

The Abdus Salam International Centre for Theoretical Physics School on Synchrotron Light Sources and their Applications

(1) Fundamentals of **Synchrotron Radiation** from Storage Rings (2) Fundamentals of X-ray **Interaction with Matter** (3) Bonus: X-ray Free Electron Lasers



Giorgio Margaritondo Ecole Polytechnique Fédérale de Lausanne (EPFL) and Istituto Italiano di Tecnologia (IIT)

# Synchrotron radiation: the biggest research network in the world!

France



Tens of thousands of researchers Over 60 active centers, more underway Research articles: over 225,000 Expenditures of over 100 billion dollars A production factory of Nobel prizes: Agre, Baker, Boyer, Kornberg, Mackinnon, Ramakrishnan, Steitz, Yonath, Walker...







ALS, USA



# Synchrotrons notably emit <u>x-rays</u>, very important because of what their wavelengths and photon energies can investigate





...where radiation is emitted by electrons that circulate in an <u>accelerator</u> (a "storage ring") at almost the speed light

Our discovery of how relativity produces xrays starts at a leading synchrotron facility: Elettra in Trieste, Italy Before seeing how, <u>A REASONABLE QUESTION</u>: why do we use big, costly accelerators instead of getting x-rays, as radio waves, from electrons oscillating in an antenna?

...indeed, oscillating electrons are <u>accelerated electric</u> <u>charges</u>, thus they do <u>emit electromagnetic waves</u>

...and the electron mass is small: this enhances the acceleration and the emission



acceleration and the emission however, antennas are good for producing <u>long-wavelength</u> radio waves, but not <u>short-wavelength</u> x-rays! inducing the oscillations cannot reach the required high frequencies (say, 10<sup>18</sup> hertz) To get x-rays, we use another strategy, combining oscillating electrons with two relativistic effects that shorten the wavelengths!



...great! But how can e get that complex electron motion?

the undulator causes transverse oscillations that enable the electron to emit radiation

....whose

wavelength is related to the

period *L*, but

is not equal to L



Then add an "undulator": a periodic series of magnets, period L

relativistic electron,

A good  $v \approx c$ solution: for the longitudinal relativistic motion, we can use a storage ring, with a system (not shown) of magnets and electric devices that forces electrons to circulate in vacuum at almost the speed of light

# Why not? To understand, you must think like an electron!

From its own point of view, the electron "sees" the undulator arriving with velocity  $-v \approx -c$ 

...so, the electron "sees" the undulator period L shrunk to  $\approx L/\gamma$ 

...and in relativity a moving object is subject to the famous "Lorentz contraction": as we have seen, its length appears shortened by  $\approx \gamma$ 

this equals the emitted wavelength as "seen" by the electron,  $\lambda_e = L/\gamma$ 

...but  $\lambda_e$  is <u>not</u> the wavelength seen in the laboratory! Why not? We already know the answer: the electron motion also causes the <u>Doppler shift</u>, further reducing the wavelength by  $\approx 2\gamma$ 

So, short wavelengths are produced by <u>two</u> combined relativistic effects:

 $\leftarrow L \rightarrow \qquad \text{large}$   $\leftarrow L \rightarrow \qquad \text{First effect:} \\ \text{Lorentz contraction} \\ \approx (L/\gamma)/(2\gamma) - M - \\ \text{Second: Doppler shift} \qquad \qquad \mathcal{X} \approx L/(2\gamma^2)$ 

Let  $2\gamma^2 \rightarrow \text{short } \lambda$ Example:  $L = 1 \text{ cm}, \gamma = 5000$  $\lambda \approx 2 \times 10^{-10} \text{ m}$ <u>x-rays!!!</u>

high energy  $\rightarrow$ 

NOTE: in relativity,

 $\gamma = \text{energy}/(m_0 c^2)$ :



large flux, small area, small divergence

Do synchrotron sources reach <u>high brightness</u>? YES INDEED: over one million billion times more than conventional x-ray sources! How? Thanks to four factors:

We shall see that <u>relativity</u> sharply reduces the <u>angular divergence</u>
 And that <u>relativity</u> also boosts the <u>emitted power</u>

- 3. Electrons in a storage ring under vacuum can handle more emitted power than those in a solid, since the solid can be damaged
- 4. The electrons travel in the ring in bunches (we shall see why), along slightly different paths; the source <u>size</u> is the transverse <u>cross section</u> of the bunch, determined by all the paths and kept small by very effective controls

### Relativity at work: extreme angular collimation

... but in  $\mathcal{R}_{\ell}$  it shrinks to a small forward cone, as the sound of a moving train but much narrower

... in the electron frame  $\mathcal{R}_{e}$ , extreme case the angular range of the emission is broad, They rade emitted in rection in  $\mathcal{R}_{\rho}$ waves from an antenna

V≈ Č

 $\mathcal{R}_{o}$ 

In  $\mathcal{R}_{c}$ , the electron motion with relativistic speed v "projects ahead" the emission: the forward wave velocity is  $\approx v$  and, since  $\theta$  is small:  $\theta \approx \sin \theta = \sqrt{c^2 - v^2}/c = \sqrt{1 - v^2/c^2}$ 

wave velocity in  $\mathcal{R}_{e}$ : magnitude c, zero longitudinal component so, from  $\mathcal{R}_e$  to  $\mathcal{R}_{\mathcal{L}}$  the velocity vector <u>rotates</u>

Relativity requires the magnitude c to be invariant

 $\theta \approx 1/\gamma$  Spread  $\approx 1/\gamma$ : milliradians!!!

### Relativity at work again: huge <u>emitted power</u>



<u>"Larmor law"</u>: the emitted power is proportional to  $a_e^2$ , the square of the transverse acceleration in  $\mathcal{R}_e$ 

If v = zero,  $a_e = a_L$ , the transverse acceleration in  $\mathcal{R}_{\mathcal{L}}$  – and the power is proportional to  $a_L^2$  electron a<sub>e</sub> emission

oscillating

but, if  $v \neq zero$ : going from  $\mathcal{R}_e$  to  $\mathcal{R}_{\mathcal{L}}$  the time is multiplied by  $\gamma$ while the <u>transverse</u> coordinate is invariant; the acceleration = coordinate/time<sup>2</sup> is divided by  $\gamma^2$ :  $a_{\rm L} = a_{\rm e}/\gamma^2$ , and  $a_{\rm e} = \gamma^2 a_{\rm L}$ 

> ...the power is proportional to  $a_e^2 = (\gamma^2 a_L)^2$ , thus to  $\gamma^4 = (\text{energy})^4 / (m_o c^2)^4$

The emission increases as the 4<sup>th</sup> power of the electron energy, to <u>very high levels</u>

...and decreases as  $1/m_0^4$ : electrons emit a lot, protons much less

Let us find more about relativistic electrons in an undulator: they behave as very collimated flashlights, causing their emitted wavelength spectrum



Bandwidth: going through the *N* undulator periods, the electron emits a wave with *N* wavelengths, of length  $N\lambda_L$ . Pulse duration:  $\Delta t_L = N\lambda_L/c$ . Fourier:  $\Delta v_L = 1/\Delta t_L = c/(N\lambda_L)$ .  $\lambda_L = c/v_L$  so  $\Delta \lambda_L/\lambda_L = I\Delta v_L/v_L I = [c/(N\lambda_L)]/(c/\lambda_L) = 1/N$ 

## Other wonderful properties of undulators:

(1) They can emit different wavelengths; (2) their angular spread is very small;
(3) they have very high brightness -- all such properties that can be explained with simple approaches, for example:

what happens if we increase the magnetic field strength *B* by changing the magnet gaps?



A stronger magnetic field *B* increases the transverse electron oscillations and their transverse speed, proportional to *B* 

The magnetic (Lorentz) force of the undulator *B*-field on the electrons does not do work and cannot change the kinetic energy, so the longitudinal speed *v* decreases

This changes the  $\gamma$ -factor in the Doppler shift, modifying  $\lambda_{L}$  from  $L/(2\gamma^{2})$  to  $\lambda_{L} = [L/(2\gamma^{2})](1 + \text{constant} \times B^{2})$  We can <u>tune</u> the wavelength!



A <u>wiggler</u>, as an undulator, is a periodic magnet array -- but its magnetic field is <u>stronger</u> and causes <u>larger transverse</u> <u>oscillations</u> of the electrons:



The third type of synchrotron sources: <u>bending</u> <u>magnets</u>, the dipoles that force the electrons to circulate in the storage ring



1E+12

Photon Energy ( KeV)

This explains the famous synchrotron radiation spectrum of bending magnets: the log-log plot of a peak!

Note -- bending magnets emit very short x-ray wavelengths: why?

...because of the same effects present for undulators (and wigglers): Lorentz contraction and Doppler shift

Intuitively, the emitted wavelengths are related to the longitudinal size D of the magnet ...which in the electron frame  $\mathcal{R}_e$  is Lorentz-contracted to  $\approx D/\gamma$ 

And in the laboratory frame  $\mathcal{R}_{\mathcal{L}}$  the wavelengths are Doppler-shifted by a factor  $\approx 2\gamma$ , so they are related to  $\approx (D/\gamma)/(2\gamma) = D/(2\gamma^2)$  The  $2\gamma^2$  factor again!

 $-v \approx -c$ 

### The time structure of synchrotron radiation The cause: electrons travel around the ring in bunches -- why?

source

To keep the electrons in the ring, the energy they lose by emitting synchrotron radiation must be restored by the periodic force of an "RF cavity": but this only works for <u>bunched</u> electrons passing through the cavity in synchrony with the force

radiofrequency (RF) cavity

at every turn, each electron bunch sends a short (nanoseconds to picoseconds) pulse of radiation in each beamline

62

detector

time

Another key synchrotron property: polarization Consider an electron traveling through an undulator or a wiggler:

### [SIDE VIEW]



undulator axis correspond to electric field perturbations in the <u>horizontal plane</u>: they are <u>linearly polarized</u>



...likewise, on-axis waves from bending magnets are linearly polarized in the horizontal plane and special (elliptical) wigglers/undulators can produce intense elliptically polarized radiation



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# Using synchrotron radiation: different interactions of x-rays with matter lead to many different experimental techniques



...let us focus now on the interactions between x-rays and solids that are most important for synchrotron applications



First, the interactions used for <u>imaging</u>, the first application of x-rays, and still the most common Originally, x-ray imaging was based on <u>absorption</u>. But synchrotron sources have a property that now leads to novel and very powerful imaging techniques: let us discover it!





In everyday life, we occasionally see wave-like effects like oil-film interference... but they are rare

Why? Because to see them the radiation source must have "coherence" = "what allows radiation to produce visible wave-like effects like interference and diffraction"

X-rays from synchrotron sources have high coherence, which is now exploited for a revolutionary new radiology!

## A simple description of coherence:



a point source emitting only <u>one</u> wavelength  $\lambda$  always produces a visible pinhole diffraction pattern: it has <u>full coherence</u>

More realistic sources reveal TWO kinds of coherence: "time" and "spatial"



different wavelengths produce different patterns...

### Multiple wavelengths: longitudinal (time) coherence

superposition blurs the fringes

### when is the fringe pattern still visible?

Spacing of adjacent fringes (from elementary optics):

 $= \mathbf{x} \approx (H|\delta)\lambda;$ if  $\lambda$  is replaced by a band  $\Delta\lambda$ ,  $\mathbf{x}$  is "blurred" to:  $\Delta \mathbf{x} \approx (H|\delta)\Delta\lambda$ 

Condition to see the pattern:

 $\bigcirc$ 

 $\Delta x < x \rightarrow \Delta \lambda / \lambda < 1 \text{ (time coherence)}$ 

 $\begin{array}{l} \mbox{defining the "coherence} \\ \underline{\mbox{length}"} \mbox{ as } L_{\rm c} = \lambda^2 / \Delta \lambda \ , \\ \mbox{time coherence} \\ \mbox{requires } L_{\rm c} > \lambda \end{array}$ 



Each point of an <u>extended source</u> produces a diffraction pattern  $\rightarrow$  <u>blurring</u>

when is a pattern still visible? Maximum distance between centers of patterns given by different source points  $M \approx \xi H/D$ Fringe spacing  $x \approx (H/\delta)\lambda$ Fringes can be seen if  $M \le x$ :  $\xi H/D \le (H/\delta)\lambda \rightarrow \delta \le \lambda D/\xi$ condition for spatial coherence

Another way to look at this condition: the radiation contributine  $\lambda o$  diffraction is that reaching the pinhole, emitted in the solid angle  $\approx \delta^2/D^2 \leq (\lambda D/\xi)^2/D^2 = \lambda^2/\xi^2$  — which corresponds to a fraction of the total emission

 $\approx (\lambda^2 / \xi^2) / \Omega = \frac{\lambda^2 / (\xi^2 \Omega)}{\lambda^2}$  This is the "<u>coherent power factor</u>": it is large if there is spatial coherence

Are synchrotron sources spatially coherent? YES! Their small size  $\xi$  and small angular spread  $\Omega$  give a large coherent power factor  $\lambda^2/(\xi^2 \Omega)$ Note, however:  $\lambda^2$  in this factor makes spatial coherence very difficult to obtain for the short  $\lambda$ 's of x-rays: synchrotron sources are required ...and  $\lambda^2$  is also present in the (time) <u>coherence length</u> causing a similar problem! Also note: the brightness is proportional to  $1/(\xi^2 \Omega)$ thus, the historical efforts to enhance the brightness by decreasing  $\xi$  and  $\Omega$  also boosted the spatial coherence 100 µm

Synchrotron x-ray coherence is very beneficial for imaging: it notably produce p<u>hase-</u> <u>contrast radiographs</u>, with sharp features and very small details radiograph of a single neuron: world record of spatial resolution

microvasculature

10 um

body of an ant

Phase-contrast imaging: the mechanism is complex, but we can grasp key features with a simple analogy: "seeing" a glass of wine

> we see the wine because it absorbs and/or scatters certain wavelengths and looks colored

but we also see the <u>edges</u> of the (transparent) glass because they deviate the light by refraction/scattering<sup>2</sup>

likewise, phase contrast (refraction/scattering of x-rays) can cause sharp, highly visible <u>edges</u> in synchrotron radiographs

...however, to create such edges x-rays must have a well-defined direction: this is guaranteed by the <u>spatial coherence</u> of synchrotron radiation, which implies angular collimation





Note: high lateral coherence is required for phase contrast, but high longitudinal (time) coherence is not needed

### An example of what can be done with phase contrast imaging: explaining the miracle of fireflies



Synchrotron microtomography of a firefly "lantern" [Y. L. Tsai, Y. Hwu et al, Phys. Rev. Letters **113**, 258103 (2014)]

...being able to detect even the smallest vessels, we could elucidate the incredibly effective light emission mechanism

### Microscopy with coherent x-rays: exploring the brain, neuron by neuron

SYnchrotrons for Neuroscience – an Asia-Pacific Strategic Enterprise (SARI/SSRF-China, PAL-Korea, AS-Taiwan, RIKEN/Spring8-Japan, NUS/SSLS-Singapore, ANSTO-Australia, SLRI-Thailand, SESAME-Jordan)





### Goal: mapping a human brain

Memorandum of Understanding

Synchrotrons Coordinated Imaging & High Performance Conjuding

The general formal background of the interactions of x-rays with solids:

Wave function in vacuum:

 $W_{o} \exp[i(kx - \omega t)]$ 

"PHASE"

In the solid: k changes to nk, where  $n = n_{\rm R} + in_{\rm I}$ (complex refractive index) Wave function:  $W_{\rm o} \exp[i(nkx - \omega t)]$  $= W_{\rm o} \exp[-n_{\rm I}kx] \exp[i(n_{\rm R}kx - \omega t)]$ 

Factor decreasing with the distance, corresponding to absorption

*n*<sub>R</sub>*k* determines the phase and corresponds to phase effects: refraction, diffraction, interference...

# The real and imaginary parts of the refractive index, $n_R$ and $n_I$ , are not independent $10^{-1}$

- They are <u>linked</u> by the so-called <u>"Kramers-Kroenig equations"</u>
- This explains the relations between different phenomena:
  - strong reflection corresponds to strong absorption (think about a metal-coated mirror)
  - phase and absorption features occur for the same wavelengths
     ...when "somet "something" els



...when "something" happens for absorption  $(n_l)$ , "something" else also happens for refraction  $(n_R)$  What causes the x-ray core-level absorption edges?

...consider the electron energies in an (insulating) solid



A core-level edge in an x-ray absorption spectrum reveals the presence of the corresponding element, its chemical status ...and more

In particular, the "**EXAFS**" = **E**xtended **X**-ray Absorption Fine Structure above each edge yields precious information on the local microscopic environment of the x-ray absorbing atom



### **EXAFS** mechanism:

neighbor

bsorbing

atom

The outgoing excited-electron wave and the backscattered electron wave interfere constructively or destructively depending on the distance d and backscattered on the electron wavelength, which corresponds electron wave to the electron energy and therefore to the photon energy hv

> This causes oscillations in the absorption vs. hv plots

atom wave of the excited electron

photon

From these oscillations (EXAFS), one can derive the local interatomic distance d, a very valuable piece of information





<u>Photoemission</u>, another fundamental class of <u>synchrotron techniques</u> ...photoemission explores the energies of electrons forming chemical bonds:



vacuum



The effect adds hv to the electron energy: by subtracting hv from electron energies measured in vacuum, one can derive the electron energies in the solid

**Photoelectric effect** 

# Solid-state photoemission detects valence electrons and core electrons:



captured photoelectrons

...synchrotron photoemission transformed my bookish quantum notions like core levels into tangible realities!

A key class of synchrotron techniques: <u>x-ray scattering</u> -- which reveals the electron charge distributions of microscopic structures

Electronic charge distribution,  $F(\vec{r})$ incoming x-ray k-vector,  $\vec{k}$ 

*k*' (scattered x-ray k-vector)

<u>Theory</u>: defining the scattering vector as  $\vec{s} = \vec{k}' - \vec{k}$ , the scattered wave  $W(\vec{s})$  is proportional to  $\int F(\vec{r}) \exp(i\vec{r} \cdot \vec{s}) d^3\vec{r}$ , which is the <u>Fourier</u> transform of the charge distribution F

Conversely, *F* is proportional to  $\int W(\vec{s}) \exp(-i\vec{r} \cdot \vec{s}) d^3 \vec{s}$ , the inverse Fourier transform

elementary volume Thus, we can find the electron charge distribution of a microscopic object by performing the inverse Fourier transform of scattered x-rays

### Inverse Fourier transform

detector

This strategy faces serious obstacles like the "phase problem", but leads to many powerful synchrotron techniques:



- Large-angle scattering
- Small-angle scattering
- Powder diffraction
- Crystallography
- Protein crystallography ...and more

### Small-angle and large-angle scattering



In a real experiment, the detector captures only a portion of the solid angle, i.e., only part of the scattered x-rays

Fourier transform properties: if scattered x-rays are only detected at small angles, the inverse transform gives the general shape of the object but not its fine details

So, small-angle scattering is useful for a first look at microstructures



inverse Fourier transforms



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## X-ray Free Electron Lasers (X-FELs): the New Generation of Synchrotron Radiation Sources

Storage-ring synchrotron sources have laser-like features: strong collimation, high intensity, high brightness and excellent coherence – are they lasers?

#### A visible/infrared laser:

Active medium, providing optical amplification

Two-mirror optical cavity, increasing the photon path and the optical amplification Storage-ring synchrotron radiation sources:

- NO optical amplification
- NO good mirrors for x-rays, thus NO optical cavities
- <u>They are NOT lasers</u>

But there is now a new class of laser-like synchrotron x-ray sources, the X-FELs, based on an <u>optical amplification process</u> due to the interaction of electron bunches with their emitted waves

### Very long undulator





### Why most undulators do not behave like x-FELs?



...to emit x-rays, high-energy electrons with large  $\gamma$ -values are required, whose relativistic "longitudinal mass"  $\gamma^3 m_0$  is very heavy: it takes a (relatively) long time to shift them to the "slices", so a very long undulator is required for microbunching

...plus, the microbunching period is very short (x-ray wavelengths) -- the structure is delicate, easily destroyed: the undulator and the electron beam must be extremely accurate

NOTE: for infrared FELs the  $\gamma$ -factor is smaller, the longitudinal  $\gamma$  mass much lighter and the wavelength much longer, so the above problems do not exist: that is why infrared FELs arrived several decades before the x-FELs

# General scheme of an X-FEL:

Electron bunches, progressively microbunched

ery long

undulato

LINAC (linear accelerator of electrons) Note: contrary to a visible laser, a two-mirror optical cavity cannot be used to increase the optical path and the amplification: mirrors <u>do not exist</u> for x-rays

X-ray pulses

High optical amplification must occur in <u>a single pass</u>: this requires electron bunches with very high density

## Duration and cross section of an x-FEL pulse:

A high electron density requires a very short electron bunch length *H* 



Microbunched electron bunch

Plus, a high electron density also requires a very small cross section *A* of the electron bunch and therefore of the photon pulse, producing high brightness

...causing a <u>very short</u> photon pulse  $H/v \approx H/c$  (femtoseconds or less, shorter than the synchrotron radiation pulses from storage rings)

[Note: most x-FELs are not based on storage rings but on LINACs, which can produce smaller cross sections *A*] COHERENCE of x-FELs: <u>spatial</u> excellent, <u>time</u> problematic

Why problematic? Because the waves that are amplified are emitted <u>at random</u> when the electron bunch enters the undulator (SASE = Self-Amplified Spontaneous Emission)



External source



Possible solution: "seeding" -- i.e., using the x-FEL undulator to amplify waves with high time coherence produced by an external source A complicated technology, recently realized X-ray Free Electron Lasers are now a fantastic reality, notably at ELETTRA

> **The seeded x-FEL "FERMI" (Free Electron Radiation for Multidisciplinary Investigations)**

Note: x-FELs emit femtosecond pulses of tens of gigawatts: how can we handle this tremendous concentrated power, and how can we use it?

...sent into a molecule or a nanoparticle, causes its explosion:



...but, with the ultrafast x-ray FEL pulses one can analyze the structure <u>during the explosion</u> and try to retrieve from the data the initial structure Some examples of what happens at the femtosecond time scale of an x-FEL pulse:

Fast chemical reactions



Novel micromachining techniques, etc...

A fascinating final aspect: X-ray FELs and the quantum foundations of physics

What causes the interference and diffraction of photons?



First-order Quantum Electrodynamics (QED):

 Wave effects like interference and diffraction are caused by interactions of each photon <u>only with itself</u> (indeed, they happen even when, on the average, there is only one photon in the apparatus)
 Multiple-photon effects <u>are negligible</u>
 BUT: with ultrabright "seeded" x-FELs, multi-photon <u>higher-order</u> QED effects are detected, leading to new techniques! [J. Stöhr, Synchrotron Radiation News **32**, 48 (2019)]

# Thanks to the school organizers for inviting me! ....and thank you for your attention: your future looks brighter than ever!

#### For further reading:

- Y. Hwu and G. Margaritondo: "Synchrotron Radiation and X-ray Free Electron Lasers (X-FELs) Explained to all Users, Active and Potential", J. Synchrotron Radiation 28, 1014 (2021)
- G. Margaritondo: "An Enlightening Procedure to Explain the Extreme Power of Synchrotron Radiation", J. Synchrotron Radiation **26**, 2094 (2019)
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