

Lecture 1: Introduction

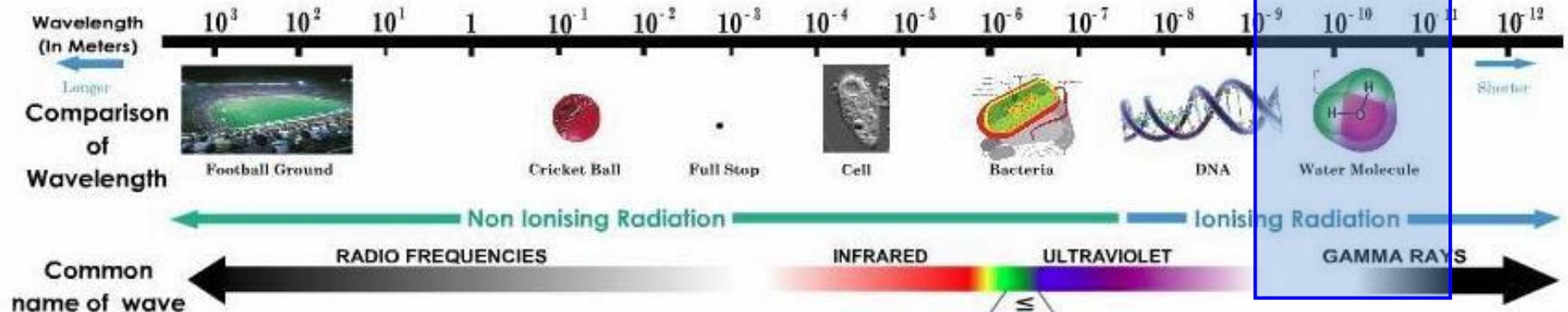
Yunhai Cai
SLAC National Accelerator Laboratory

June 12, 2017

USPAS June 2017, Lisle, IL, USA

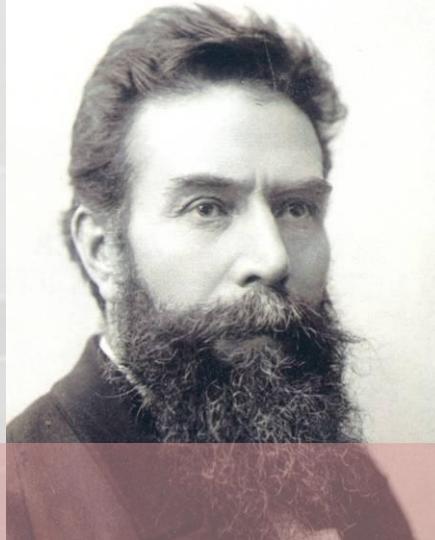
WHY X-RAYS?

THE ELECTROMAGNETIC SPECTRUM



X-rays - as electrons - are ideally suited to achieve sub-nano-metre spatial resolution:

- No diffraction limit (visible light)
- X-ray Synchrotron nano-imaging
achieved already resolution below $10 \times 10 \text{ nm}^2$



Röntgen discovered X-rays in 1895 and received the FIRST NOBEL PRIZE in Physics in 1901.

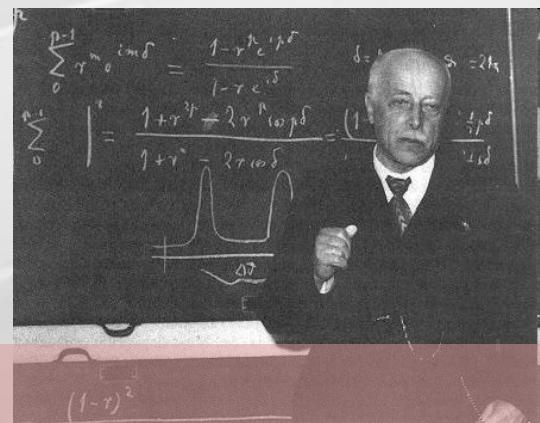
X-rays



2012

SLAC: 50 years
X-ray Diffraction: 100 years

Laue and the Braggs discovered in 1912-13 that X-rays can be used to study the structures and properties of materials. They received Nobel Prizes in physics in 1914 and 1915, respectively.

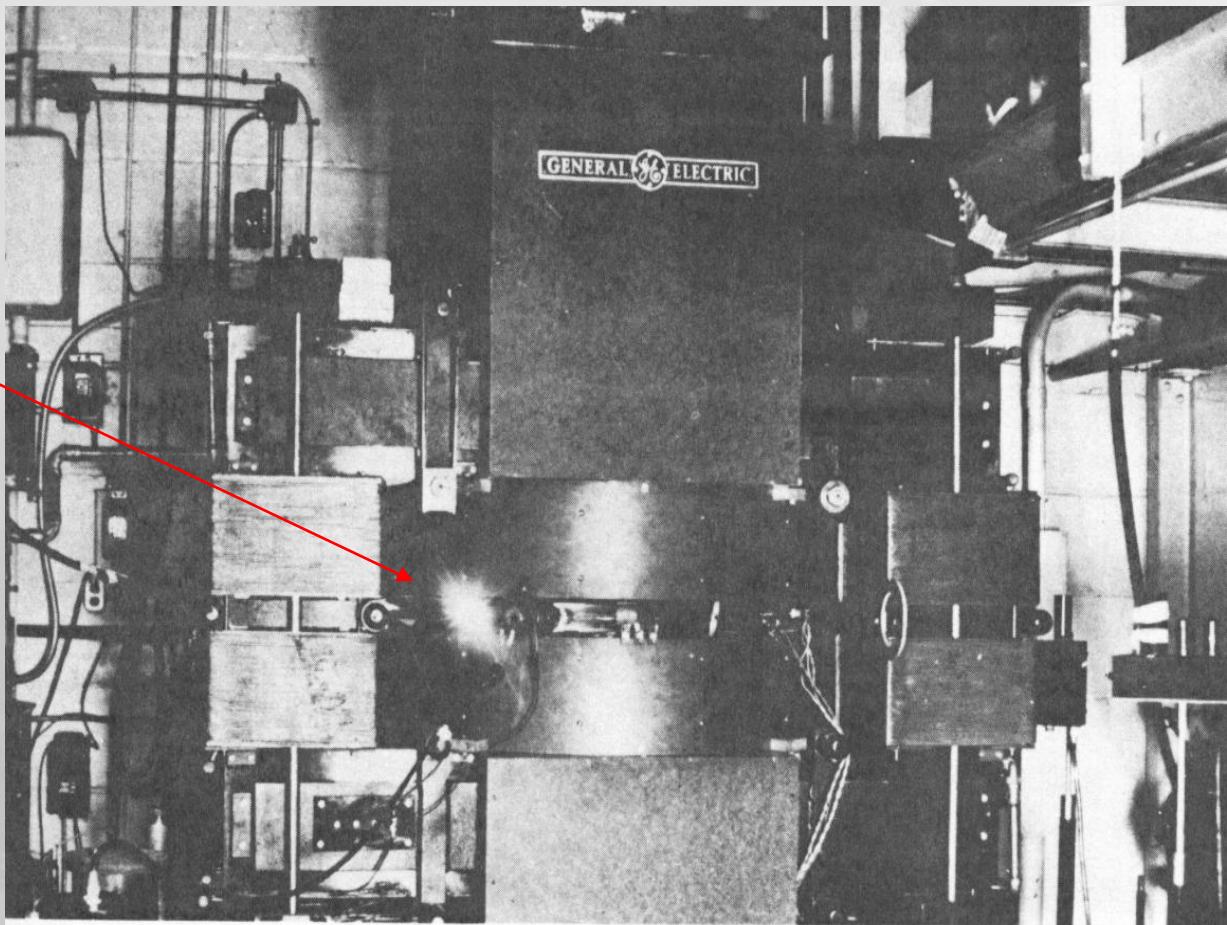


Max von Laue

W. Bragg father and son



First Observation of Synchrotron Radiation



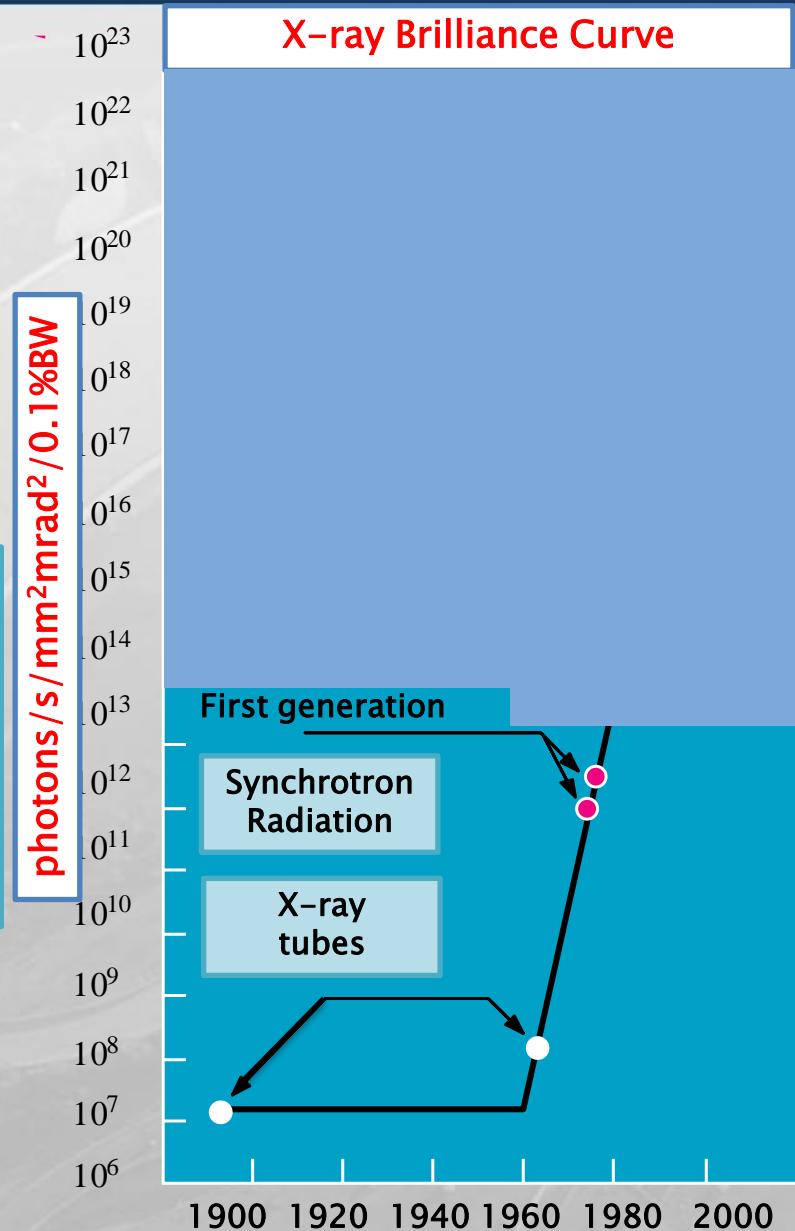
The General Electric team (Langmuir, Elder, Gurewitsch, Charlton and Pollock) looking at the vacuum chamber of the 70 MeV synchrotron (1947).

Synchrotron Radiation: A Revolution in the use of X-rays

**Storage Ring, 1961–1964
Key Time for Synchrotron
Radiation**



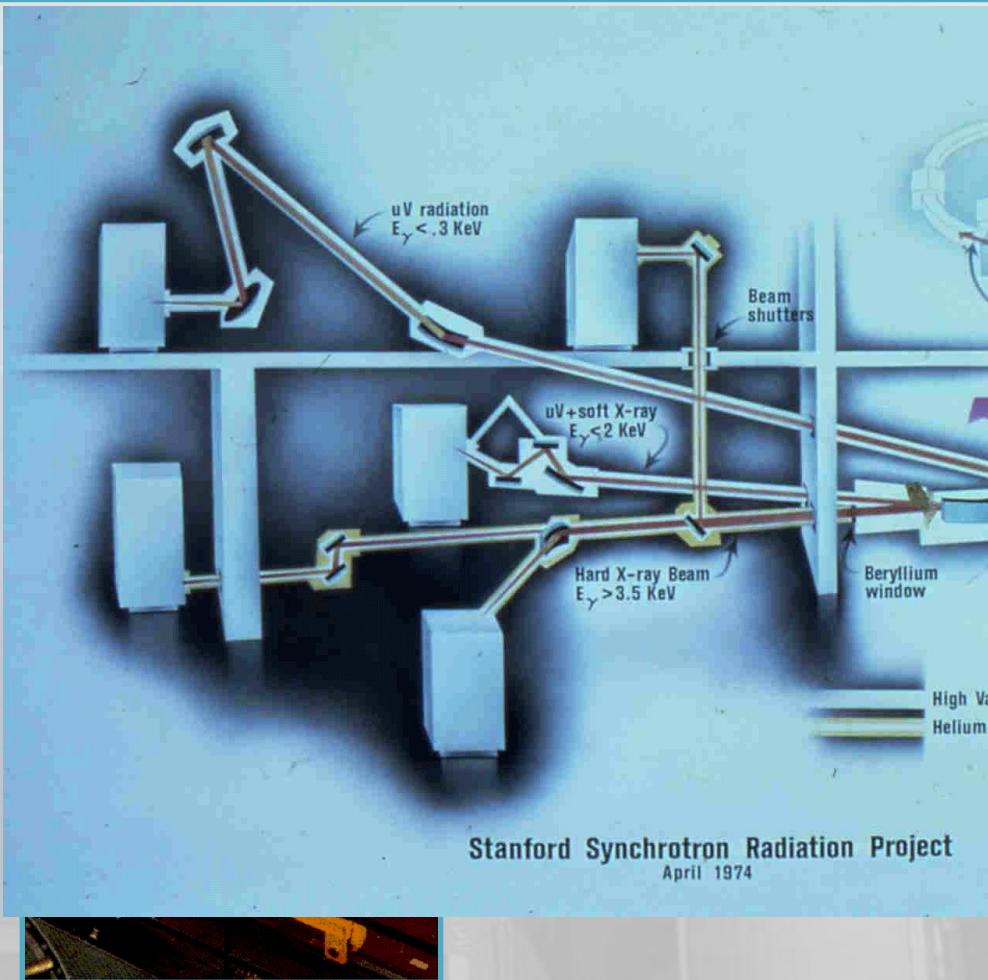
Construction of ADA,
the first storage ring for
electron and positron
beams rotating in opposite
Directions.
Proposed by Bruno Touschek
(1921–1978), in 1960



Synchrotron Radiation: A Revolution in the use of X-rays

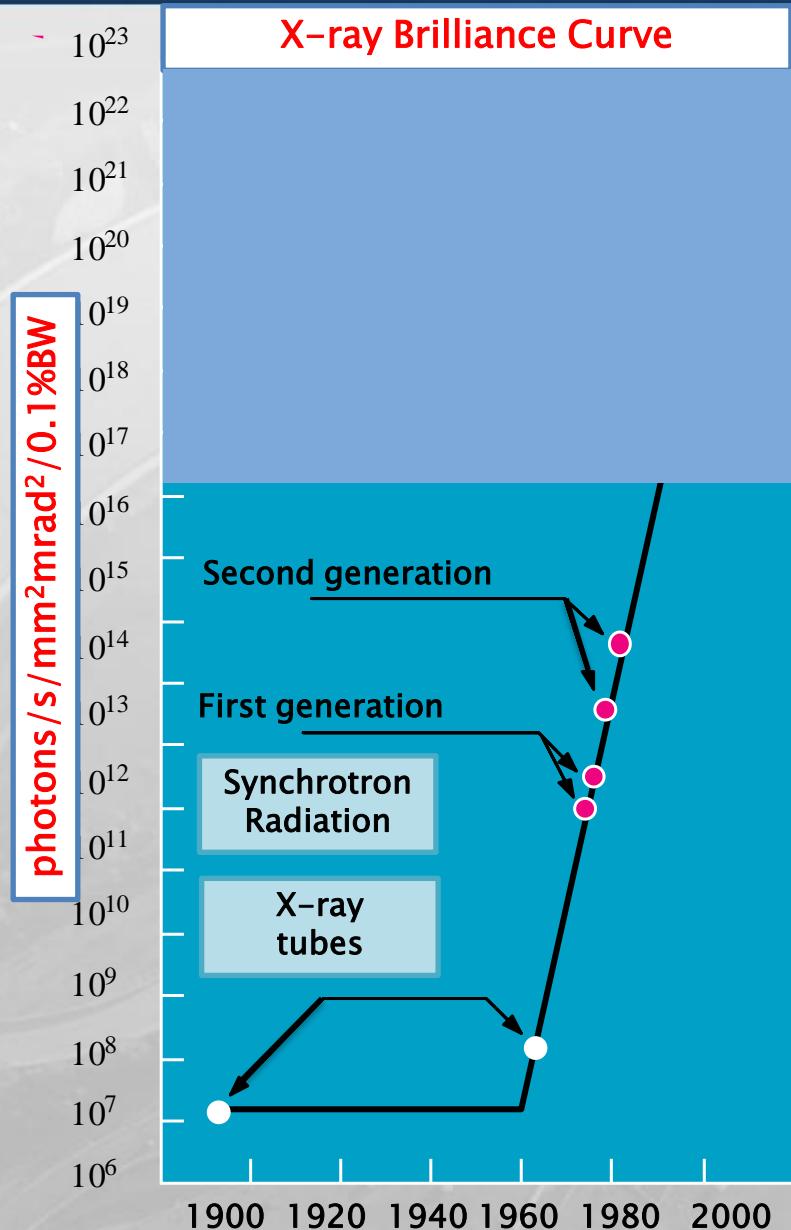
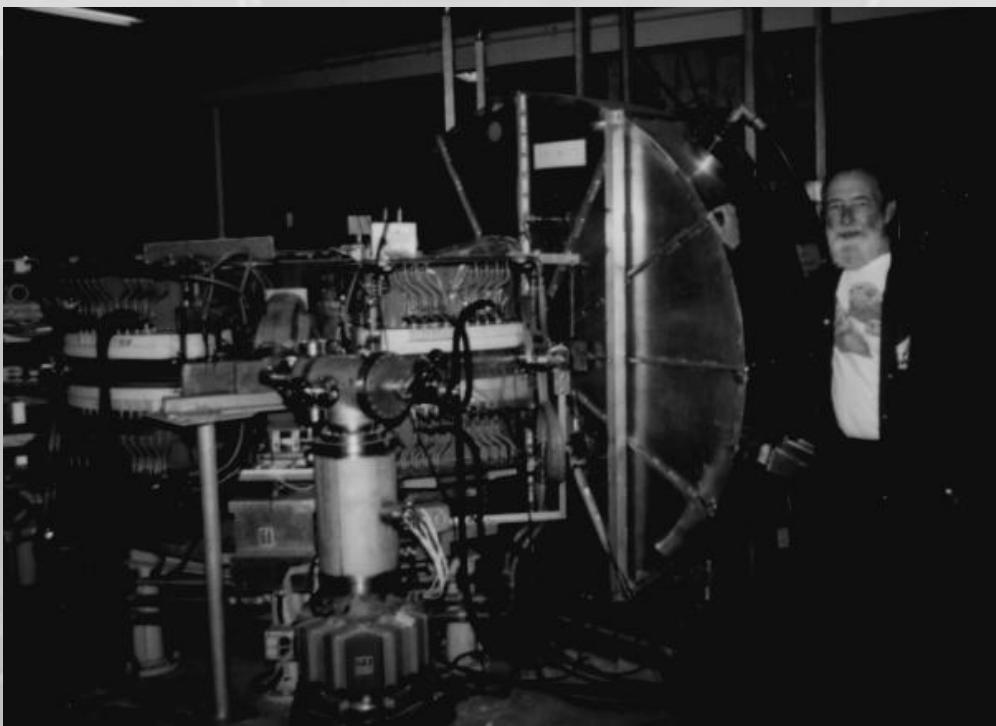
10²³
10²²
10²¹

X-ray Brilliance Curve

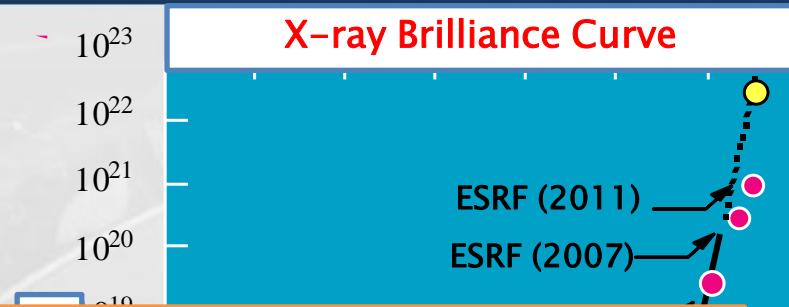


Synchrotron Radiation: A Revolution in the use of X-rays

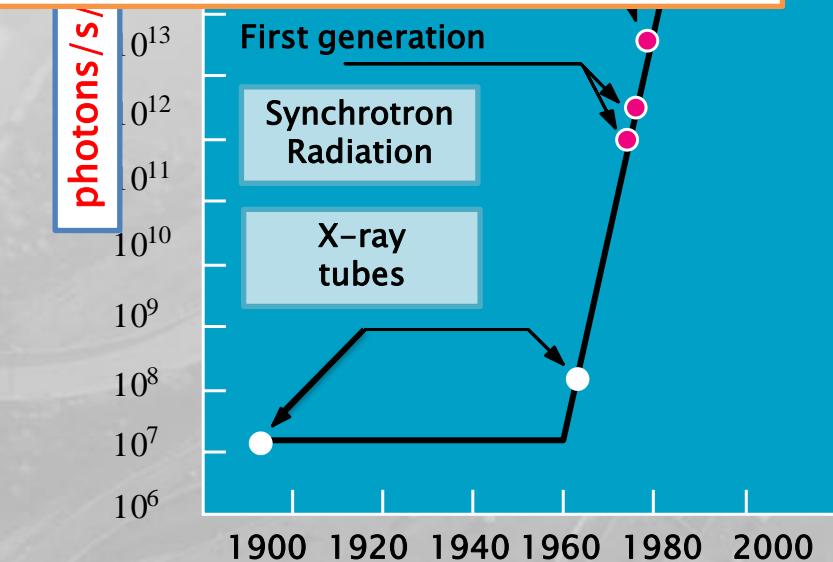
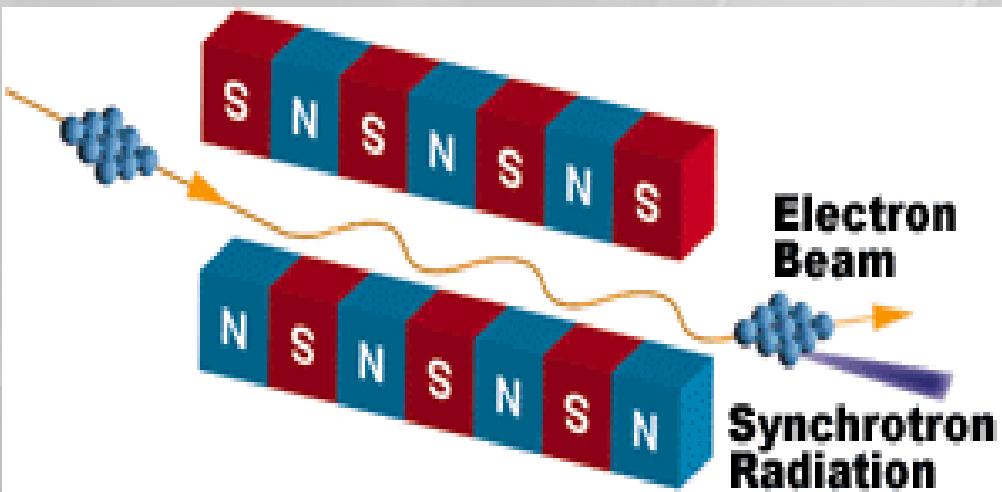
Tantalus I:
The first dedicated source of
Synchrotron Radiation, 1968



Synchrotron Radiation:
A Revolution in the use of X-rays



$\sim 10^{11}$ brighter than a
Laboratory Source



The European Synchrotron Radiation Facility: the 1st Third Generation Source



Investigating matter, materials and living matter

Fields of application

Understanding matter down to the single atom links many scientific disciplines at Synchrotrons:



Solid-state
physics

- Atomic structure
- Magnetic / electronic properties of materials



Chemistry

- Structure / dynamics of new materials
- Structure of interfaces



Medicine

- Pharmaceutical molecules
- New therapy protocols



Life
sciences

- Protein cristallography
- Protein dynamics

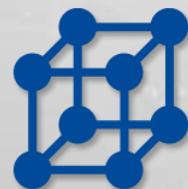
Investigating matter, materials and living matter

Fields of application

Understanding matter down to the single atom links many scientific disciplines at Synchrotrons:



Engineering



Material science



Earth sciences



Environment



Cultural heritage

- Development of new manufacturing / processing technologies
- Material failure

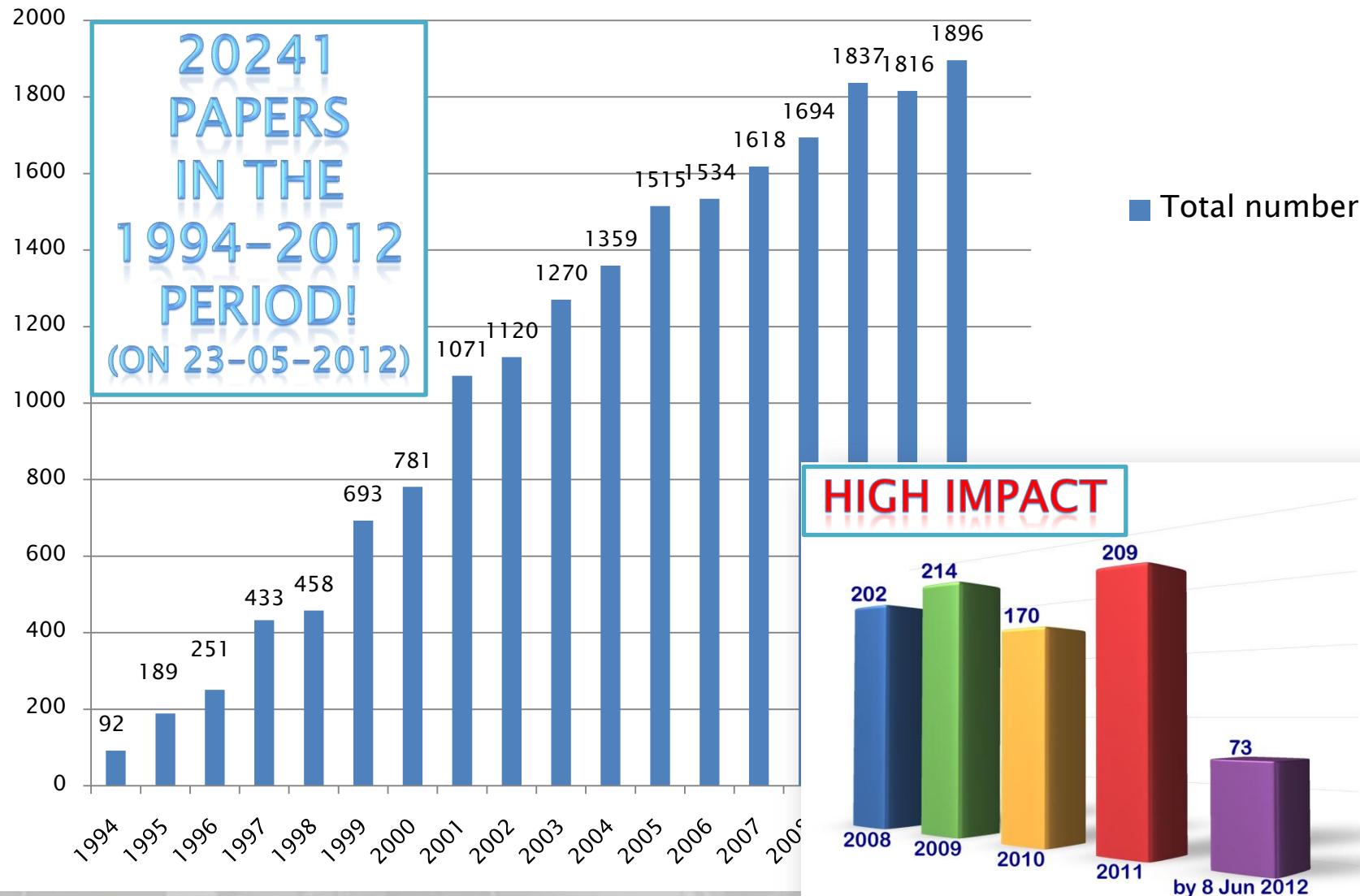
- Structural properties of high-performance materials
- Soft-condensed matter

- Structure and formation of earth's crust
- Geo-dynamics

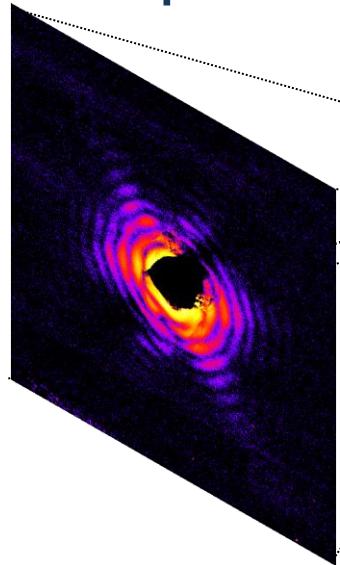
- Behaviour of bacteria under extreme conditions
- Heavy Metals in the Environment: origin, interaction and remediation

- Non-destructive X-ray imaging
- Artefacts
- Palaeontology

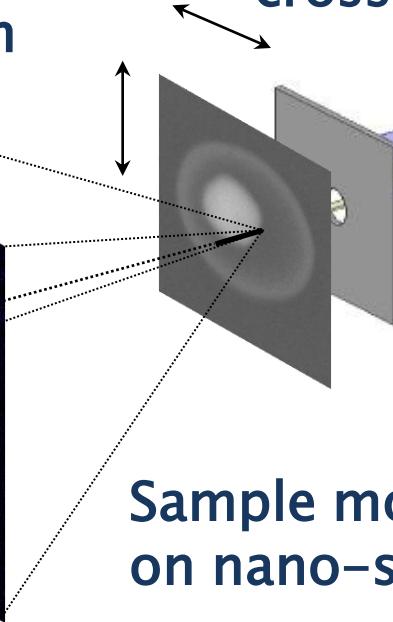
Refereed Publications from work at the ESRF



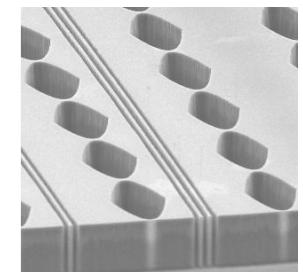
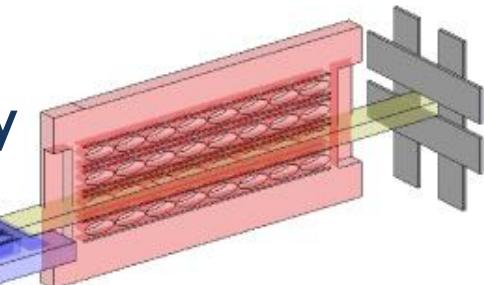
coherent diffraction pattern



crossed geometry

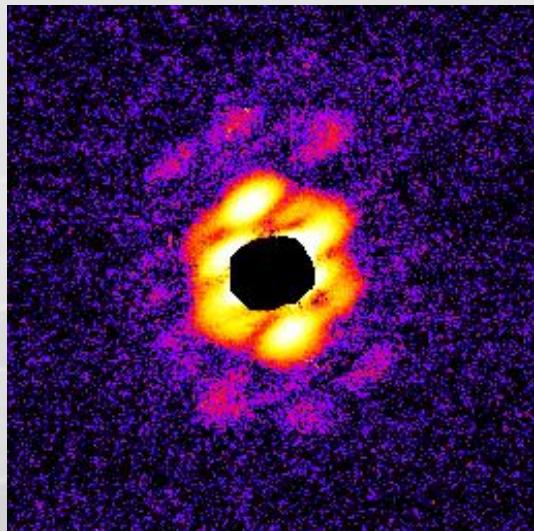


Sample mounted
on nano-scanner

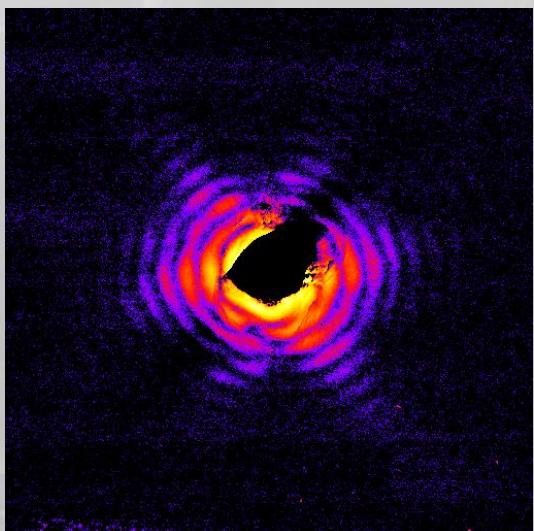
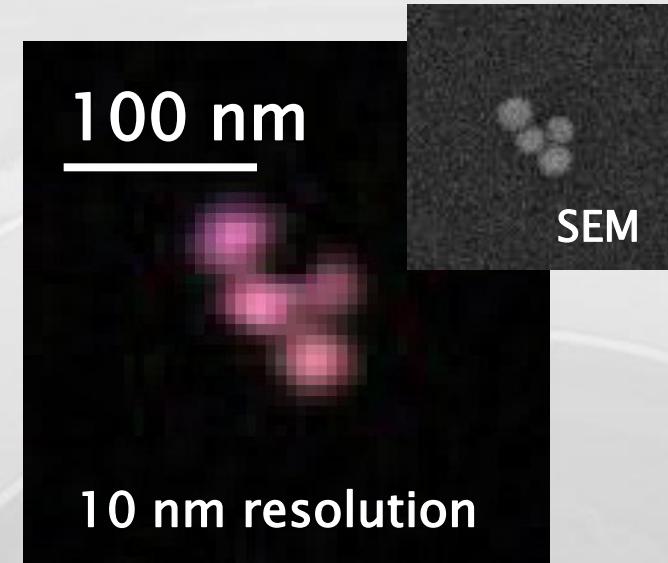


Si-NFL lenses
100 nm beam
15.25 keV energy

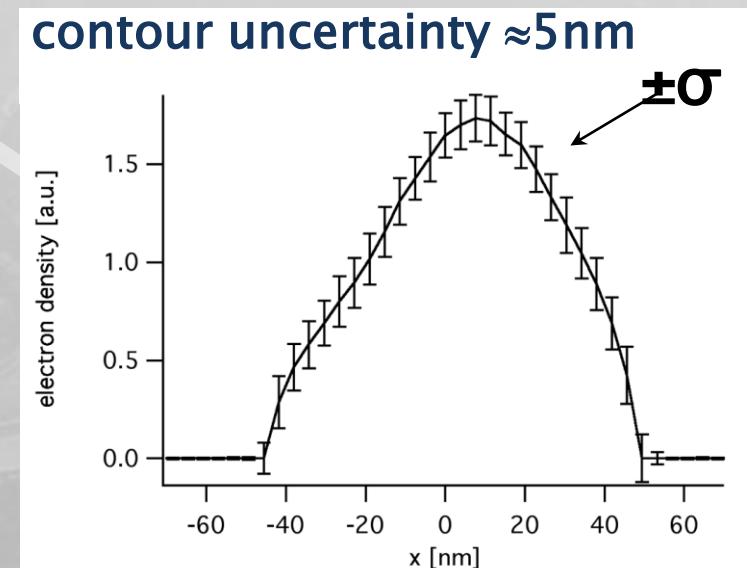
- *nano*-beam coherent X-ray diffraction imaging (CXDI)
- 100 nm beam generating gaussian illumination function
- *nano*-focusing silicon compound refractive lenses (NFL)



reconstruction
via
iterative
phase retrieval

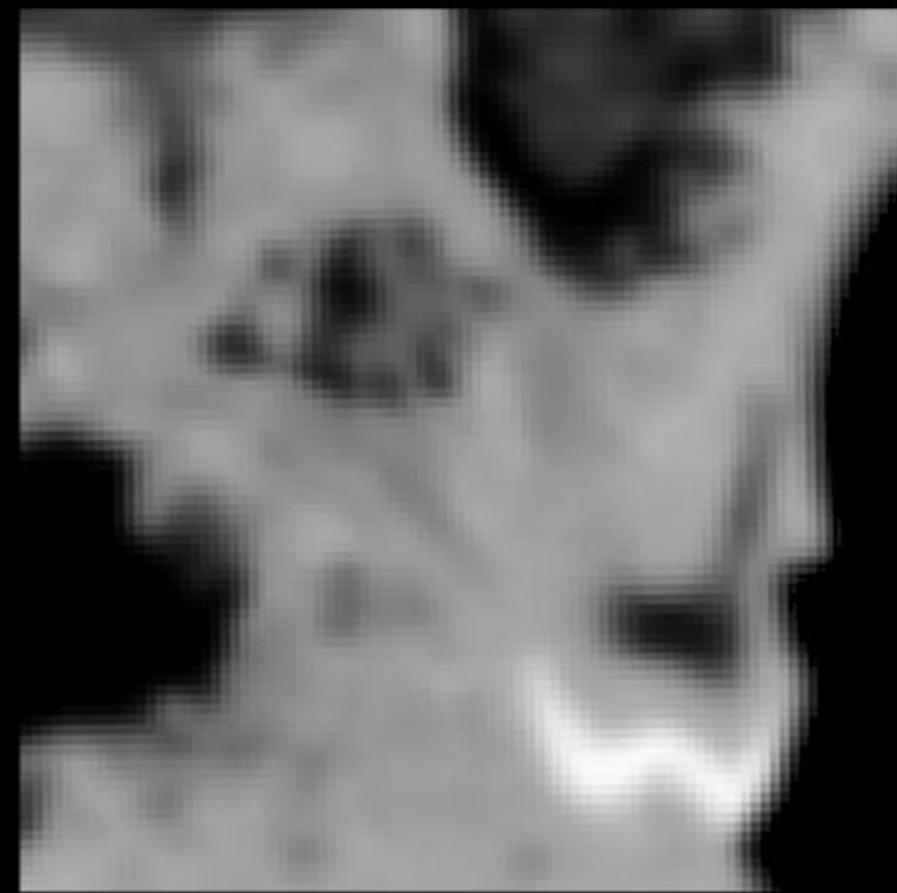
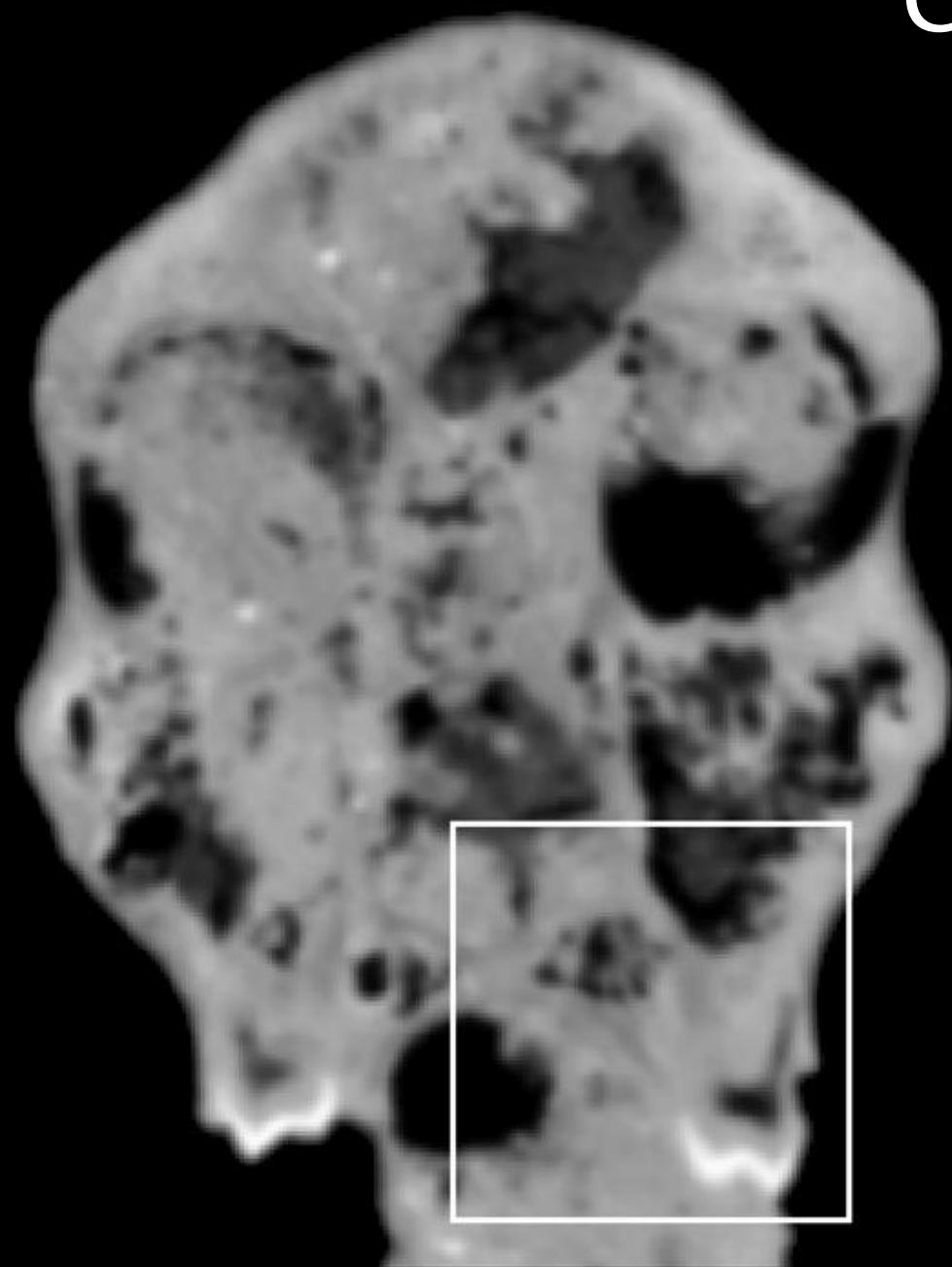


gold *nano*-particle
reconstructed
projection
5 nm resolution

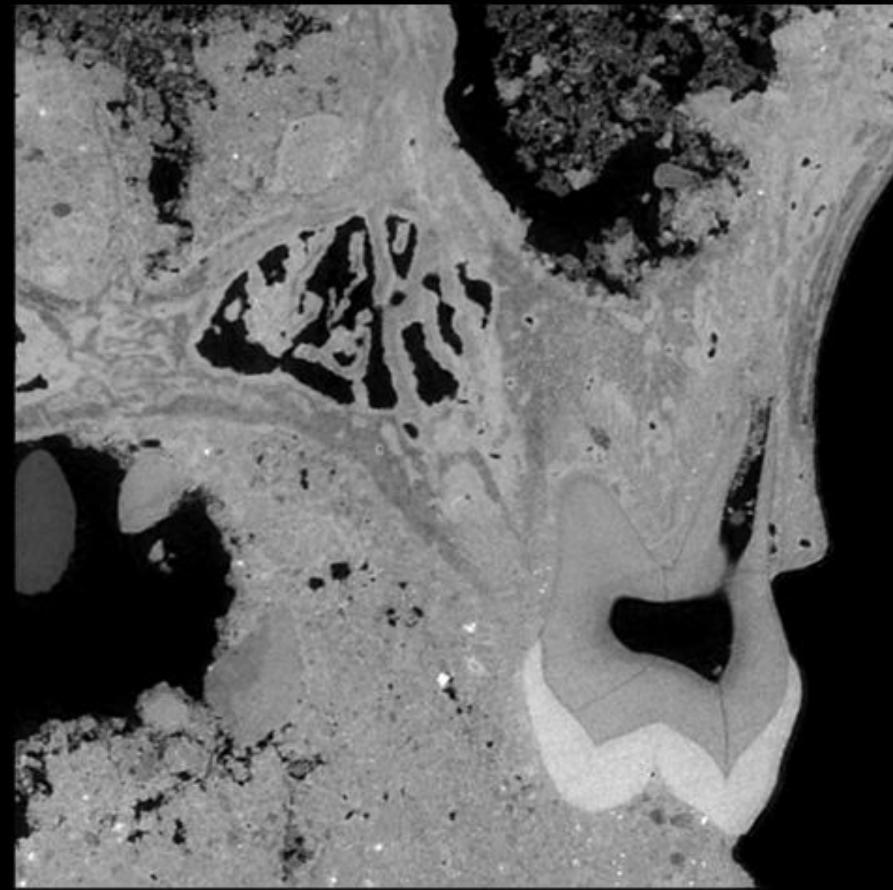
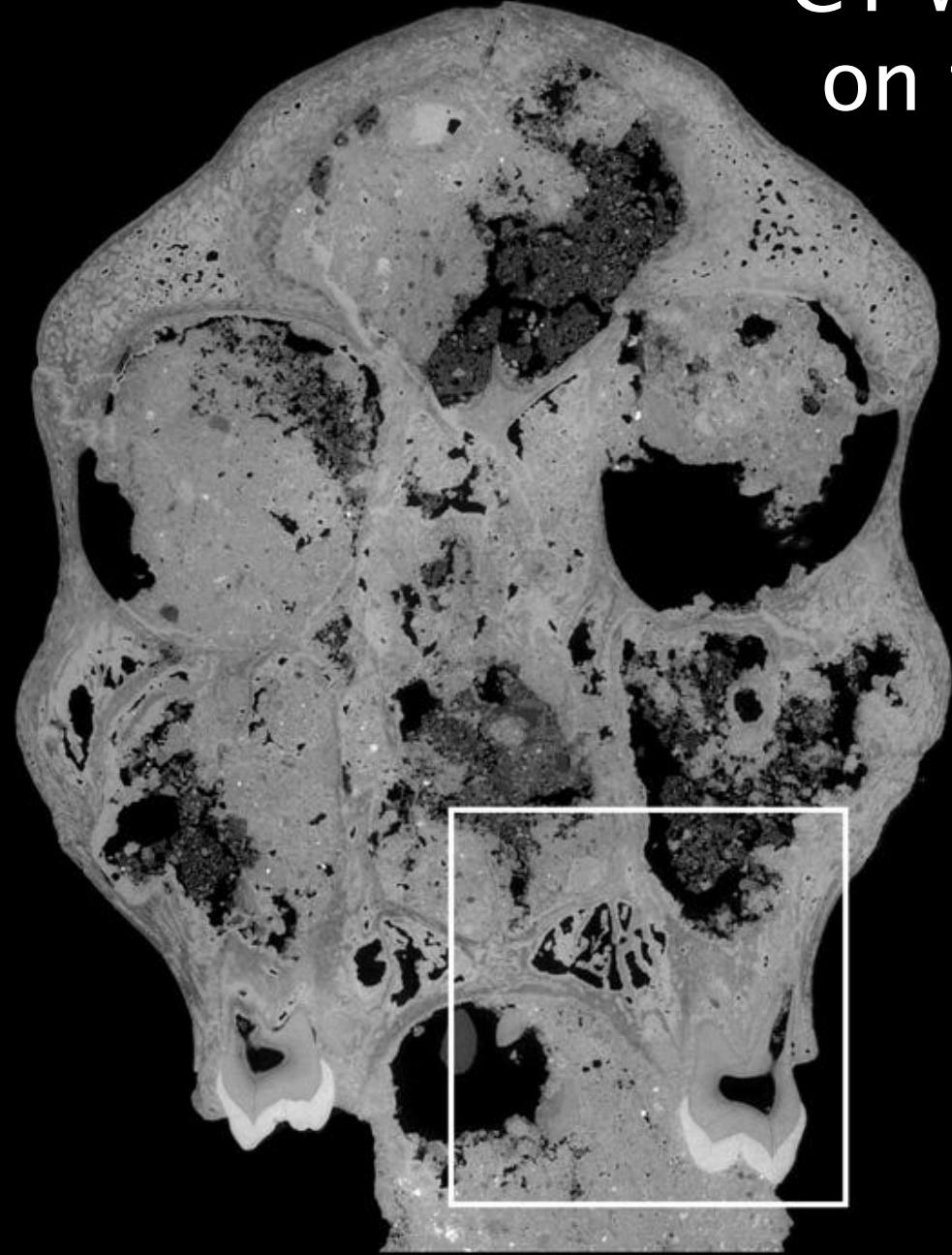


C. G. Schroer et al. Phys. Rev. Lett. 101, 090801 (2008)

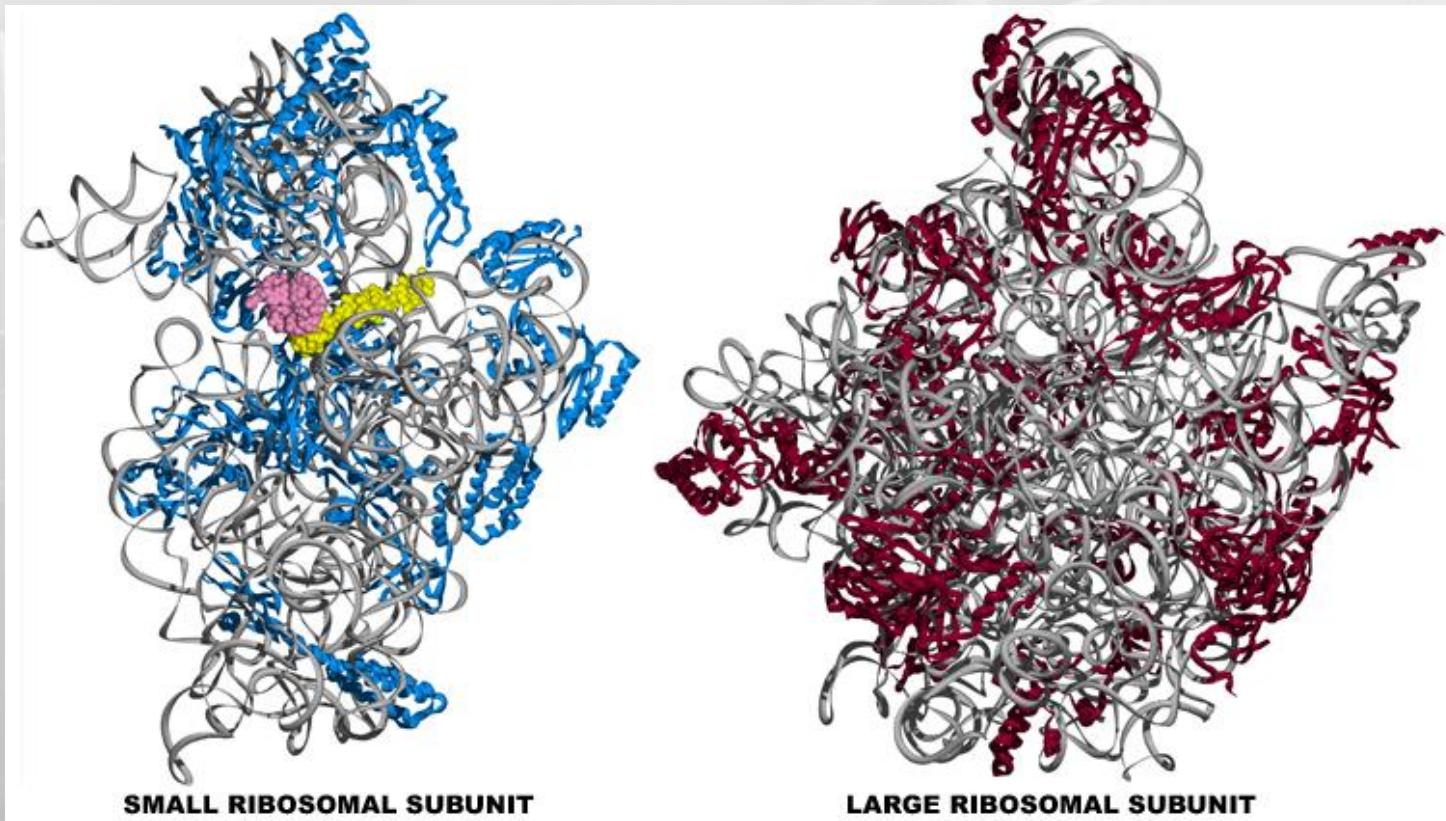
CT with a Hospital Machine



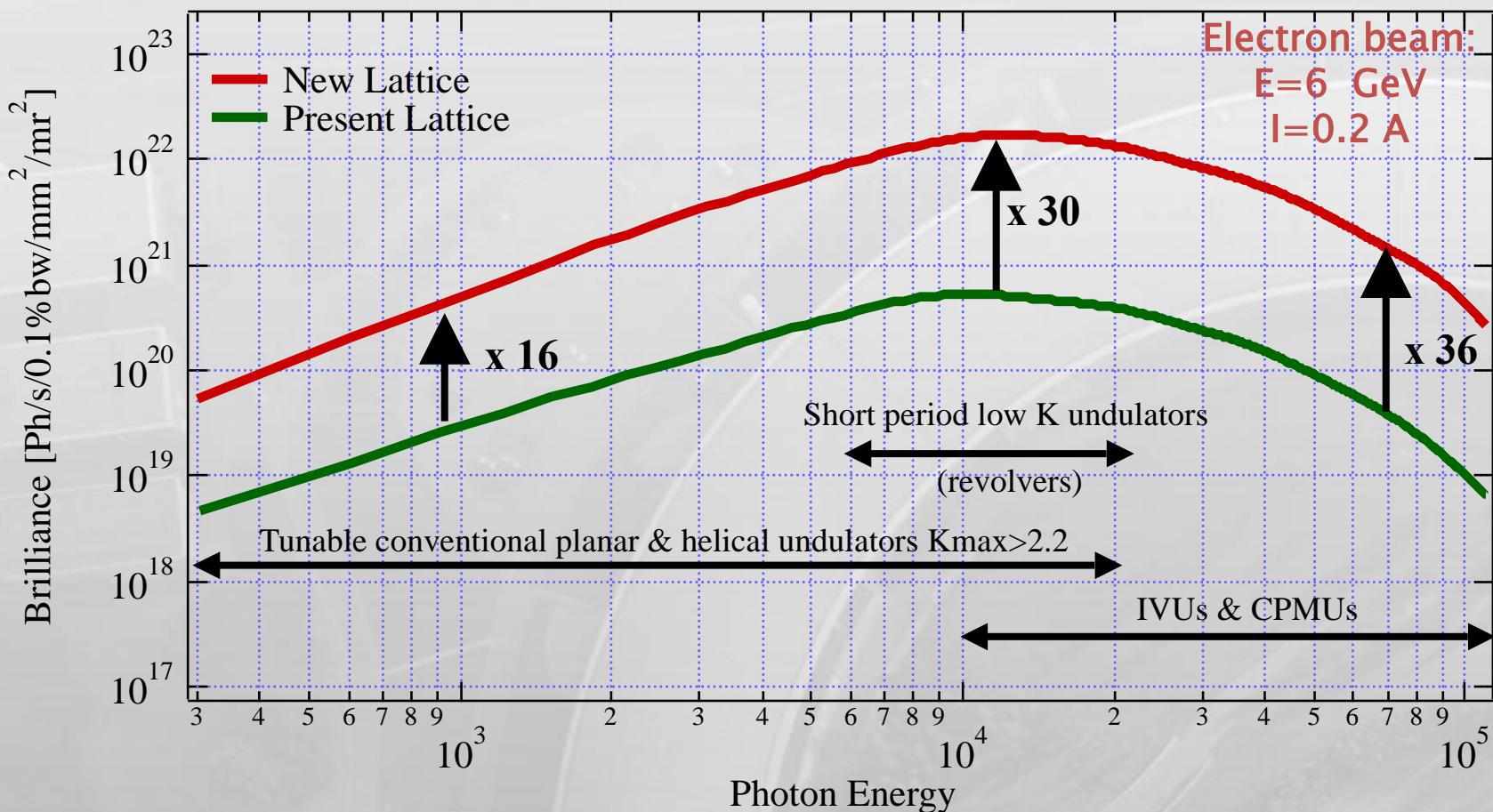
CT with Synchrotron Light on the ID17 Line at ESRF



Ribosome sub-units at atomic resolution.

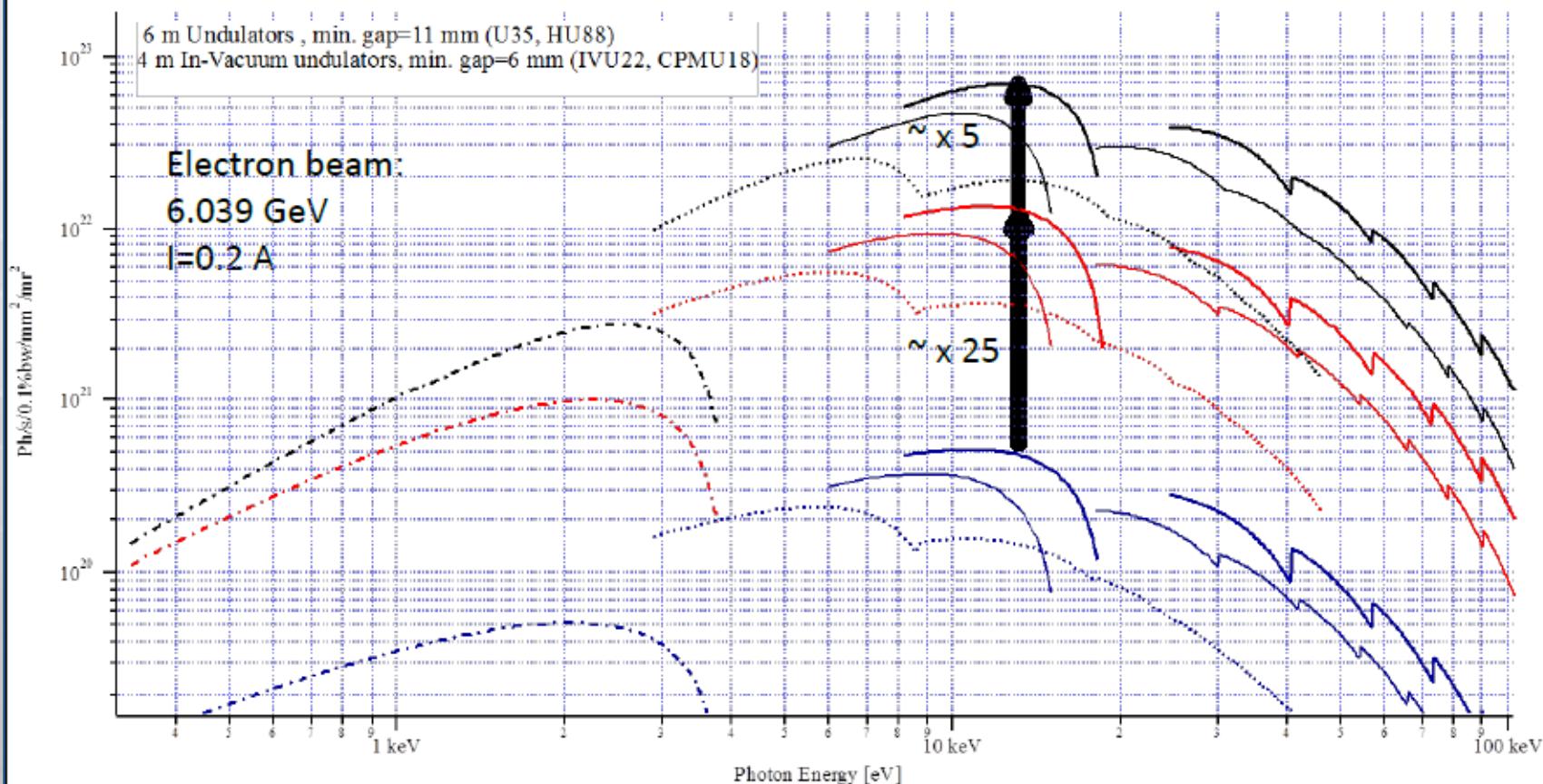


SSU from Ramakrishnan's work with A-site Anticodon Stem Loop bound
and mRNA LSU from Steitz and Moore labs



	Emittance	Coupling [%]	Energy spread [%]
Present	4 nm	0.12	0.1
New lattice	0.13	1	0.09

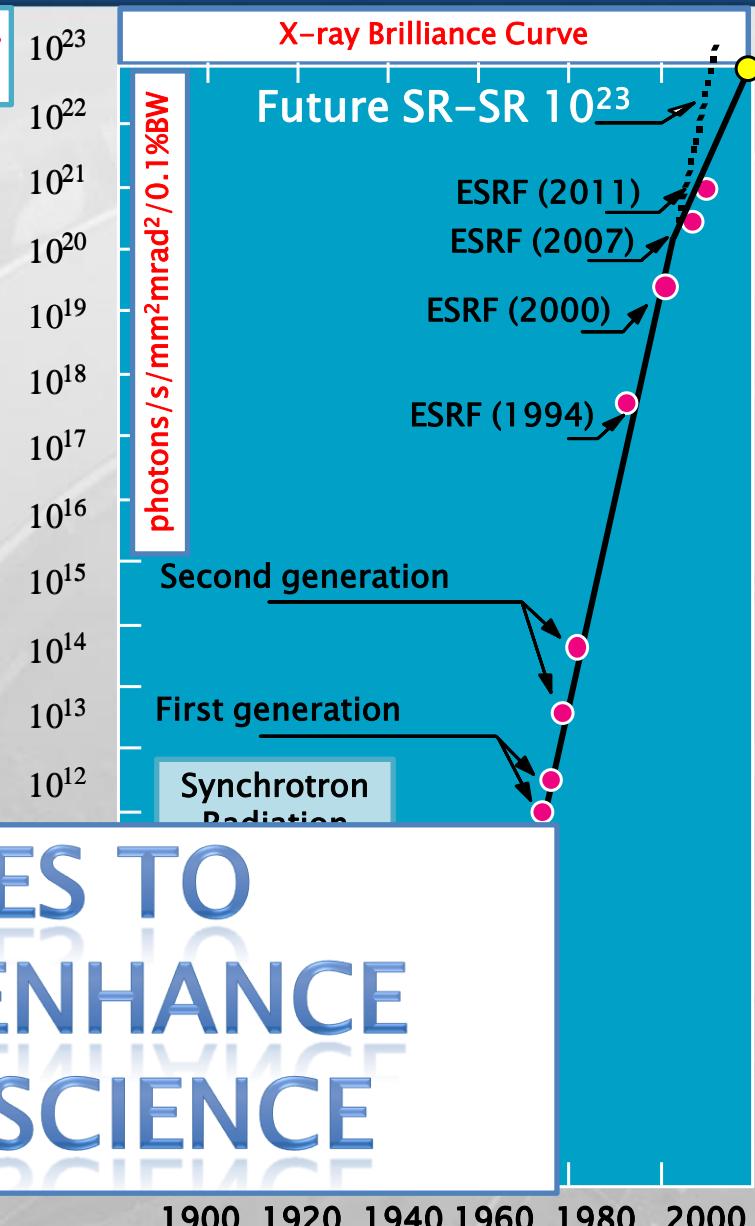
Gain in brilliance due to reduction of horizontal emittance



Hor. Emittance [nm]	4	0.15	0.01
Vert. Emittance [pm]	3	2	2
Energy spread [%]	0.1	0.09	0.09
Betax[m]/Betaz [m]	37/3	6/2	6/2

The SR Grand Challenges

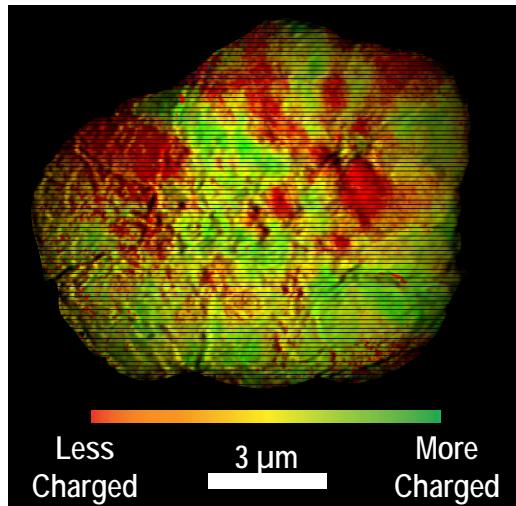
- To be increasingly useful:
 - Powered by scientific excellence
 - Faithful and committed Users' service
- To enlarge the Users' Community:
 - More then PHOTONS!
- Quest for the “Future SR–SR source”:
 - Improved horizontal emittance: $10 \times 10 \text{ pm}^2$??
 - 10^{23} Brilliance (ph/s/mm²mrad²/0.1%BW) ??



OPPORTUNITIES TO
QUALITATIVELY ENHANCE
SYNCHROTRON SCIENCE

Motivation: Desire to Probe Nature at Atomic Length (\AA) & Time (fs) Scales

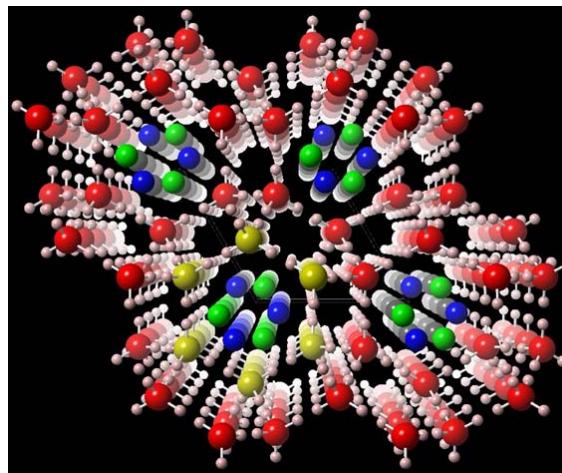
Seeing the Invisible in Real Materials



Compositional heterogeneity in a $\text{LiNi}_{1/3}\text{Co}_{1/3}\text{Mn}_{1/3}\text{O}_2$ battery hundreds of hours after charging

Adv. Materials (2016)

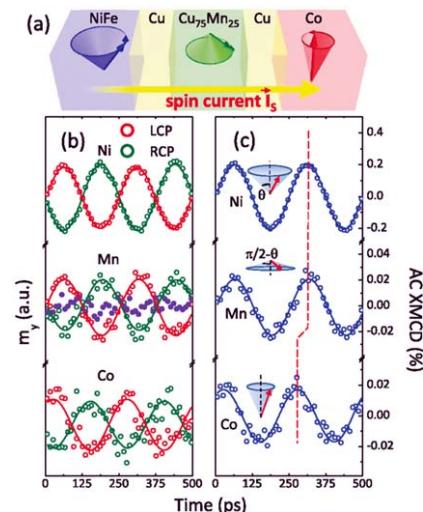
Where are the Atoms?



Newly discovered structure of a hydrogen-stuffed, quartz-like form of ice

JACS (2016)

Where are the Electrons & Spins?

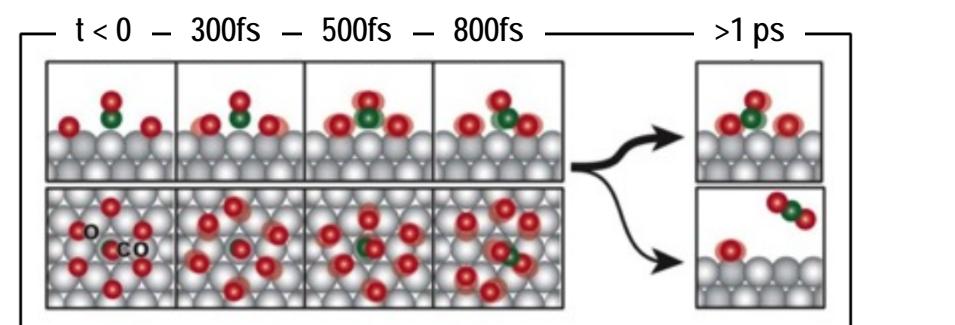


Direct measurements of "pure" ac spin currents (flow of spin angular momentum without flow of charge)

PRL (2016)

What are the Dynamics?

Capturing the transient behavior of catalytic bond formation



Science (2015)

Light Sources Are Alive & Kicking: 60+ Facilities Worldwide & Growing



ALS



APS



NSLS-II



SSRL



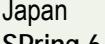
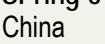
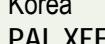
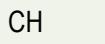
LCLS

BES Light Sources
of
ENERGY
Office of
Science

*Many other new & upgraded facilities are in the design stage...
Take Away Message: It's a very competitive landscape!*

NORCE	North Sea Ring	DESY	FLASH I & II	SACLA FEL 2011 8.5 GeV, 30 Hz NC
APS	Canada: LCLS	Japan: SPring-6	China: BLS	PAL XFEL 2016 10 GeV, 60 Hz NC
NSLS-II	Germany: PETRA 3/4	Brazil: SIRIUS	SWISS FEL 2017 5.8 GeV, 100 Hz NC	Sweden: MAX-IV
LCLS	France: ESRF II	New Rings	Upgraded & New FELs	EU XFEL 2017 17.5 GeV, 3000 x 10 Hz SC

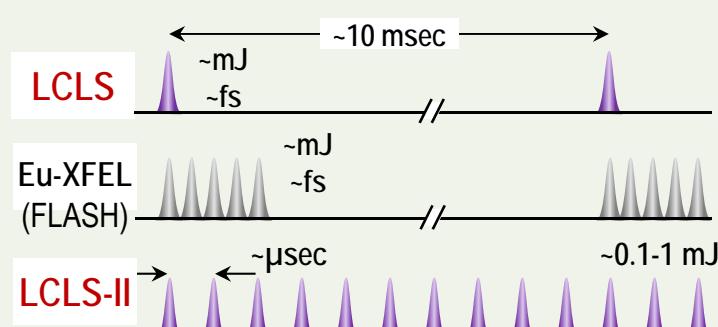
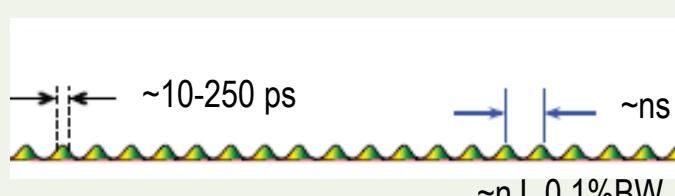
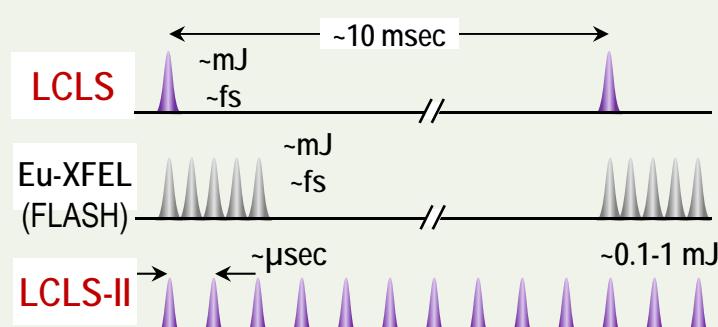
USA Response: BESAC Report on Light Source Facility Upgrades (June 2016)

	Storage Rings		FEL
Project	ANL APS-U	LBNL ALS-U	SLAC LCLS-II-HE
Project Scope	Hard X-ray ~Diffraction Limited 6 GeV Multi-Bend Achromat (MBA) Ring	Soft X-ray ~Diffraction Limited 2 GeV Multi-Bend Achromat (MBA) Ring	High Rep-Rate, High Energy X-ray FEL, 8 GeV SC Linac
Current Status of Facility	APS is operational since 1996; ring will be replaced	ALS is operational since 1993; ring will be replaced	LCLS is operational since 2010; LCLS-II is under construction
Worldwide Competition	 EU  ESRF  Germany  PETRA 3,4  Japan  SPring-6  China  BLS	 Sweden  MAX-IV  Brazil  SIRIUS  CH  SLS-II	 EU  XFEL  Japan  SACLA  Korea  PAL XFEL  CH  Swiss FEL
Dark Time	~1 yr	~0.75 yr	0 yr
Status FY2017	CD-3b	CD-0	CD-0

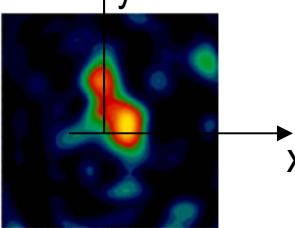
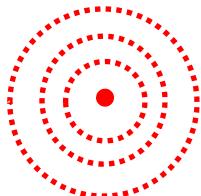
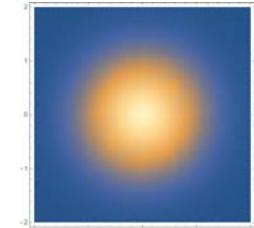
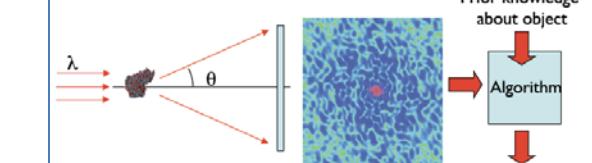
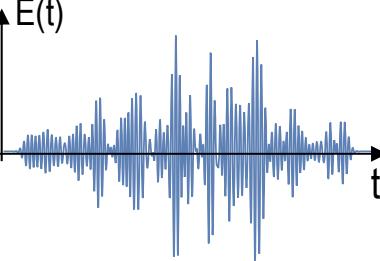
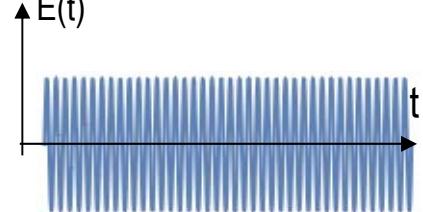
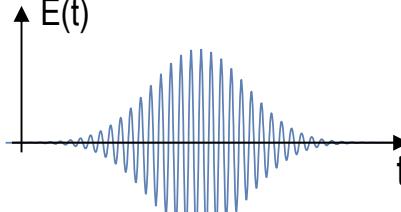
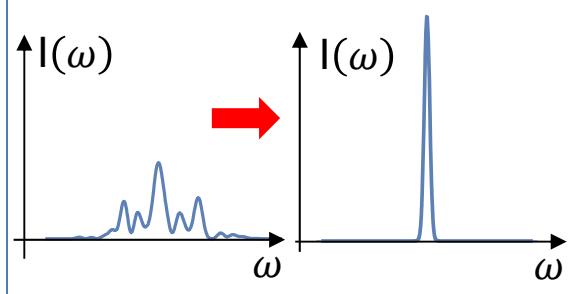


The ALS-U, APS-U & LCLS-II-HE proposals were each deemed “absolutely central to contribute to world leading science & ready to initiate construction”

Storage Rings & Free Electron Lasers are Complementary

Parameter	Storage Rings	FELs
Beam Stability	Excellent	Very Good
Number of Beamlines	Up to 70+	1-5
Brightness (Ave, Peak)	(High, Low)	(Up to Very High, Extreme)
Transverse Coherence	Partial-Full	Full (@ Saturation)
Longitudinal Coherence	Poor	Moderate (SASE)-Very Good (seeding)
Pulse Time Structure		
Pulse Energy		

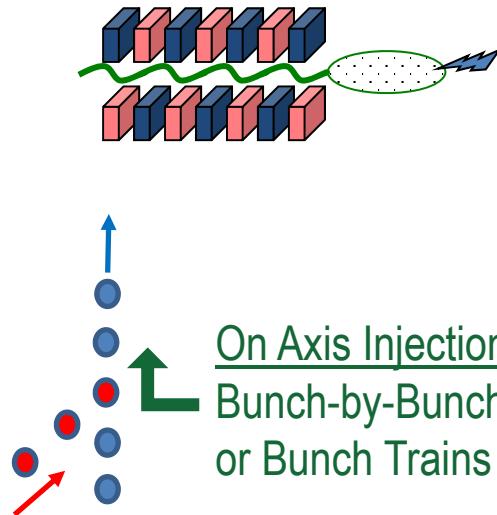
New Sources Will Provide Enhanced Transverse & Longitudinal Coherence

Coherence Level	Realistic Partial	Idealized Full	Realistic Full	Coherence Advantages
Transverse (Spatial Profile)	<p>Multi-Mode</p>  $\Delta x \cdot \Delta \theta_x > \lambda / 4\pi$	<p>Point Source (Spherical Waves)</p>  $\Delta x, \Delta y \rightarrow 0$	<p>Gaussian Laser Mode</p>  $\Delta x \cdot \Delta \theta_x = \lambda / 4\pi$	<p>Coherent Diffractive Imaging, Ptychography & Nanoprobes</p>  <p>Imaging w/o Lenses</p>
Longitudinal (Temporal Profile)	<p>Noisy Pulse</p>  $c \Delta t \cdot \frac{\Delta \omega}{\omega} > \lambda / 4\pi$	<p>Monochromatic Wave Train</p>  $\Delta \omega \rightarrow 0, \Delta t \rightarrow \infty$	<p>Gaussian Laser Pulse</p>  $c \Delta t \cdot \frac{\Delta \omega}{\omega} = \lambda / 4\pi$	<p>FEL SASE vs Seeded Spectrum</p>  <p>Maximize Number of Photons in Minimum BW</p>

Physics & Technology for Maximizing the Photon Beam Brightness, B_{ave}

Rings $\sim 10^{22}$

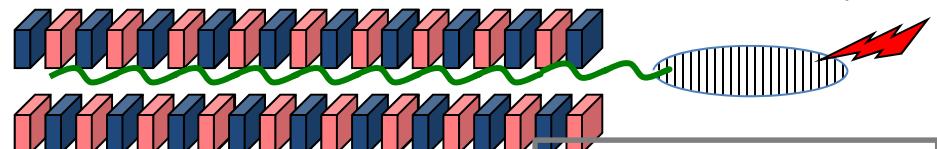
Spontaneous Emission from a Random Beam



$$N_{ph}^{spon} \approx \alpha N_e \approx \frac{N_e}{137}$$

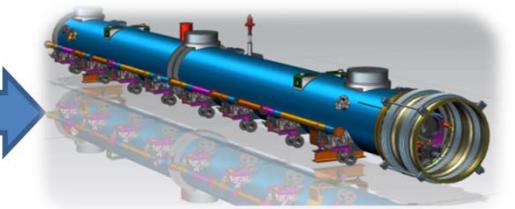
FELs $\sim 10^{25}$

Stimulated Emission from a Self Bunched Beam (SASE)



$$N_{e/coop} \approx 10^6$$

$$N_{ph}^{stim} \approx 10^6 N_{ph}^{spon}$$

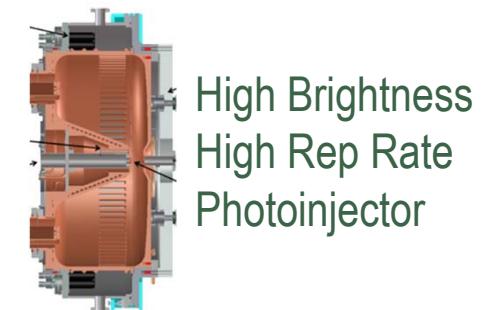


$$\mathcal{E}_x \propto \frac{E_e^2}{N_{dipole}^3}, \quad N_{MBA} \approx 2,3 \rightarrow 7,9$$

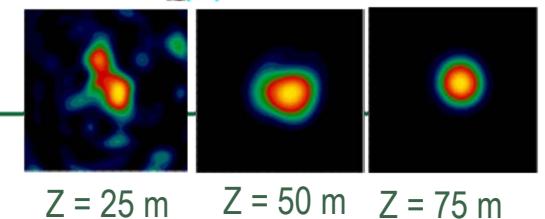


Diffraction Limit

$$\mathcal{E}_{Lx} \mathcal{E}_{Ly} \rightarrow \left(\frac{\lambda}{2}\right)^2$$



$$B_{peak} = \frac{B_{ave}}{\tau_e \cdot f_{repre}} \xrightarrow{FEL} 10^{10} B_{ave}$$

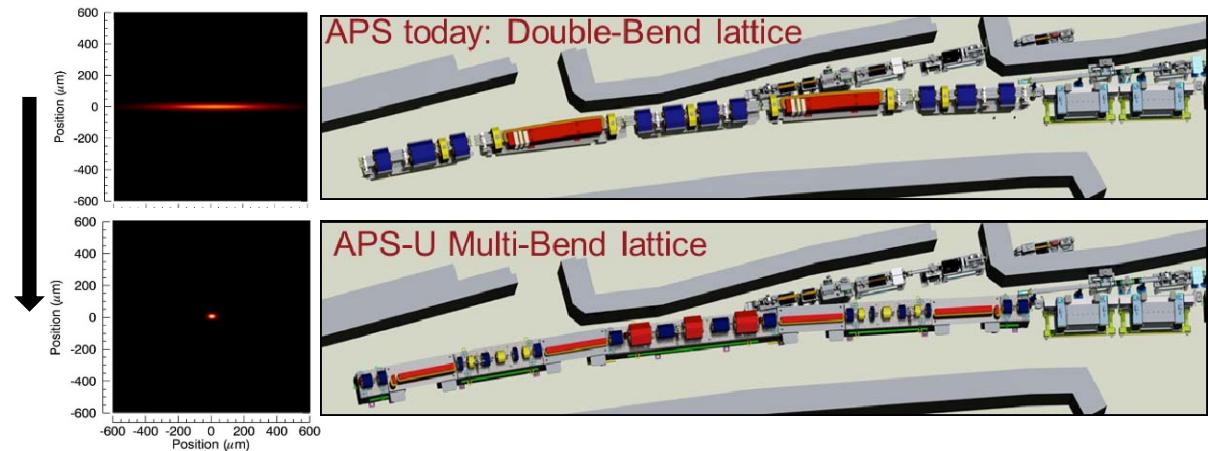


Advanced Photon Source Upgrade (APS-U) at ANL

Project Developments:

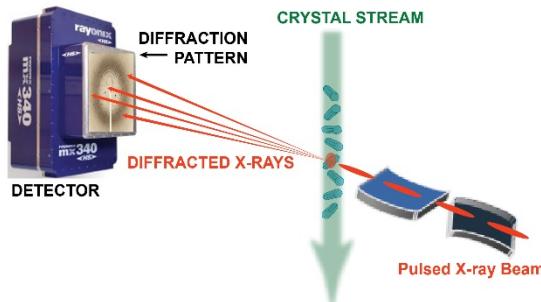
- Design optimized to provide penetrating high-energy x-rays
- MBA-7 lattice incorporating reverse bends to reduce emittance from 67pm to 41pm
- Beamlime proposal selection and roadmap complete
- Technical prototypes well along; Preliminary Design Report underway; ready for next step

APS-U MBA-7 lattice uses 7 bending magnets/sector (was 2)



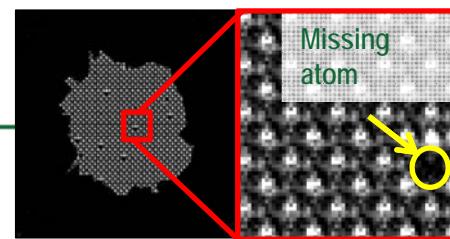
Small-Beam Scattering & Spectroscopy

- Nanometer imaging with chemical and structural contrast; few-atom sensitivity
- Room-temperature, serial, single-pulse pink beam macromolecular crystallography



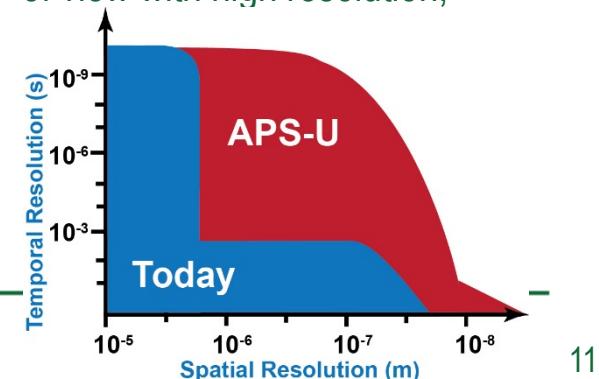
Coherent Scattering & Imaging

- Highest possible spatial resolution: 3D visualization; imaging of defects, disordered heterogeneous materials
- XPCS to probe continuous processes from nsec onward, opening up 5 orders of magnitude in time inaccessible today,



Resolution @ Speed

- Mapping all of the critical atoms in a cubic millimeter
- Detecting and following rare events
- Multiscale imaging: enormous fields of view with high resolution;

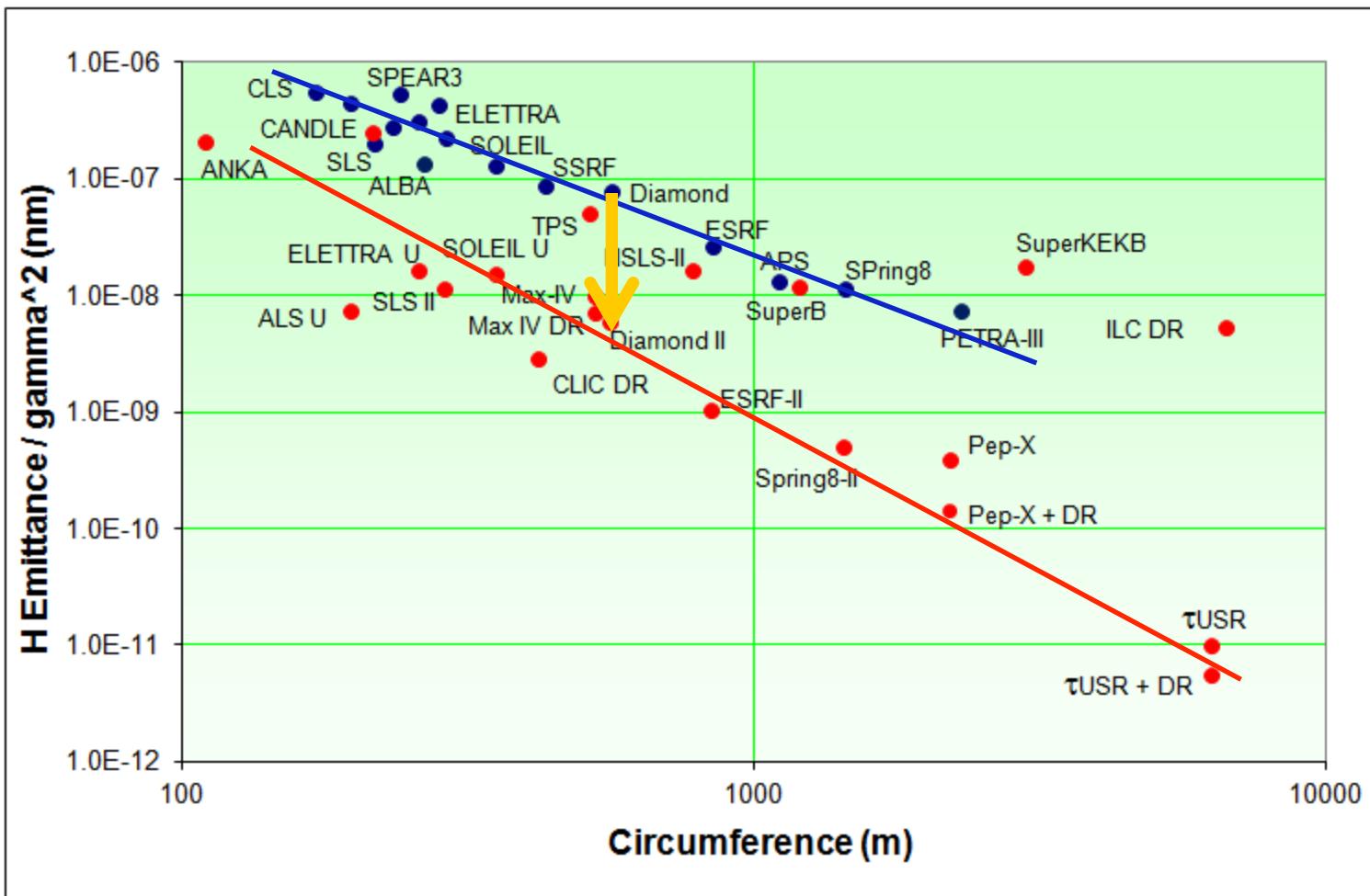


Ring Based Light Sources



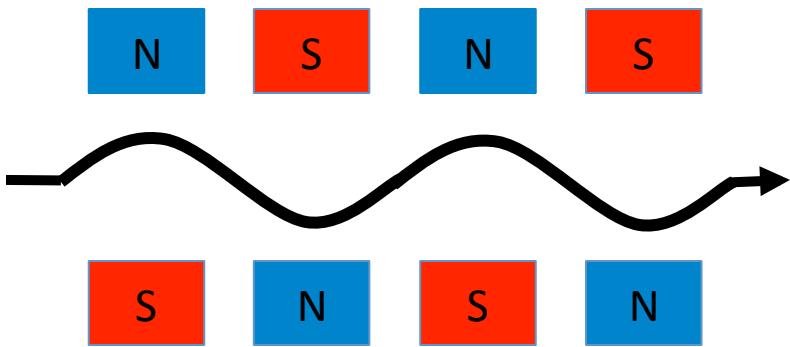
Start a new trend:
MBA

Survey of low emittance lattices



Synchrotron Radiation

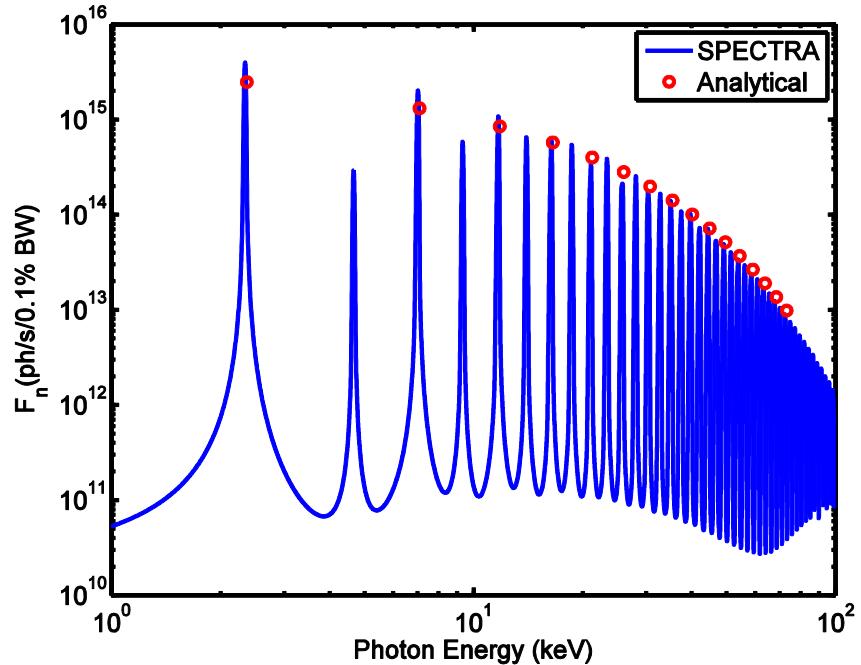
Electron beam in undulator



n^{th} harmonic wavelength:

$$\lambda_n = \frac{\lambda_u}{2n\gamma^2} \left(1 + \frac{K^2}{2}\right)$$

Photon spectral flux in 0.1% BW



$$F_n = \frac{\pi}{2} \alpha N_u Q_n \left(\frac{n K^2}{4 + 2 K^2} \right) \frac{\Delta\omega I}{\omega e}$$

Spectral Brightness

Brightness of electron beam radiating at n^{th} (odd) harmonics in a undulator is given by

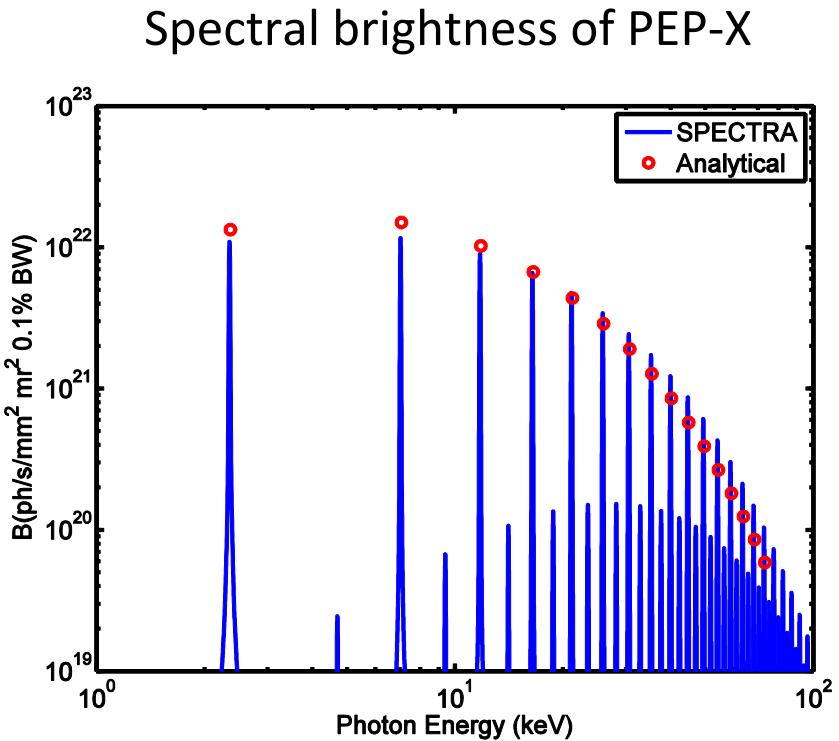
$$B_n = F_n / (4\pi^2 \sum_x \sum_x' \sum_y \sum_y')$$

If the electron beam phase space is matched to those of photon's, the brightness becomes optimized

$$B_n = \frac{F_n}{4\pi^2 (\varepsilon_x + \lambda_n / 4\pi)(\varepsilon_y + \lambda_n / 4\pi)}$$

Finally, even for zero emittances, there is **an ultimate limit** for the brightness

$$B_n = \frac{4F_n}{\lambda_n^2}$$



A diffraction limited ring at 1 angstrom or 8 pm-rad emittance

Energy Spread and Emittance

Balance between the quantum excitation and radiation damping results in an equilibrium Gaussian distribution with relative energy spread σ_δ and horizontal emittance ε_x :

$$\sigma_\delta^2 = \frac{\tau_s}{2E_0^2} \langle \dot{N}_{ph} \langle u^2 \rangle_s \rangle_s = C_q \frac{\gamma^2}{J_s} \frac{\langle 1/\rho^3 \rangle_s}{\langle 1/\rho^2 \rangle_s},$$

$$\varepsilon_x = \frac{\tau_x}{4E_0^2} \langle \dot{N}_{ph} \langle u^2 \rangle H_x \rangle_s = C_q \frac{\gamma^2}{J_x} \frac{\langle \mathcal{H}_x / \rho^3 \rangle_s}{\langle 1/\rho^2 \rangle_s},$$

where

and

$$C_q = \frac{55}{32\sqrt{3}} \frac{\hbar}{mc}, \quad \mathcal{H}_x = \beta_x \eta_{px}^2 + 2\alpha_x \eta_x \eta_{px} + \gamma_x \eta_x^2$$

- The quantum constant $C_q = 3.8319 \times 10^{-13}$ m for electron
- γ is the Lorentz factor (energy)

Minimization of Emittance

For an electron ring without damping wiggles, the horizontal emittance is given by

$$\varepsilon_0 = F_c \frac{C_q \gamma^2}{J_x} \theta^3$$

where F_c is a form factor determined by choice of cell and θ is bending angle of dipole magnet in cell. In general, stronger focusing makes F_c smaller. Often there is a minimum achievable value of F_c for any a given type of cell. For example, we have

$$F_{min}^{DBA} = \frac{1}{4\sqrt{15}}$$

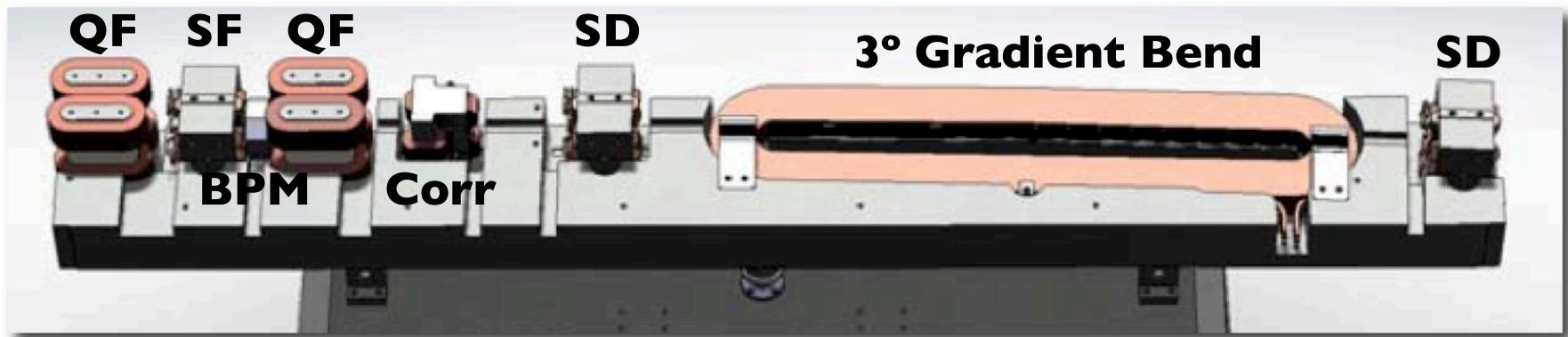
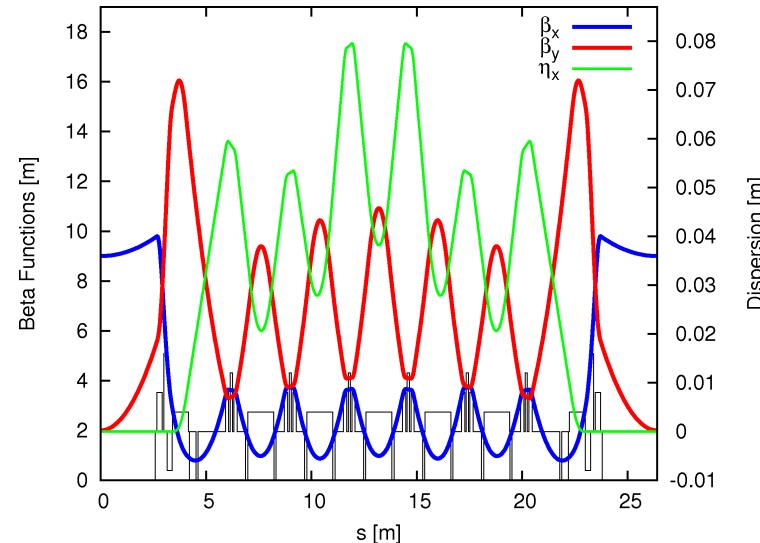
$$F_{min}^{TME} = \frac{1}{12\sqrt{15}}$$

There is a factor of **three** between the minimum values of DBA and TME cells. That's the price paid for an achromat, namely fixing the dispersion and its slope at one end of dipole.

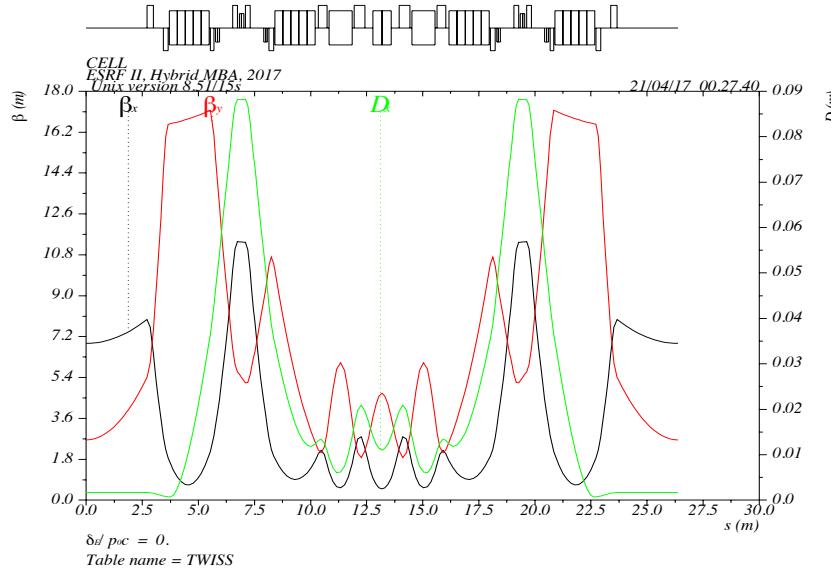
MAX-IV Synchrotron Light Source

Innovation:

- 7 bend achromat
- Combine function dipoles
- Compact magnets
- Resonance minimization
- OPA optimization code
- Harmonic Sextupoels
- Octupoles



ESRF-II Synchrotron Light Source

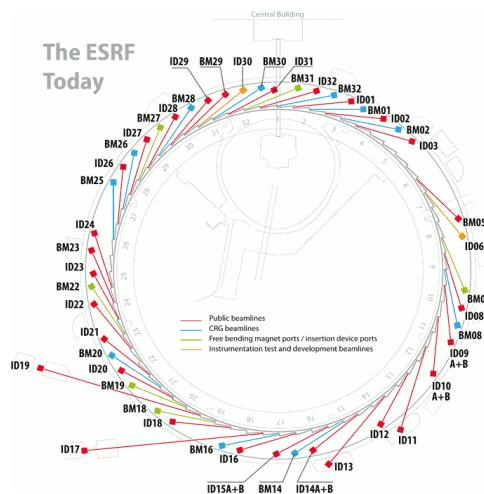


Innovations:

- Hybrid 7 bend achromat
 - Dispersion bump
 - “-l” paired sextupoles
 - Variation dipoles

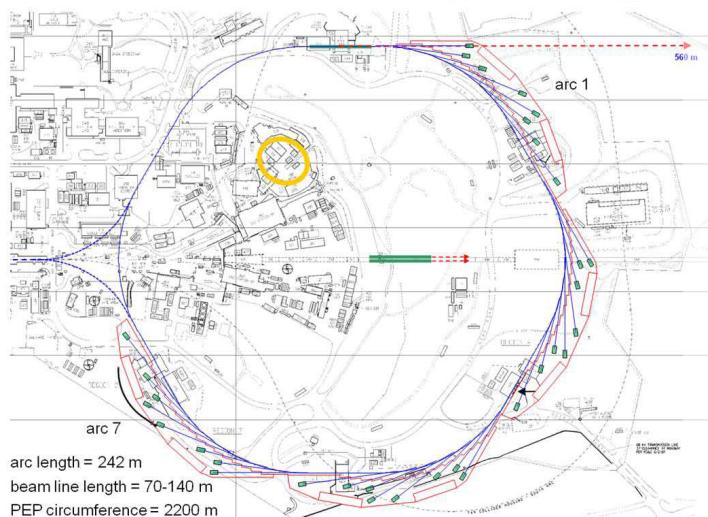
An approximated symmetry:

$$\mu_x \sim (2+3/8) \times 360^\circ, \mu_y \sim (1-1/8) \times 360^\circ$$



PEP-X Layout & Parameters

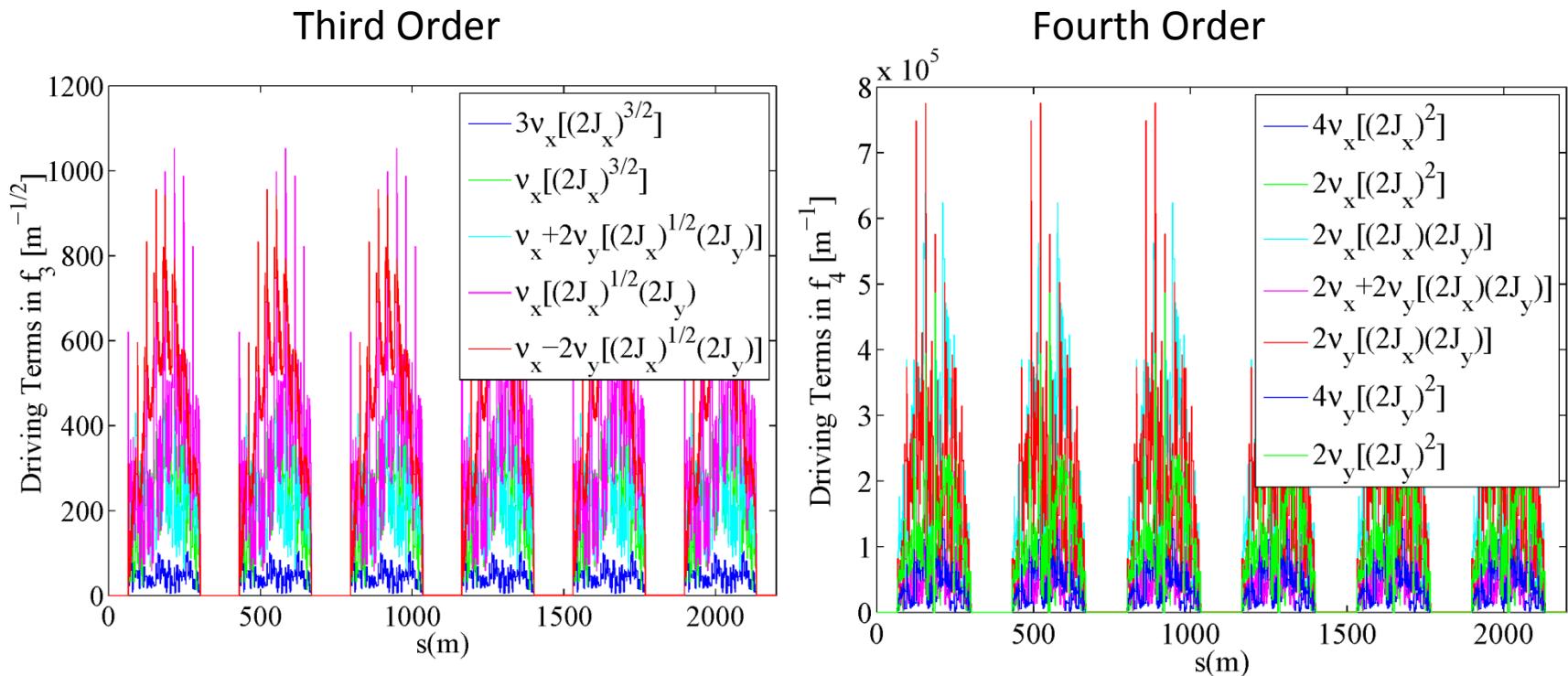
An ultimate storage ring



Energy, GeV	4.5
Circumference, m	2199.32
Natural emittance, pm	11
Beam current, mA	200
Emittance at 200 mA, x/y, pm	12 / 12
Tunes, x/y/s	113.23 / 65.14/0.007
Bunch length, mm	3.1
Energy spread	1.25×10^{-3}
Energy loss per turn, MeV	2.95
RF voltage, MV	8.3
RF harmonic number	3492
Length of ID straight, m	5.0
Wiggler length, m	90.0
Beta at ID center, x/y, m	4.92 / 0.80
Touschek lifetime, hour	10
Dynamic aperture , mm	10

To be Built with 4th-order geometrical achromats in the PEP tunnel.

Cancellation of All Geometric 3rd and 4th Resonances Driven by Strong Sextupoles except $2v_x - 2v_y$



K.L. Brown & R.V. Serfranckx

Nucl. Inst. Meth., A258:480–502, 1987

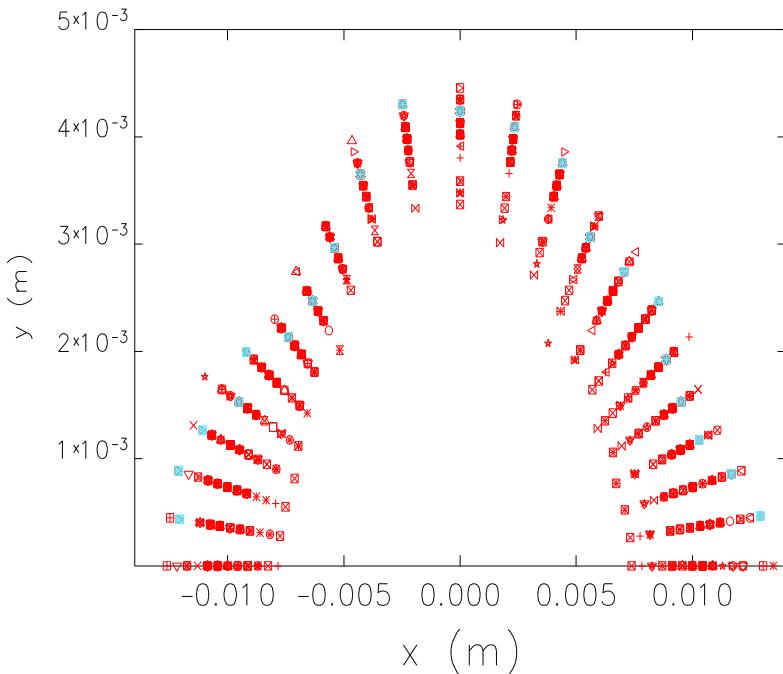
Cell phase advances: $\mu_x = (2+1/8) \times 360^\circ$, $\mu_y = (1+1/8) \times 360^\circ$ (8 cells for cancellation)

Yunhai Cai

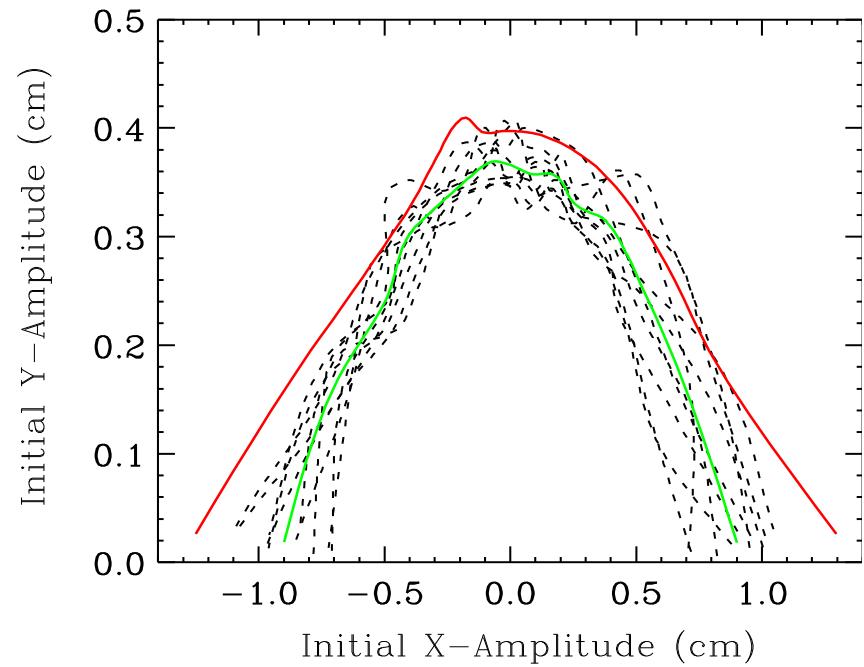
Nucl. Inst. Meth., A645:168–174, 2011.

Dynamic Aperture

ELEGANT Tracking



LEGO Tracking



Presentations for Magnetic Elements

Lie factors

$$M^{-1} e^{:f_3:} e^{:f_4:} \dots$$

Dragt-Finn

- engine in MARYLIE (A. Dragt)
- violates symplecticity when evaluates

Taylor map

$$M^n(z)$$

TPSA

- engine in TRANSPORT, MAD, COSY (K. Brown and M. Berz), simple R-matrix
- but high-order one violates

Symplectic Integrator

$$\prod_{i=1}^n e^{-\frac{|H_0|}{2}\Delta s} e^{-|H_1|\Delta s} e^{-\frac{|H_0|}{2}\Delta s}$$

- engine in TEAPOT, SAD, TRACY, **LEGO**, PTC (E. Forest, R. Ruth, and K. Hirata)
- preserves symplecticity
- simple and based on several known solutions
- emphasis on numerical process

Lie Method Bases Analysis and Tracking Code

Element

Hamiltonian
Lie form
 $e^{(-:H:s)}$

Similarity
transformation
CBH theorem

Accelerator

$A^{-1}e^{(-:H:)A}$
 $e^{(:f_2:) \dots e^{(:f_n:)} e^{(-:H:)}}$

Symplectic
Integrator

Symplecticity

Factorization
Normal form

Solvable
Solution (Map)

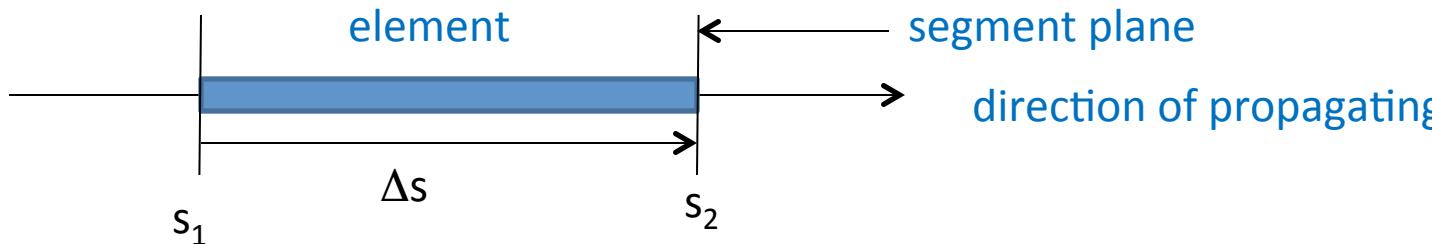
Tracking map

Taylor map

Tracking phase vector

Dynamic aperture?

Concept of Transfer Map

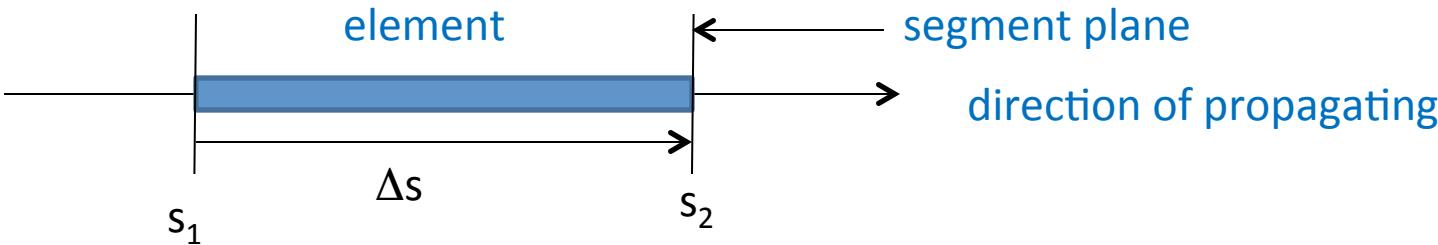


$$z(s_1) = \begin{pmatrix} x \\ p_x \\ y \\ p_y \\ \delta \\ \ell \end{pmatrix}_{|s_1} \quad \mathbf{M}_{1 \rightarrow 2} \quad \begin{pmatrix} x \\ p_x \\ y \\ p_y \\ \delta \\ \ell \end{pmatrix}_{|s_2} = z(s_2)$$
$$z(s_2) = \mathbf{M}_{1 \rightarrow 2}(z(s_1)).$$

↑
abbreviated map notation

A set (six) of functions of canonical coordinates. It's called symplectic if its Jacob is symplectic.

Exponential Lie Operator



For any function $f(s)$, we have the Taylor expansion

$$f(s_2) = \sum_{n=0}^{\infty} \frac{\Delta s^n}{n!} \frac{d^n f}{ds^n} \Big|_{s_1} \equiv e^{\frac{\Delta s}{ds} \frac{d}{ds}} f(s) \Big|_{s_1} \quad \leftarrow \text{a symbolic notation}$$

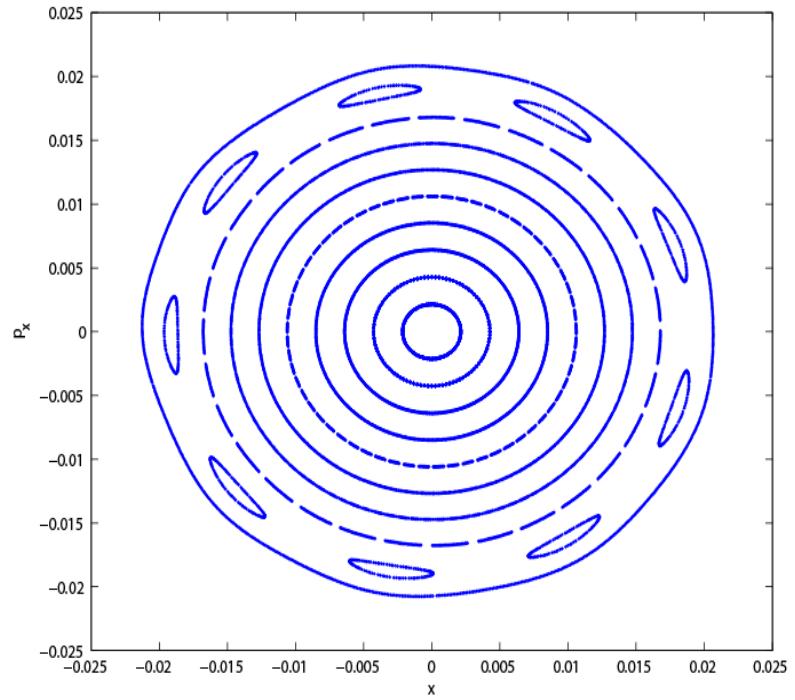
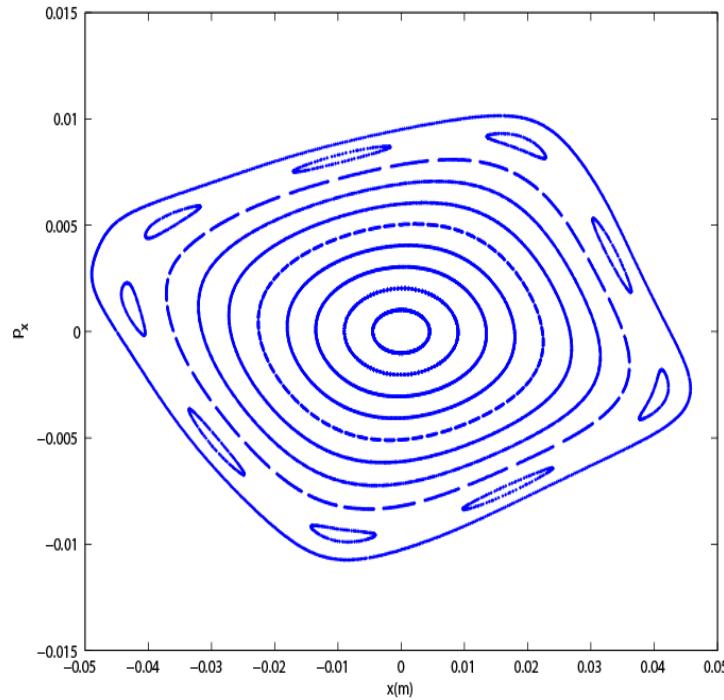
In particular, if there is no explicit dependent of s in the function $f(s)$, namely $f(s) = f(x(s), p_x(s), \dots)$, we have

$$\frac{df}{ds} = -[H, f] \equiv -:H:f, \quad \leftarrow \text{another symbolic notation}$$

Used Hamiltonian equation and the definition of the Poisson bracket.
Combining these symbolic notations, we have the exponential Lie operator

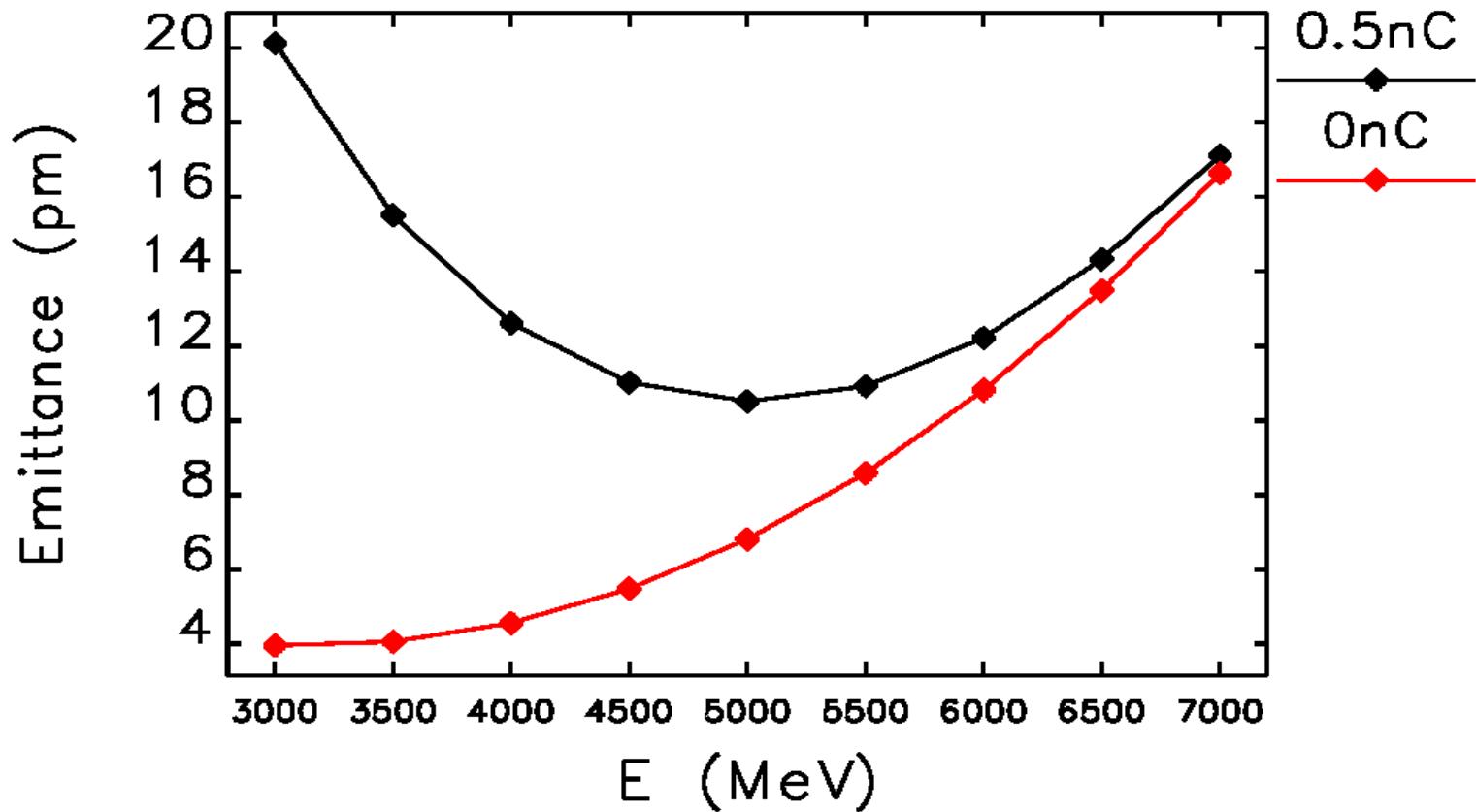
$$f(s_2) = e^{-\Delta s :H:} f(s) \Big|_{s_1}$$

Nonlinear Normal Form



Physical coordinates \longrightarrow Normalized coordinates
Transformation approximated by a 10th order Taylor map

Intra-Beam Scattering



Touschek Lifetime

When a pair of electrons go through a hard scattering, their momentum changes are so large that they are outside the RF bucket or the momentum aperture. This process results in a finite lifetime of a bunched beam. The lifetime is given by

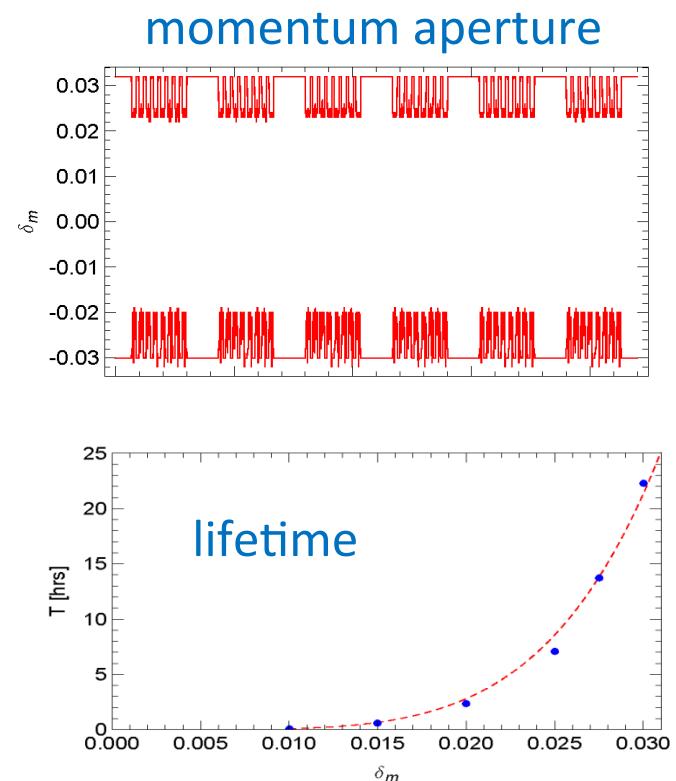
$$\frac{I}{T} = \frac{r_e^2 c N_b}{8\sqrt{\pi}\gamma^4 \varepsilon_x \varepsilon_y \sigma_z \sigma_\delta} \langle \sigma_H F(\delta_m) \rangle,$$

with

$$F(\delta_m) = \int_{\delta_m^2}^{\infty} \frac{d\tau}{\tau^{3/2}} e^{-\tau B_+} I_0(\tau B_-) \left[\frac{\tau}{\delta_m^2} - 1 - \frac{1}{2} \ln\left(\frac{\tau}{\delta_m^2}\right) \right],$$

$$B_{\pm} = \frac{1}{2\gamma^2} \left| \frac{\beta_x (\beta_x \varepsilon_x + \eta_x^2 \sigma_\delta^2)}{\varepsilon_x (\beta_x \varepsilon_x + \beta_x H_x \sigma_\delta^2)} \pm \frac{\beta_y}{\varepsilon_y} \right|,$$

where d_m is the momentum acceptance.

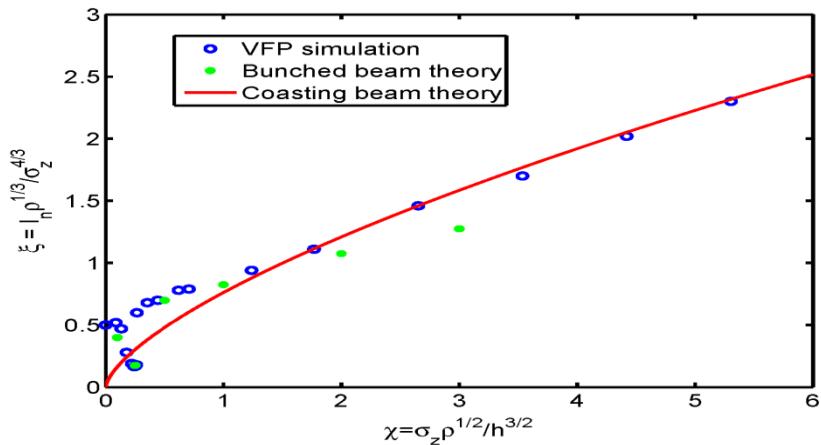


Threshold of Instability Driven by CSR

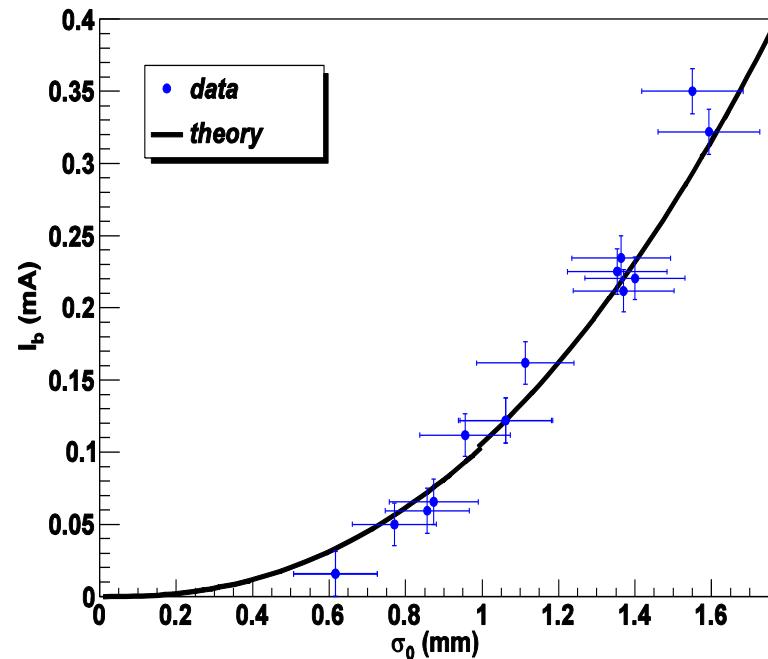
Based on the bunched beam theory,
the threshold can be written as

$$\sigma_z^{7/3} = \frac{c^2 Z_0}{8\pi^2 \xi^{\text{th}}(\chi)} I_b^{\text{th}} \rho^{1/3} / (V_{rf} \cos \varphi_s f_{rf} f_{rev})$$

where ξ^{th} is given by



Measured bursting threshold at ANKA
See M.Klein et al. PAC09, 4761 (2009)



(courtesy of M. Klein, $\xi^{\text{th}}=0.5$ used.)

My talk, IPAC 2011, San Sebastian, Spain

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- Francesco Sette, SLAC 50th Anniversary talk, 2012
- Persis Drell, BESAC talk, 2017