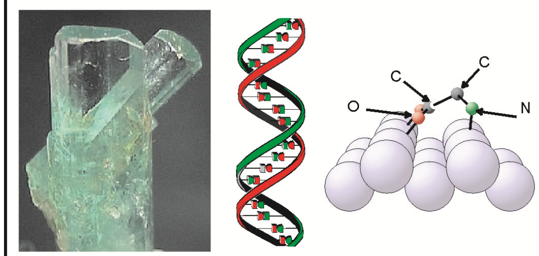


X-Rays and the World of Atoms, Electrons & Spins

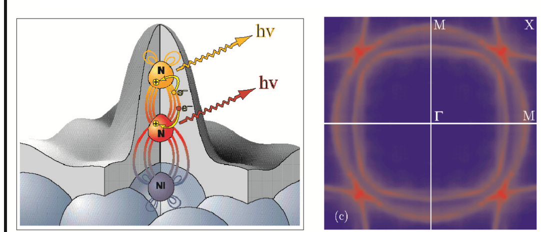
- **X-Ray diffraction and imaging can determine atomic and nanoscale structure in materials and bio-systems**

- **X-Ray spectroscopy can reveal the electronic and spin structure**

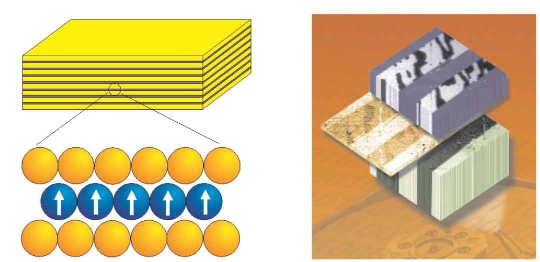
Where are the atoms?



Where are the electrons?



Where are the spins?

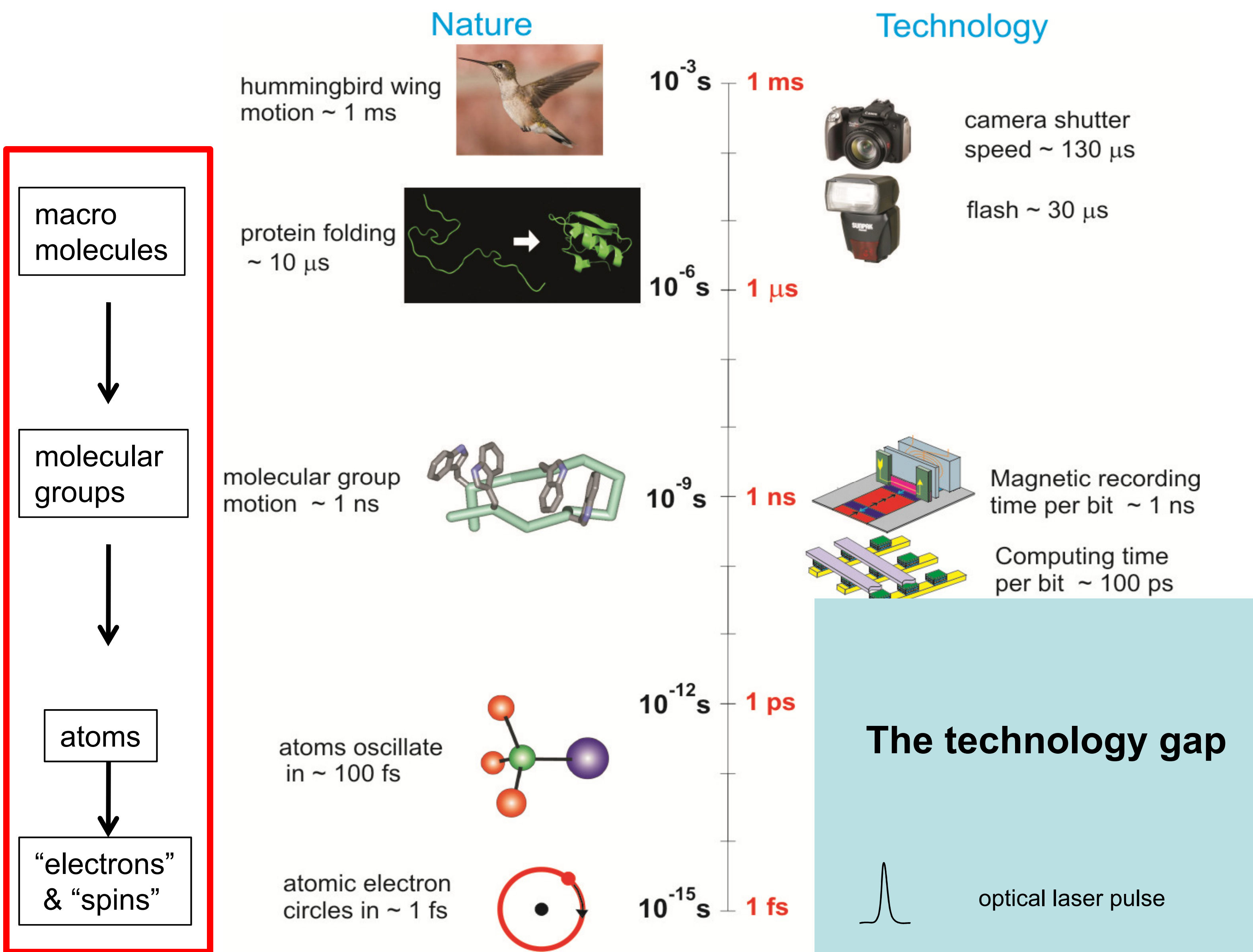


Two X-FEL science examples:

or

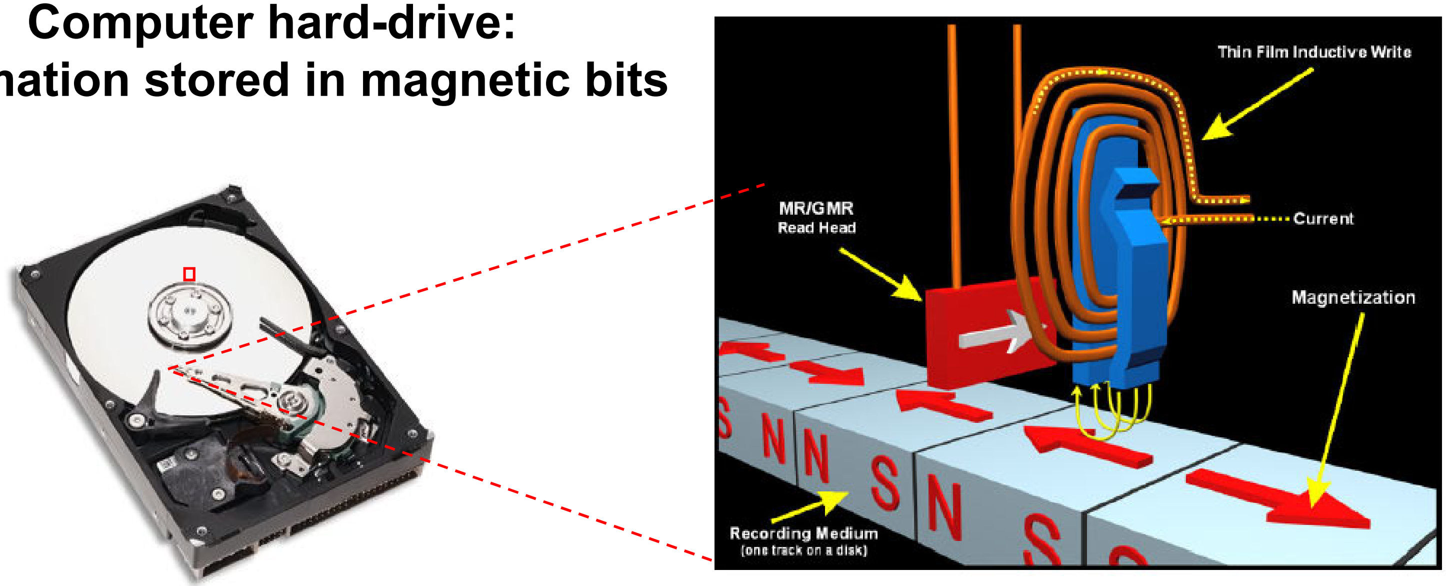
The need for speed !

The speed of things – the smaller the faster



Data manipulation at the speed of light

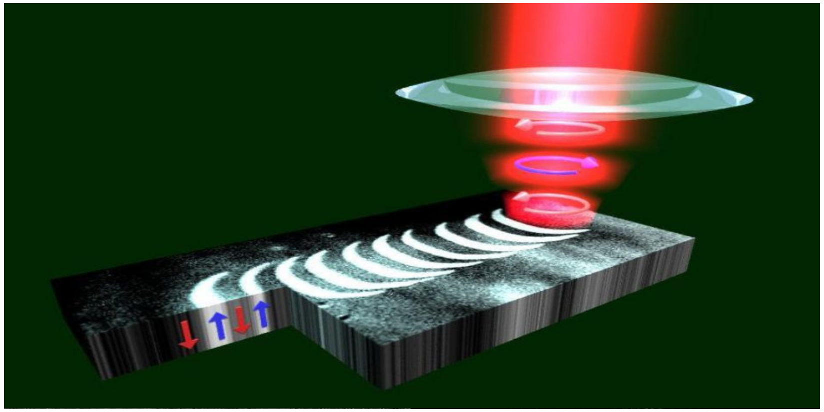
Computer hard-drive:
information stored in magnetic bits



Today: Data storage speed (writing and reading) limited by electron transport in wires (~100 ps pulses)

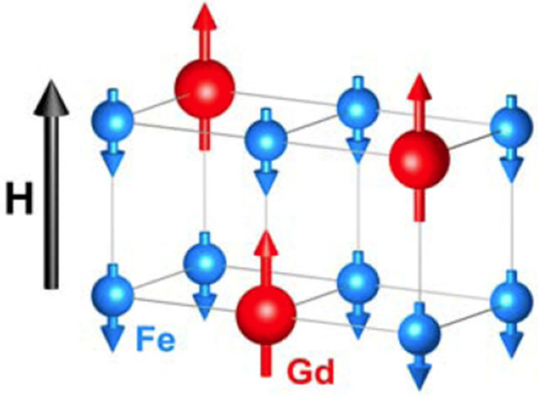
Future: Can magnetic bits be switched by light pulses (<1 ps)?

All-optical magnetic switching has been observed



Stanciu *et al.*,
PRL **99,** 047601 (2007)

Ostler *et. al.*,
Nature Comm. **3,** 1 (2012)

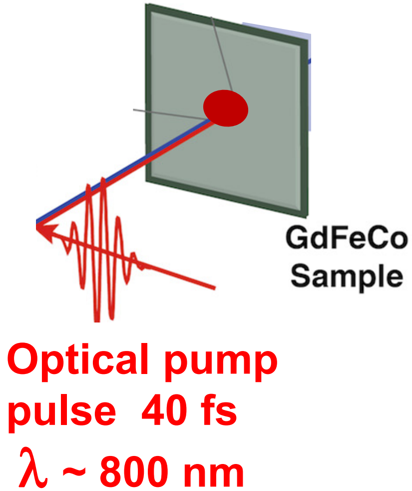


Switching works:

- ultrafast - 40 fs optical light pulses
- independent of light polarization
- only for one material – ferrimagnetic metallic GdFeCo alloy

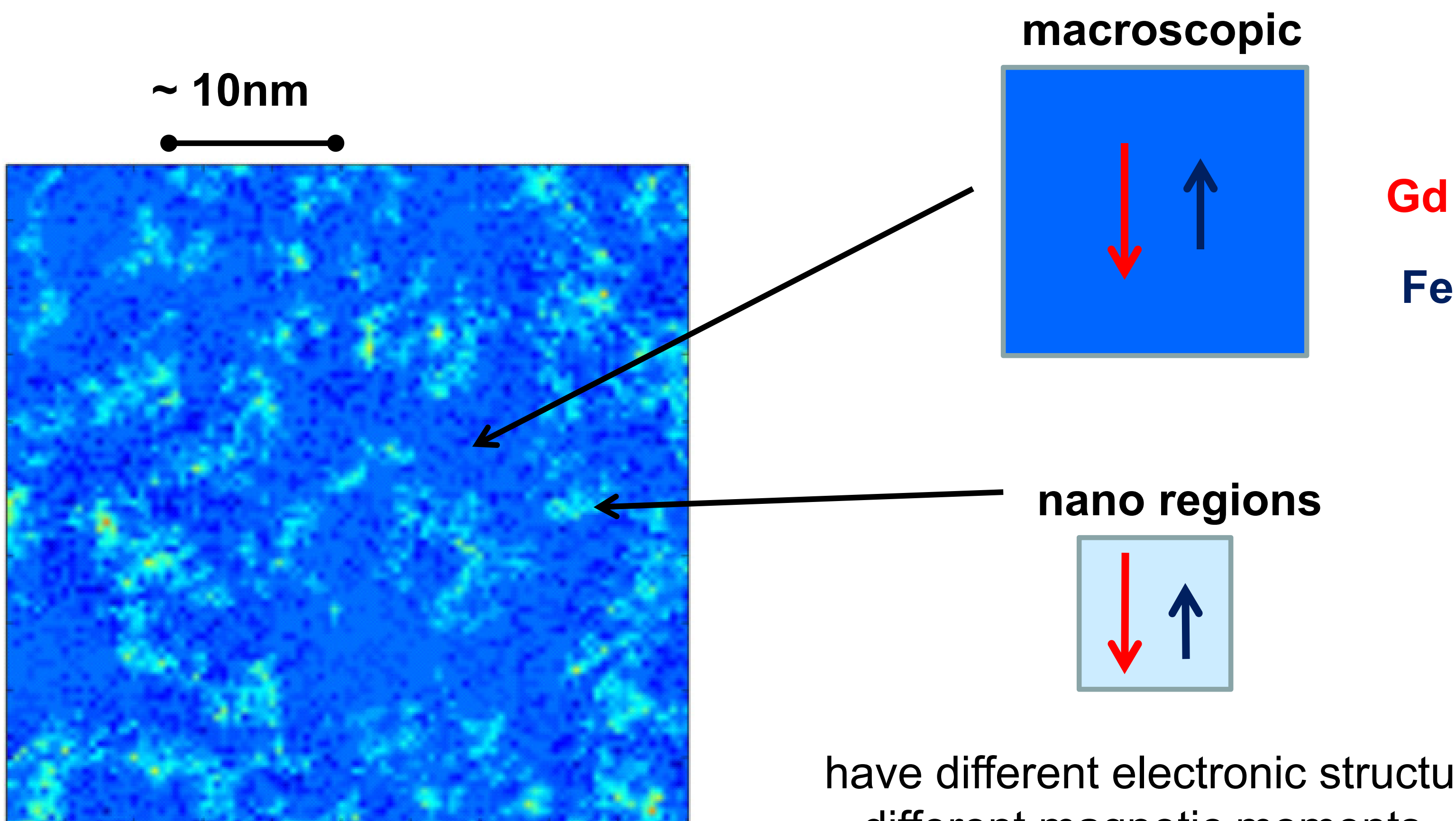
What is the secret that makes GdFeCo work?

Use x-ray pulses to probe optical switching



Obtain information what happens after optical pulse
- as function of Δt
- as function of q (size)

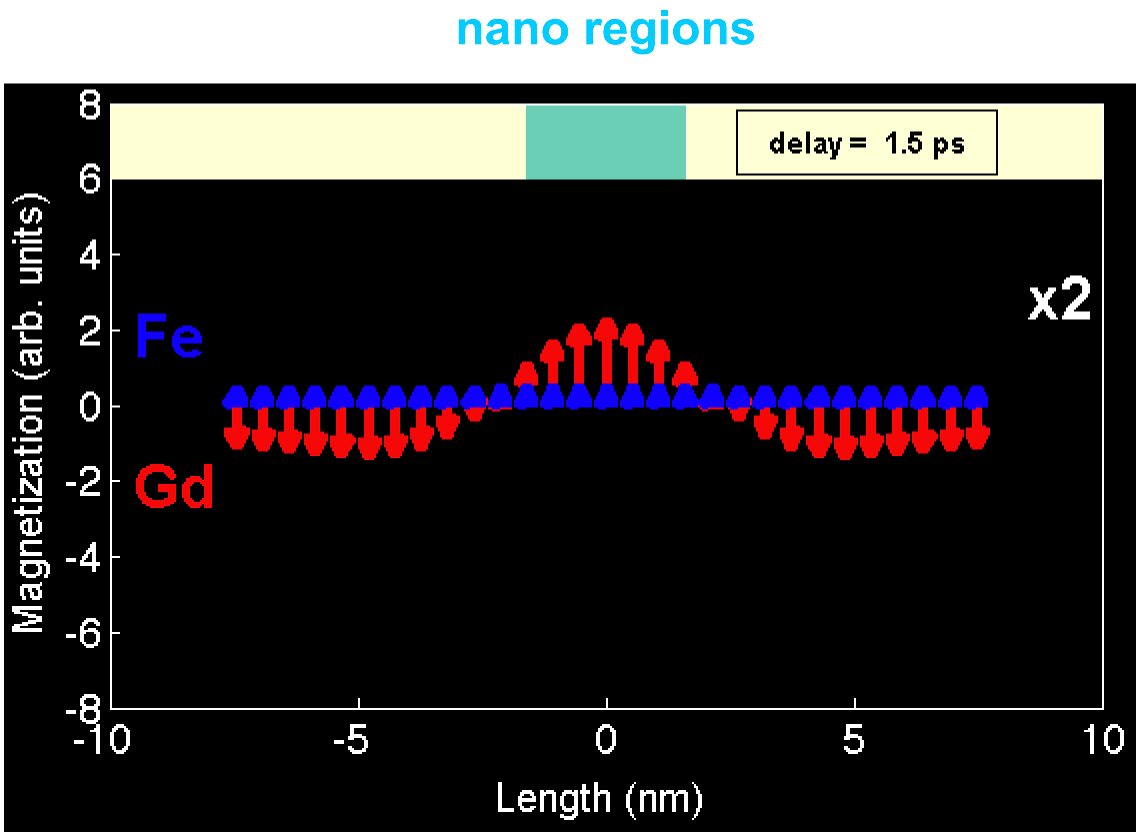
GdFeCo is inhomogeneous on nanoscale



schematic picture

have different electronic structure
different magnetic moments
and faster time response

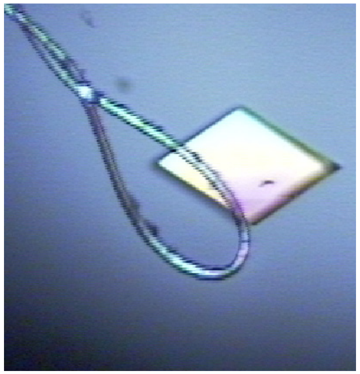
Evolution of Fe and Gd moments with time

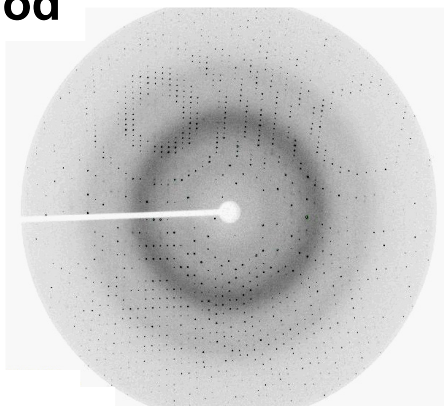


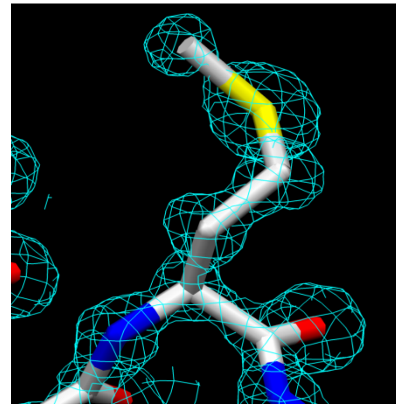
- GdFeCo contains nanoregions which respond faster
- Gd atoms in nano-regions switch first
- Nanoregions form nucleation centers for macroscopic switching

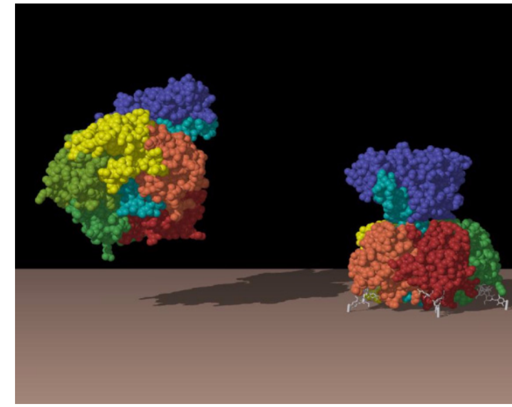
Toward a new Paradigm in Macromolecular Crystallography

conventional method









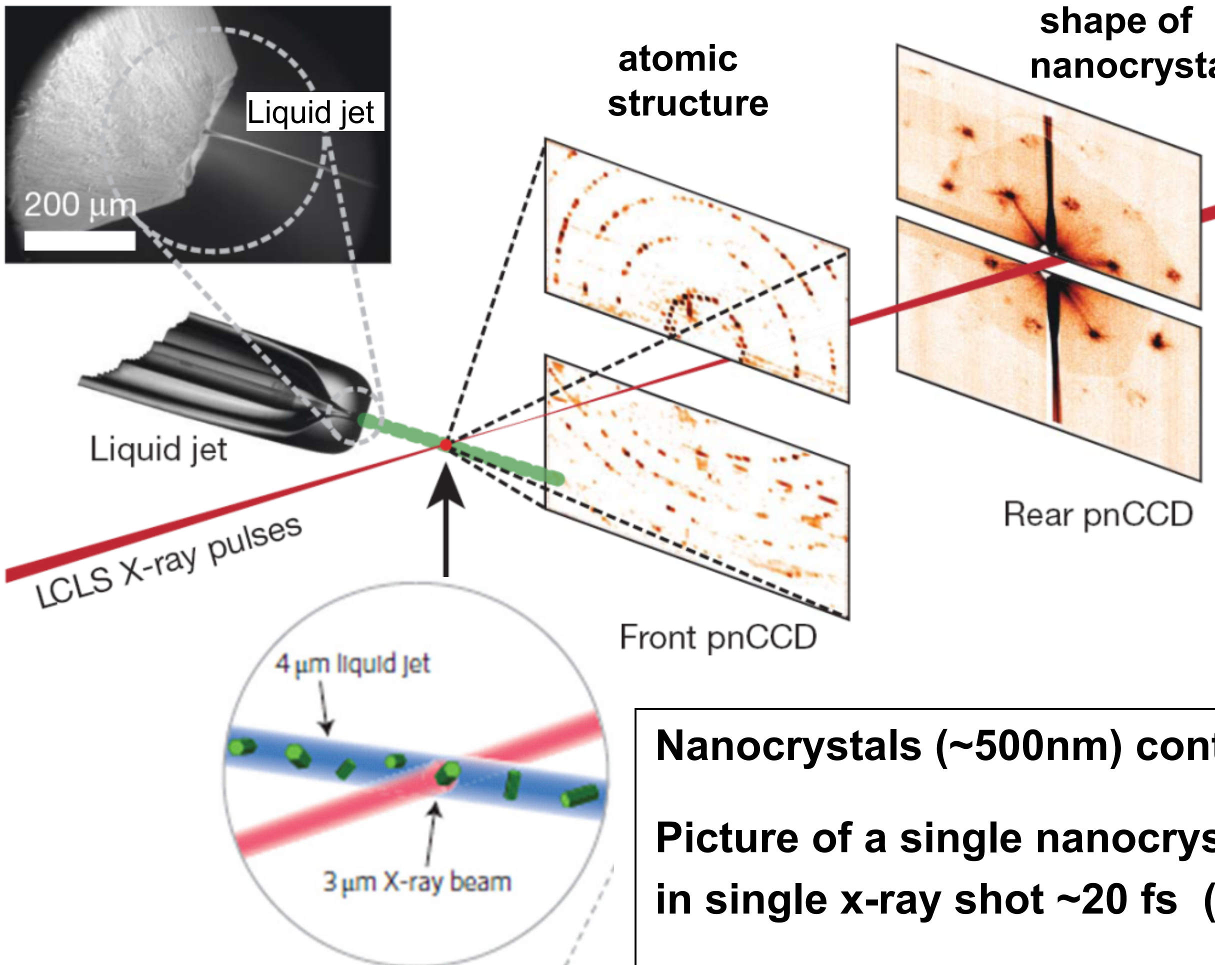
Protein crystal → *Diffraction data* → *Electron density* → *Molecular model of protein suggests its function*

In 1980s synchrotron x-rays revolutionized macromolecular crystallography

- Understanding how proteins function has allowed the developments of drugs
- However, synchrotron studies limited to large (> 5 microns) crystals
- Data for smaller crystals limited by x-ray beam damage

Studies of nanocrystals at X-FELs leads to a new paradigm

Femtosecond Protein Nanocrystallography



Nanocrystals (~500nm) contained in water jet

Picture of a single nanocrystal is recorded in single x-ray shot ~20 fs (“speed of light”)

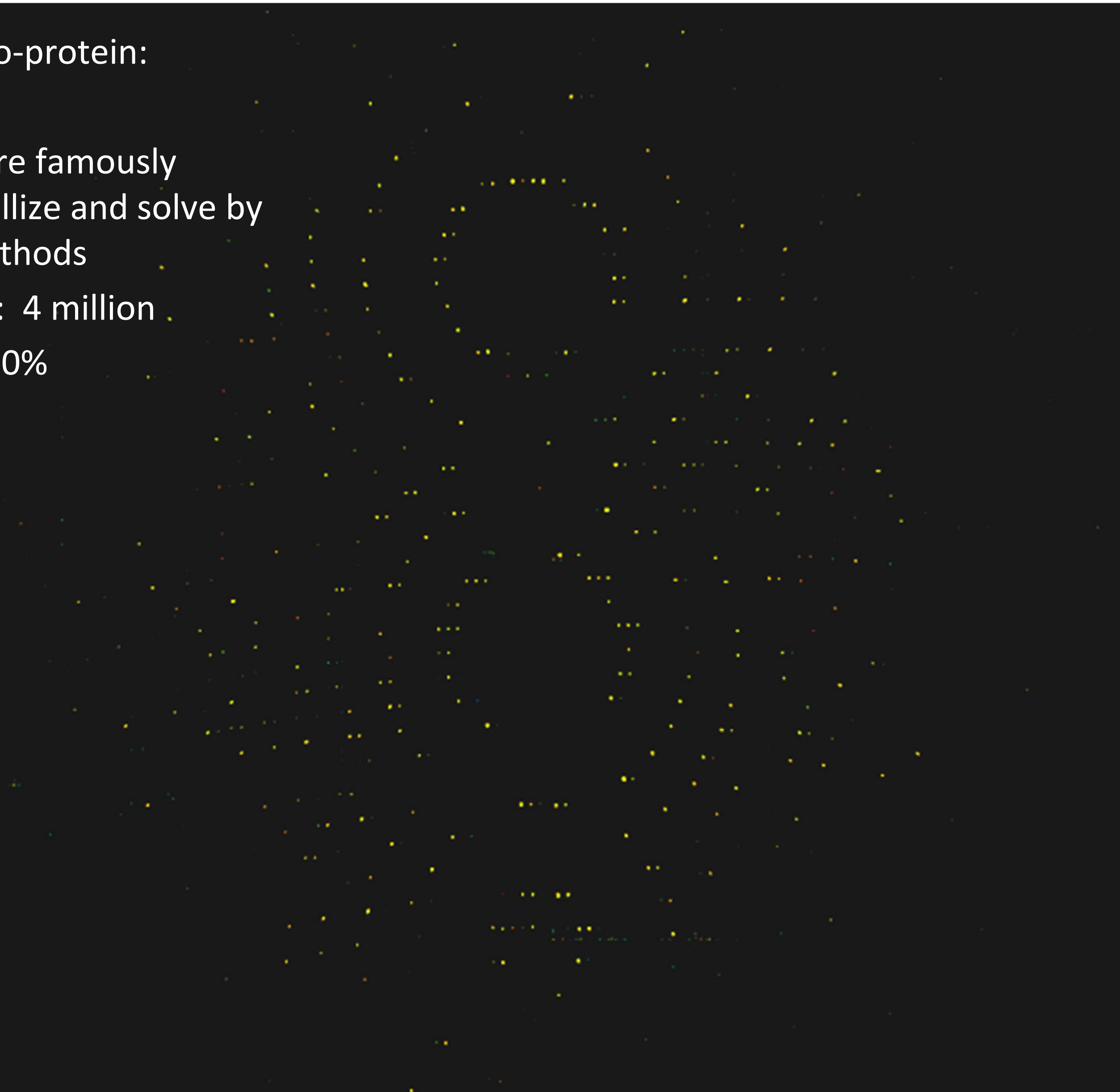
Crystal blows up later (“speed of sound”)

Complete structure from ~1 million shots

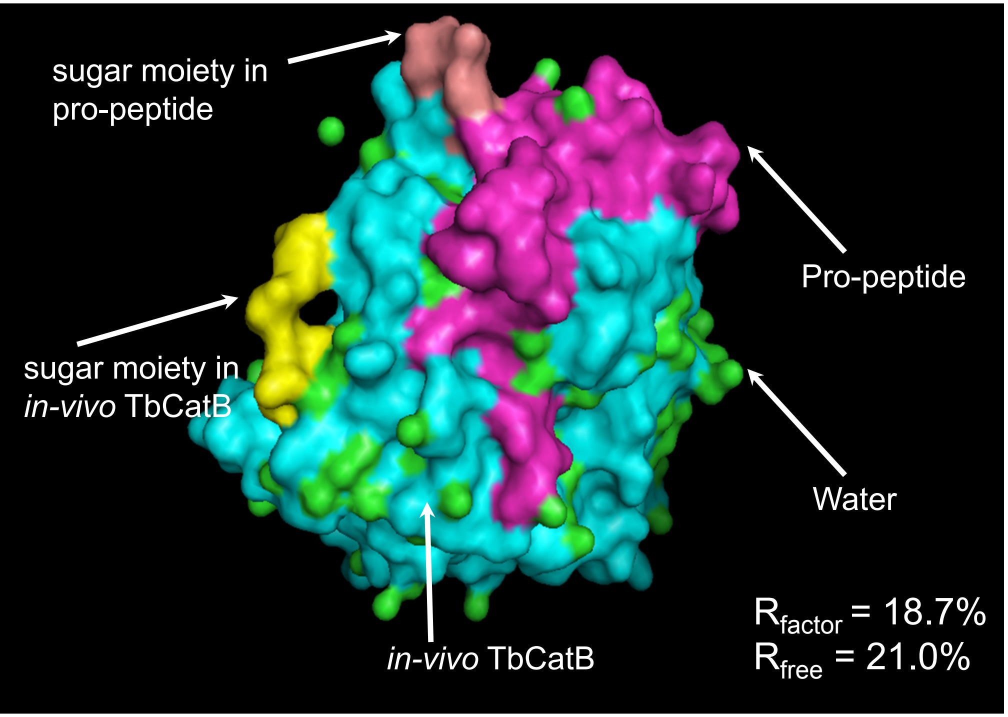
First X-FEL solved protein structure

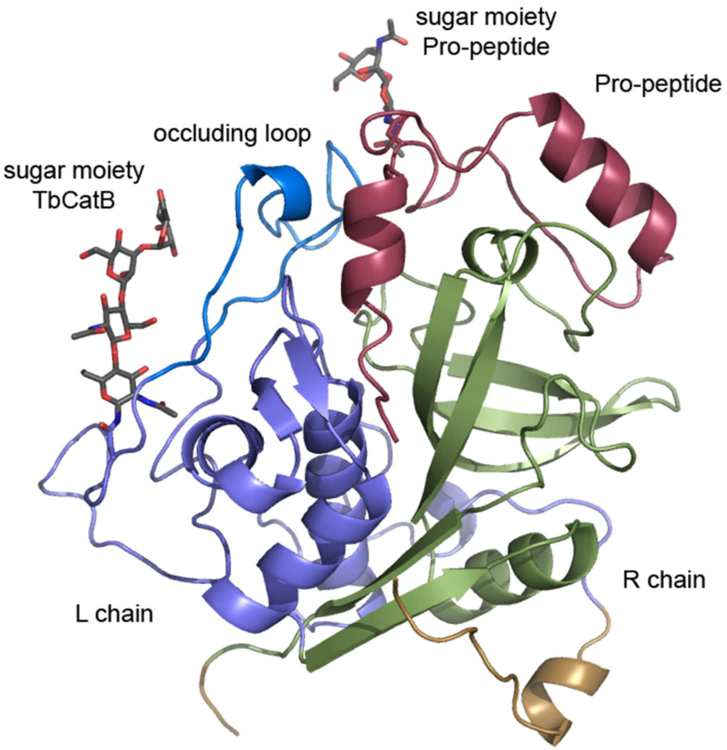
Cathepsin B enzyme protein - part of the African sleeping sickness parasite

- Cathepsin B glyco-protein:
  <3Å resolution
- Glyco-proteins are famously difficult to crystallize and solve by conventional methods
- number of shots: 4 million
  number of hits 10%



The structure of Cathepsin B





Karol Nass (CFEL) &
Lars Redecke (U. Hamburg)

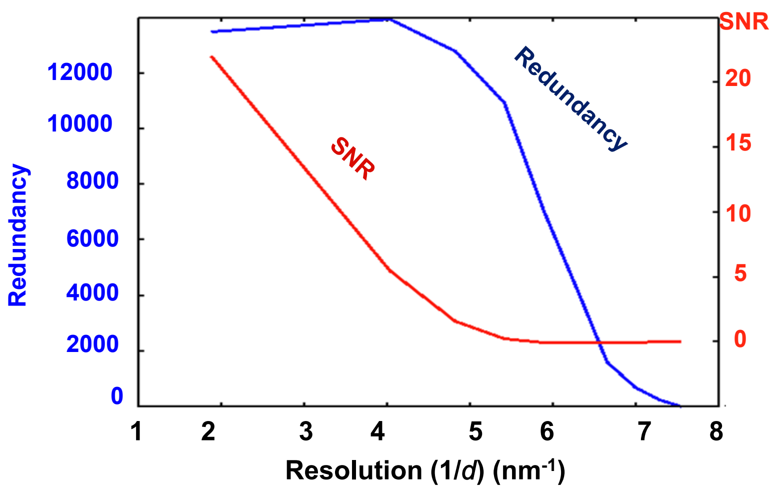
The Advent of X-Ray Lasers: Evolution or Revolution?

- 1879 - Light bulb
- 1895 - X-Rays
- 1960 - LASER
- 1970 - Synchrotron radiation
- 2010 - X-ray lasers

The end

TbCathepsin B Statistics

Data collected @ CXI in Feb 2011	
Number of shots (40 fs. pulses)	3,953,201
Number of "crystal hits"	357,555 (9% of above)
Number of indexed patterns	156,565 (44% of above)
Collection time	8 hours



Structure Refinement	
R factor	18.6%
R free	21.0%
Overall B factor	42.2
Completeness	99.6%
Highest resolution shell	1.9 Å – 1.95Å
$R_{int}(I)$	5.0%
Redundancy	10,955

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The new paradigm in understanding atomic matter

Structure and Properties

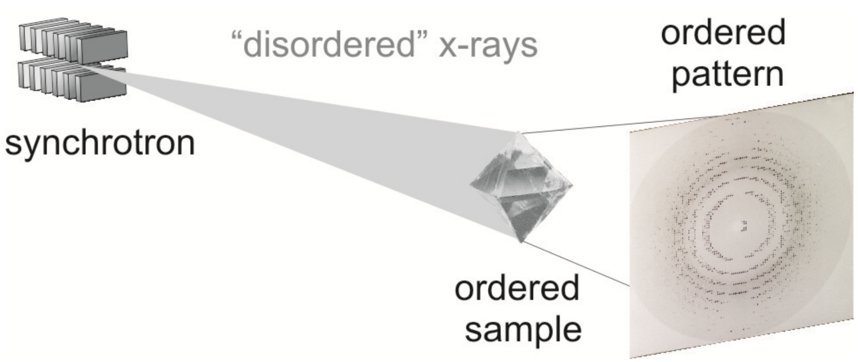
- Long range order
- Static disorder
- Equilibrium States

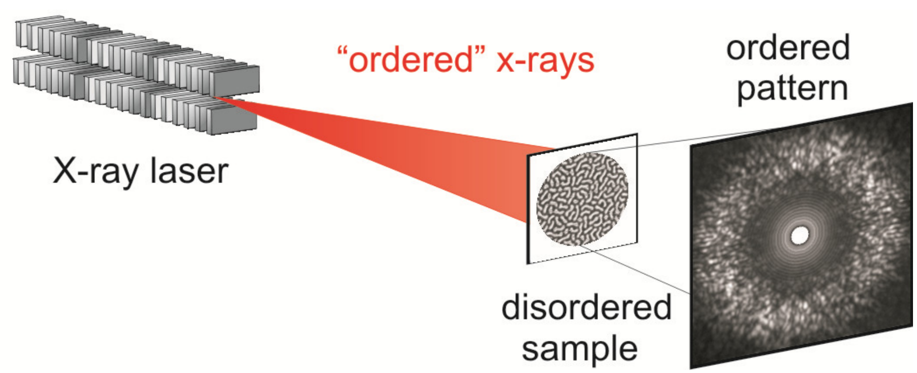
Function and Control

- Nanoscale order
- Dynamic order
- Transient States

1900 **2000** **future**

- most reliably calculated
- difficult to measure and calculate





User Input at Workshop

- **Atoms = electronic cores move slow enough (inertia) that "probe before atomic motion" concept works**

future vision:

- Maximum intensity for signal-to-noise – seeding, Terawatt beams
- Short pulse length (< 10 fs) to minimize effects of atomic motion
- Pursue first killer application: Bio-structures of small crystals
- Extend to single macromolecule imaging - requires TW beams < 5keV

- **Electrons respond faster, take advantage of non-linear phenomena**

future vision:

- Control photon energy, pulse intensity and shape – seeding
- Control polarization to distinguish charge & spin
- Explore x-ray/electronic interactions with controlled pulses
- Develop x-ray beam manipulation toolbox for non-linear x-ray optics

What determines the speed of atoms, electrons and spins?

rule of thumb…"the smaller the faster"….

Classically, "speed" of motion related to concept of inertia or mass
Quantum mechanically, time and energy are correlated

• **Atoms:**	**speed of sound:**	**1 nm / ps** (phonon energy 10 meV)
• **Electrons:**	**Fermi velocity:**	**1 nm / fs** (Fermi energy 10 eV)
for reference:	**speed of light:**	**300 nm / fs**

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The new science paradigm:
Static nanoscale "structure" plus its dynamic "function"