

MSAE E8235x – Selected Topics in Materials Science

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Overview

- In this seminar course scientists from Brookhaven National Laboratories will introduce advanced characterization and fabrication techniques deployed at BNL
- Both the underlying theory and cutting-edge applications will be covered.
- At the end of the course the participants should be able to select the instruments suitable for their particular applications, contact the instrument scientist with relevant questions, and contribute to writing competitive proposals for facility access.

Ground Rules

- Enrollment: The course is open only to graduate students. Enrollment is limited to 20 students.
- Auditing requires written permission from the Course Coordinator.
- There are no required textbooks. Course notes will be provided and weekly reading will be assigned.
- Grading will be based on weekly HW, a midterm and a final exam.
 - Midterm ~October 21
 - Final~ Dec. 17
- Both exams will be take-home exams with open book/notes.
- The exams are non-cumulative: Those who teach before the midterm contribute midterm questions.

GOAL

- This is a survey class with a very wide scope:
 - Each lecture deserves its own textbook(s) and its own semester or year-long course.
- By necessity we will have broad but so deep discussions on most topics. However, certain issues will be treated in depth and you will be asked to remember them.
- At the end of the semester all students should be familiar with the experimental techniques available at BNL/NSLS-II for advanced materials fabrication and research.

Textbooks and Reference Books

- Jens Als-Nielsen & Des McMorrow, *Elements of Modern X-ray Physics*, John Wiley & Sons (2001).
- J.D. Jackson, *Classical Electrodynamics*, Wiley (1975): Ch. 7, 9.
- J.M. Cowley, *Diffraction Physics*, North-Holland (1975).

Reference Books and Databases:

- *International Tables for Crystallography*, Kluwer Academic Publishers (1989).
- X-ray Interactions with Matter, http://henke.lbl.gov/optical_constants/
- Electromagnetic wave fields emitted by electrons, <http://www.shintakelab.com/en/enEducationalSoft.htm>

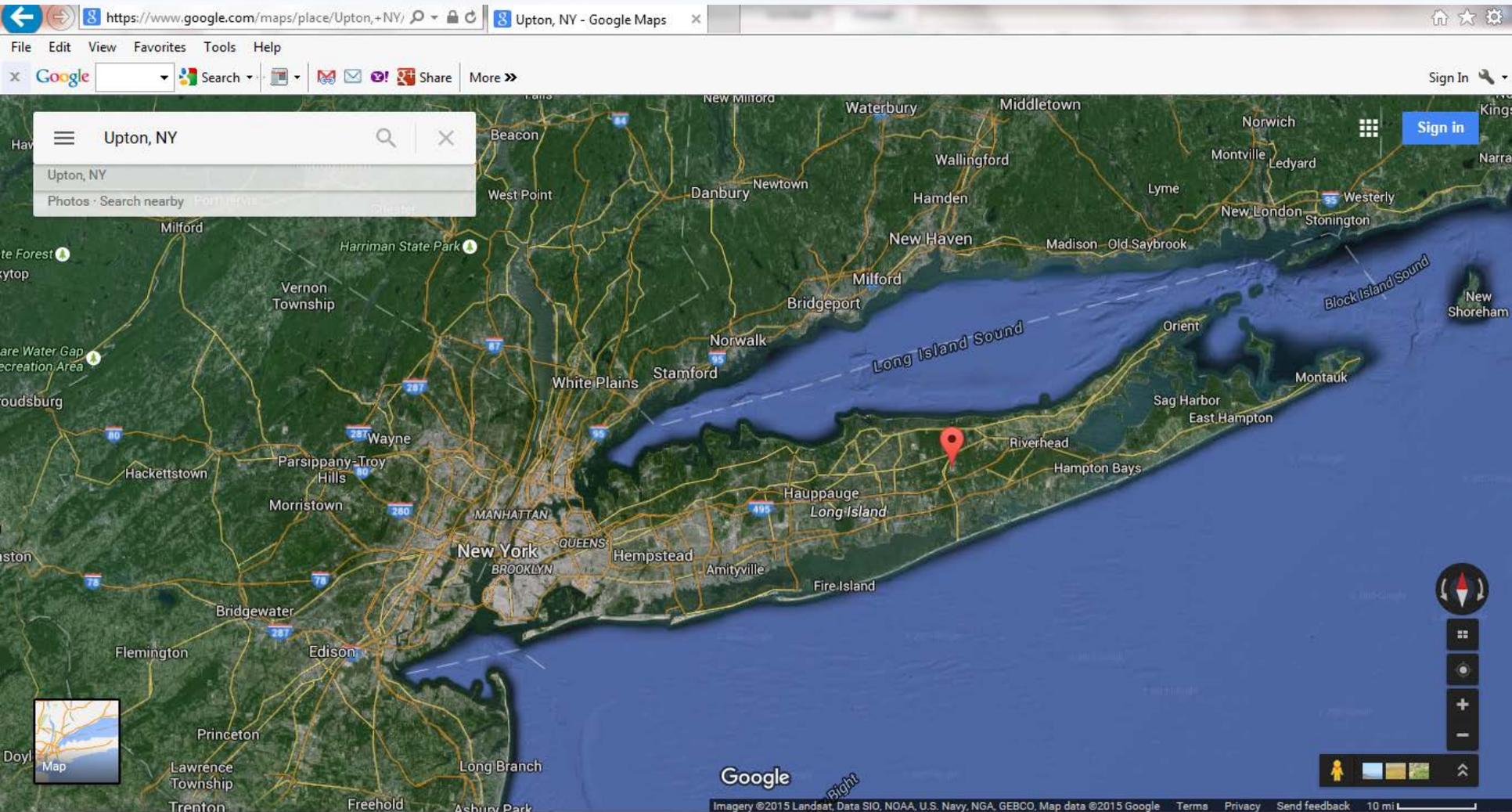
Lecture Schedule

Columbia Course 2015: MSAE E8235x, Wednesdays, 16:10 - 18:40			
Date	Lecturer	Topic	Confirmed
9/9/2015	Qun Shen	Introduction / X-ray Interactions with Matter	Y
9/16/2015	Timur Shaftan	Synchrotron Radiation	Y
9/23/2015	Eric Dooryhee	X-ray Powder Diffraction	Y
9/30/2015	Bruce Ravel	X-ray Spectroscopy	Y
10/7/2015	Sean McSweeney	Biological Crystallography	Y
10/14/2015	Anibal Bosbonboinic	X-ray Photoelectron Spectroscopy/Microscopy	Y
10/21/2015	Mid-term		
10/28/2015	Oleg Gang	Small-Angle & Wide-Angle X-ray Scattering	Y
11/4/2015	Ignace Jarrige	X-ray Emission Spectroscopy & RIXS	Y
11/11/2015	Wah-Keat Lee	X-ray Imaging	Y
11/18/2015	Eric Stach	Transmission Electron Microscopy & EELS	Y
11/25/2015	Thanksgiving Break - no class		
12/2/2015	Qun Shen	X-ray Microscopy	Y
12/9/2015	Ming Lu	Nanofabrication	Y
12/16/2015	Final Exam		

Today's Lecture

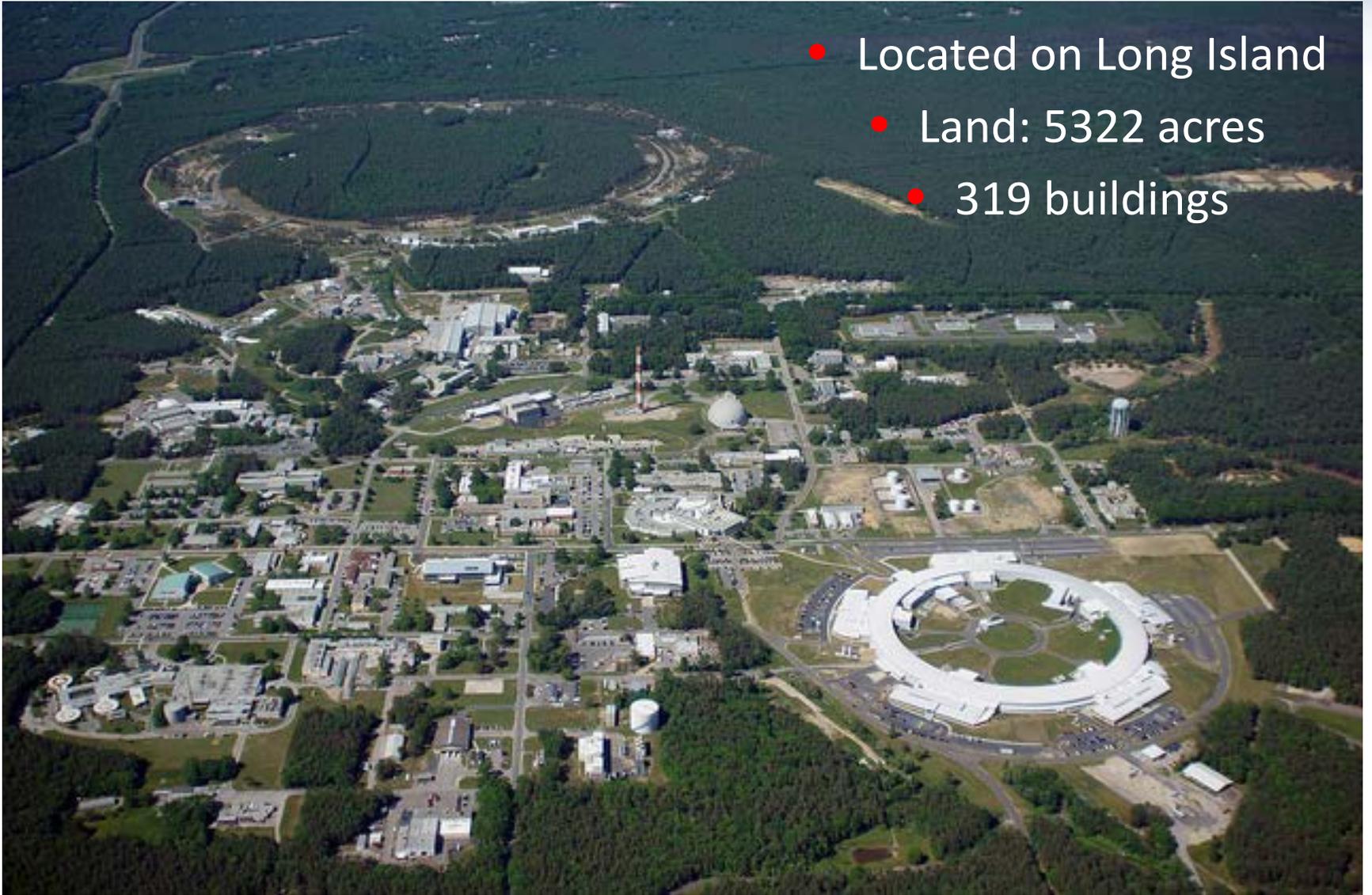
- Introduction to the Course
- About Brookhaven National Laboratory
- Overview of Synchrotron Sources and to NSLS-II
- X-ray Interactions with Matter
- Quick survey of synchrotron techniques

Brookhaven National Laboratory



Brookhaven National Laboratory

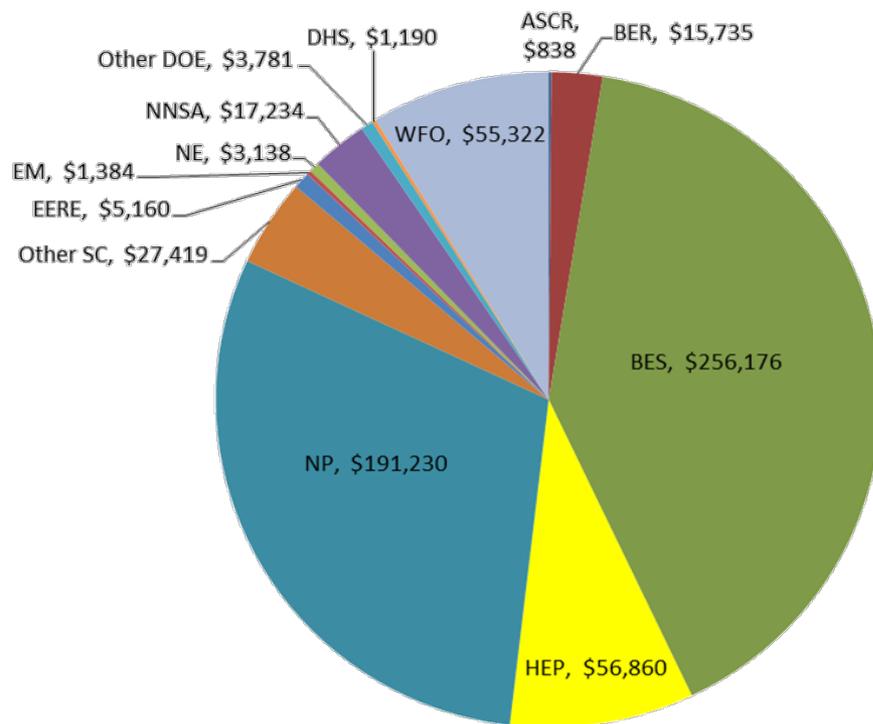
- Located on Long Island
- Land: 5322 acres
- 319 buildings



Brookhaven National Laboratory

- One of the ten DOE Office of Science, multi-program national laboratories with recognized impact on national science needs
- Employees & Staff
 - 2800 Employees
 - 26 Joint/Dual appointments
 - 137 Postdocs
 - 420 undergrad/graduate students (paid by Lab)

FY 2014 Funding by Source (\$K)



FY 2014 Total Lab Operating Costs: \$635.5 million

FY 2014 Total DOE/NNSA Costs: \$17.2 million

FY 2014 WFO (Non-DOE/Non-DHS) Costs: \$55.3million

FY 2014 WFO as % Total Lab Operating Costs: 8.7%

FY 2014 DHS Costs: \$1.2 million

Recovery Act Costed from DOE Sources in FY 2014: \$0.5 million

DOE Office of Science Graduate Student Research (SCGSR) Program

The SCGSR Program provides supplemental awards to outstanding graduate students to spend 3 to 12 months conducting part of their doctoral thesis/dissertation research at a DOE national laboratory in collaboration with a DOE laboratory scientist.

- Graduate students must apply online through the online application system.
- The application requires a research proposal and letters of support from both the graduate student's thesis advisory and the collaborating DOE laboratory scientist.
- Student's research and proposed SCGSR project must be aligned with one of the identified SCGSR priority research areas defined by the SC Program Offices and specified in the solicitation.
- Applications proposing to use an SC user facility must apply for user facility time separately.

Award Benefits:

- A monthly stipend of up to \$3,000/month for general living expenses
- Reimbursement of inbound/outbound traveling expenses to/from the DOE laboratory of up to \$2,000.

(Award payments are provided directly to the student.)

Eligibility:

- U.S. Citizen or Permanent Resident
- Qualified graduate program & Ph.D. Candidacy
- Graduate research aligned with an SCGSR priority research area
- Establishment of a collaborating DOE laboratory scientist at the time of application

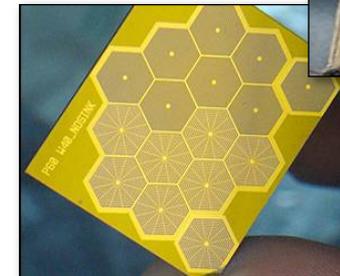
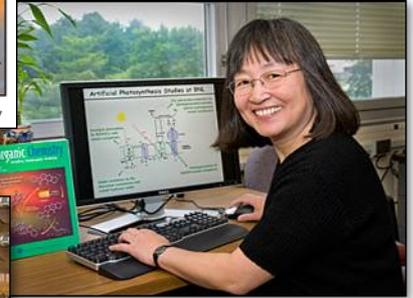
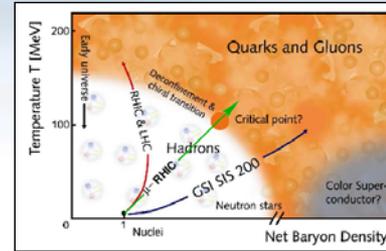
2015 Solicitation 2 – Applications Due: December 15, 2015 5:00PM ET

Full details, requirements, FAQs, and link to application at: <http://science.energy.gov/wdts/scgsr/>

Program Contact : sc.scgsr@science.doe.gov

Lab Core Capabilities

- Particle Physics
- Nuclear Physics
- Accelerator Science
- Condensed Matter Physics & Materials Science
- Chemical & Molecular Science
- Climate Change Science
- Biological Systems Science
- Applied Nuclear S&T
- Applied Materials Science & Eng.
- Chemical Engineering
- Systems Engineering and Integration
- Large Scale User Facilities/Advanced Instrumentation



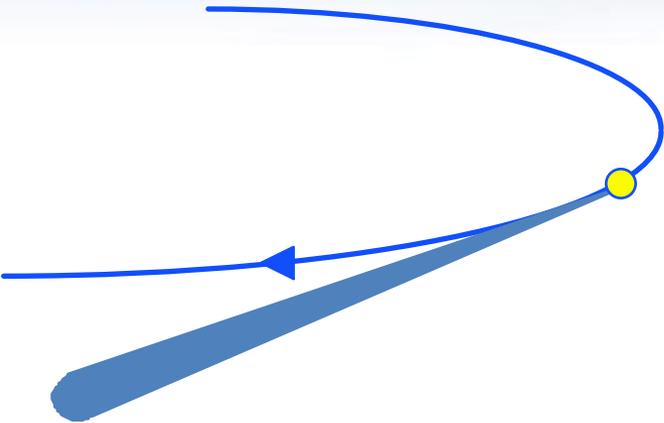
NSLS-II and CFN

- NSLS-II is the newest & most advanced synchrotron in the world; It will enable world-leading programs in imaging and dynamics with unprecedented resolution, providing impact in condensed matter physics, materials physics, chemistry and life sciences
- The CFN is one of the five Nanoscale Science Research Centers created by the Department of Energy to investigate, understand, and exploit the unique characteristics of materials and phenomena at the nanoscale
- SYNERGY: colocation of the CFN and the NSLS-II at Brookhaven allows integrated suites of instruments for multi-scale in-situ & operando research across multiple techniques



Synchrotron Light Source

T. Shaftan's Lecture 9/16/2015



- Particles called electrons are accelerated to extremely high speeds, injected in the synchrotron ring to move in a large circle.
- As the electrons pass through magnets around the ring, they lose energy in the form of light, emitted as a narrow pencil directed forward.

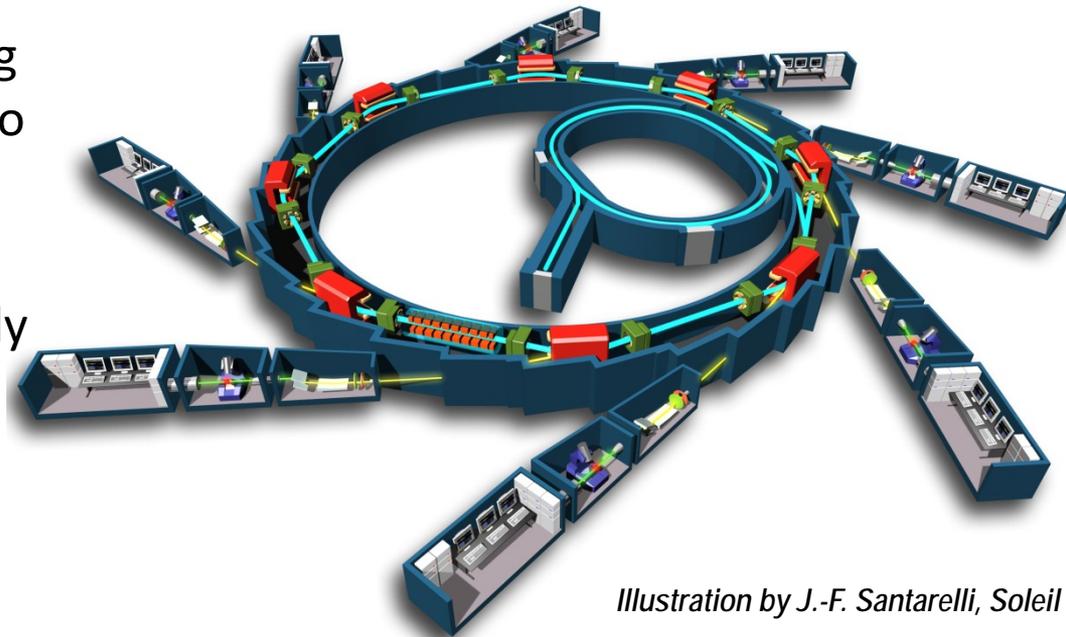
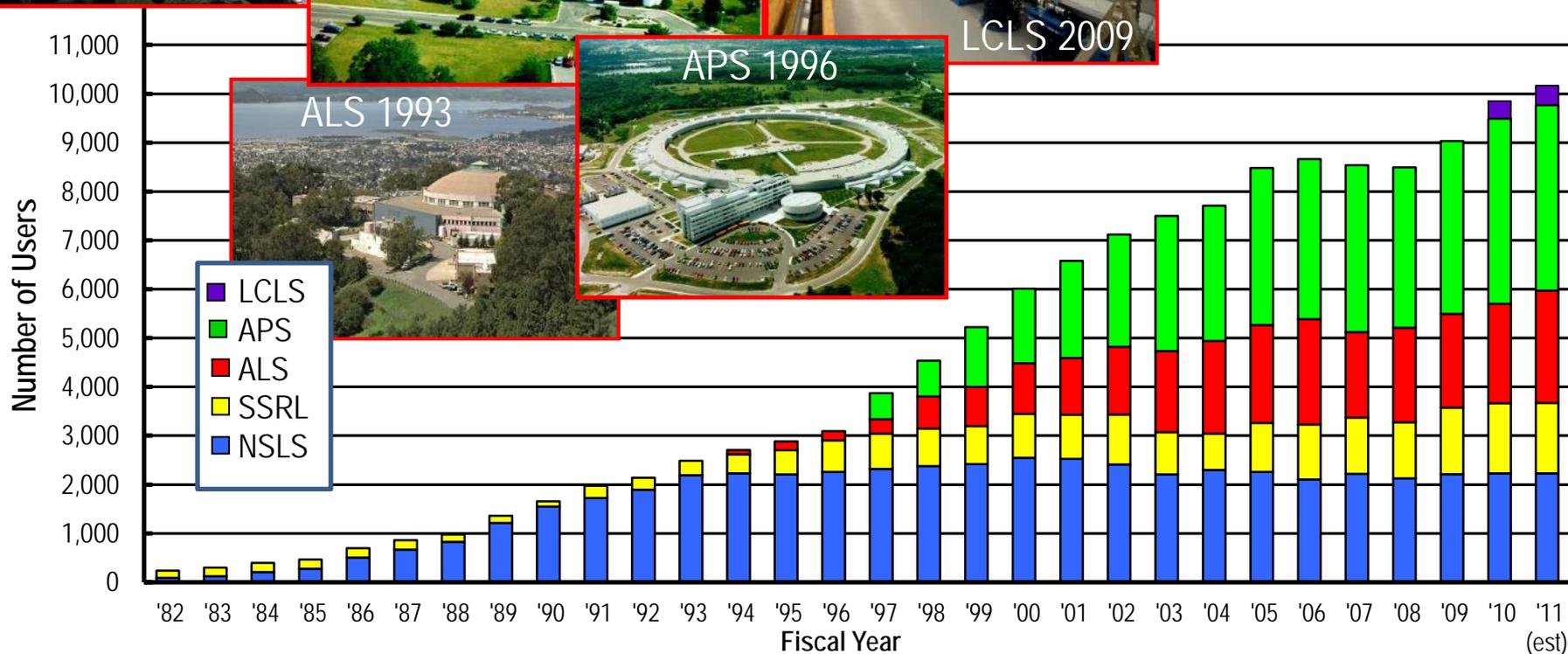
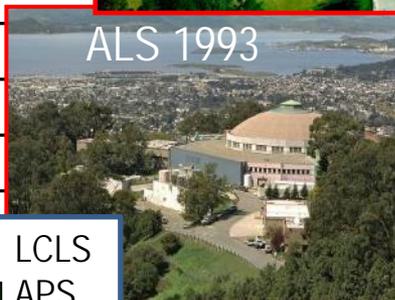
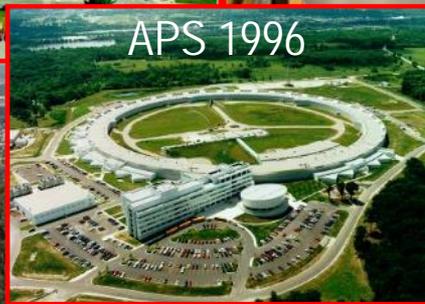
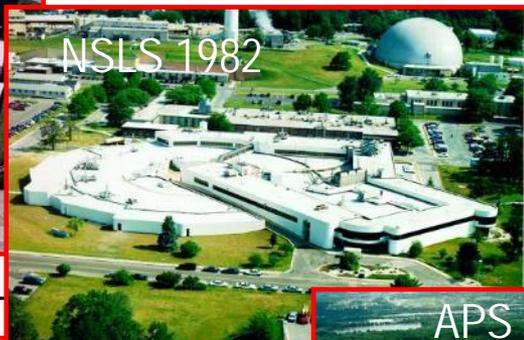


Illustration by J.-F. Santarelli, Soleil

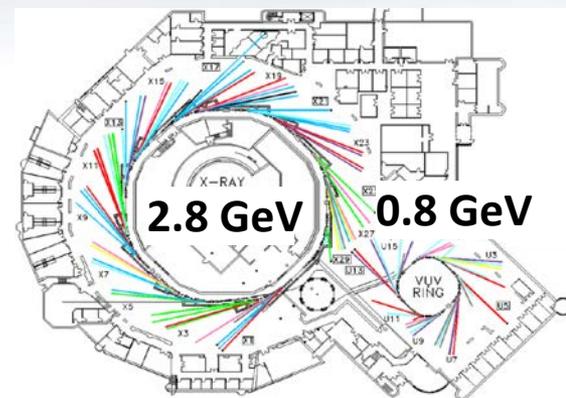
- This light is channeled out of the ring into beamlines, where it is tailored to accommodate specific needs of the research conducted
- All beamlines operate simultaneously
- Each beamline is designed for use for a specific type of research
- Experiments run 24 hours a day

DOE-BES Light Source Facilities



NSLS hosted ~23% of all users of DOE light sources

NSLS – Outstanding Scientific User Facility

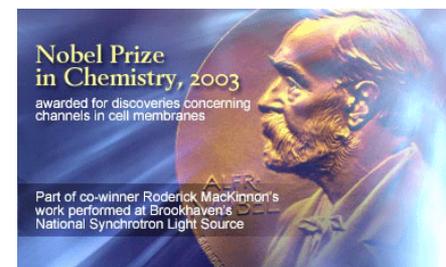


55 Beamlines in FY14
Operation ended 9/30/2014

- **NSLS Tradition and Strengths:**
Broad range of science programs
Diverse capabilities over broad spectral range
Highly engaged and productive user community

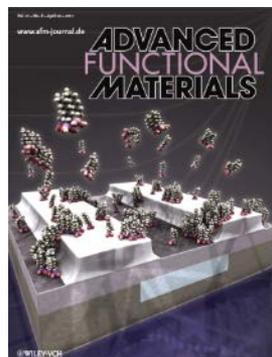
- **Highly Productive & High Impact**

	<u>FY13</u>	<u>Since 1982</u>
• Users	2,367	~ 57,000
• Publications	881	17,182
• Protein Databank Deposits	~ 600	7,122
• 2 Nobel Prizes (2003, 2009)		



- **Crucial Resource**

- Universities: SBU, Columbia, MIT, Yale, Rutgers, ...
- Industry: IBM, ExxonMobil, GE, Pharmaceuticals, ...
- BNL: CFN, CMP, Catalysis, Biology, Environ Sci, ...



Societal Impact – Over 100 Companies Have Conducted Research & Development at NSLS



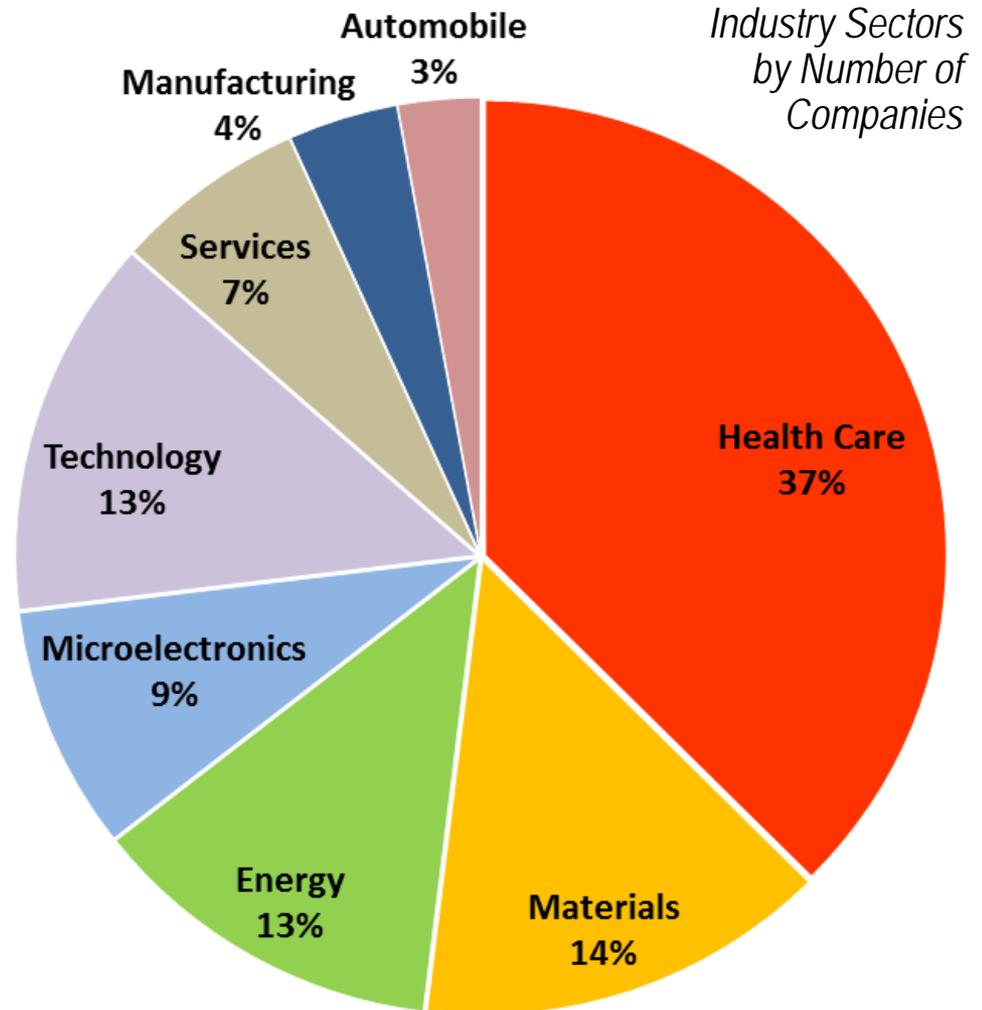
Work Conducted at NSLS Supports a Wide Range of Private Sectors Today

- Majority of industrial research is on basic material structures at the molecular and atomic levels

- Petrochemicals
- Polymers
- Nanostructures
- Catalysts
- Pharmaceuticals
-

- Significant work on in-situ systems engineering and prototype manufacturing processes

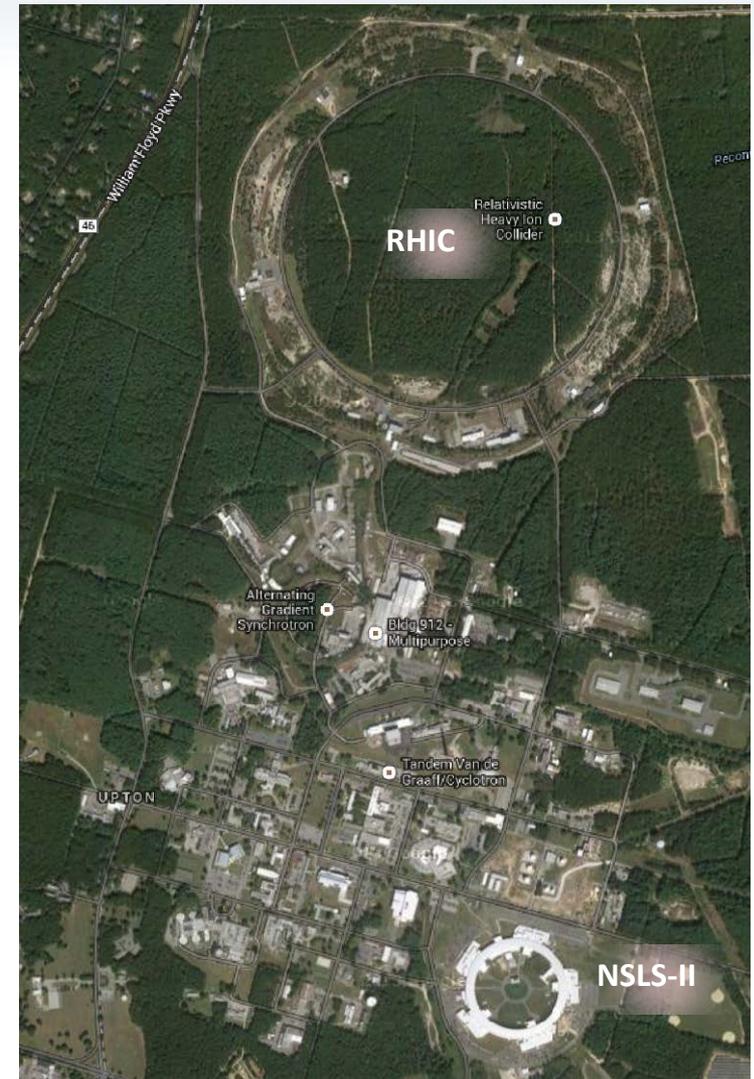
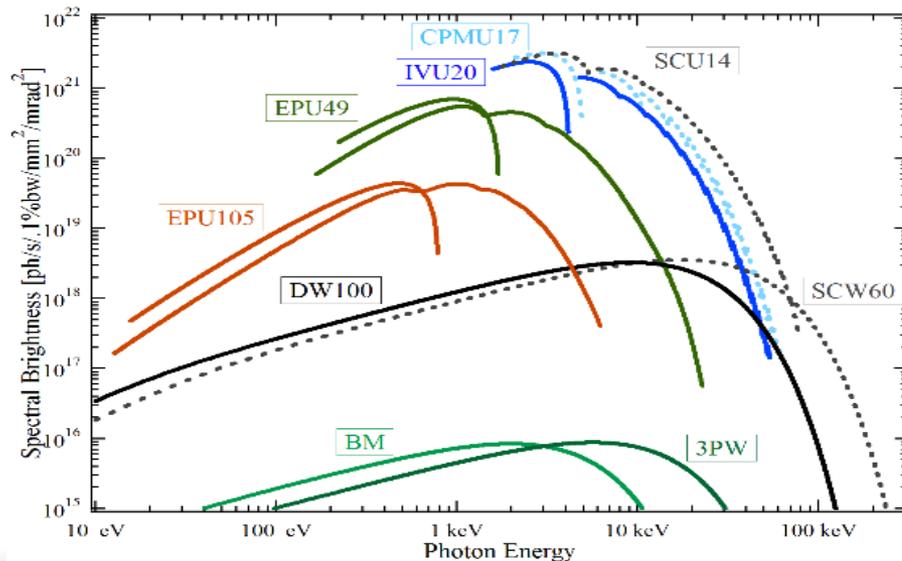
- Thermal annealing
- Purification process
- Battery cycling
- Mechanical stress tests
-



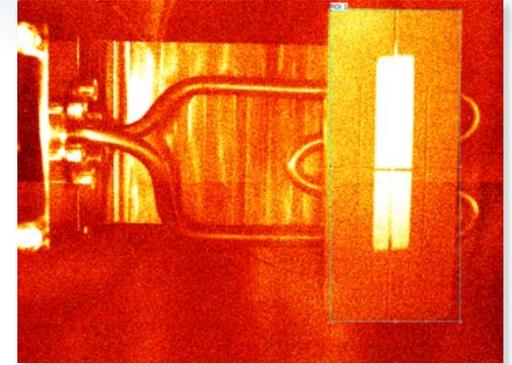
National Synchrotron Light Source II

NSLS-II At-A-Glance

Storage ring circumference: 792 meters
Electron energy: 3×10^9 electron volt
Electron current: 0.5 amperes
Photon energy: from IR to hard X-rays
Capacity: >70 simultaneous experiments
Visiting users: > 4000 per year



NSLS-II First X-ray Light!



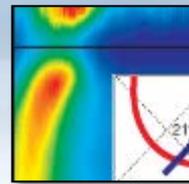
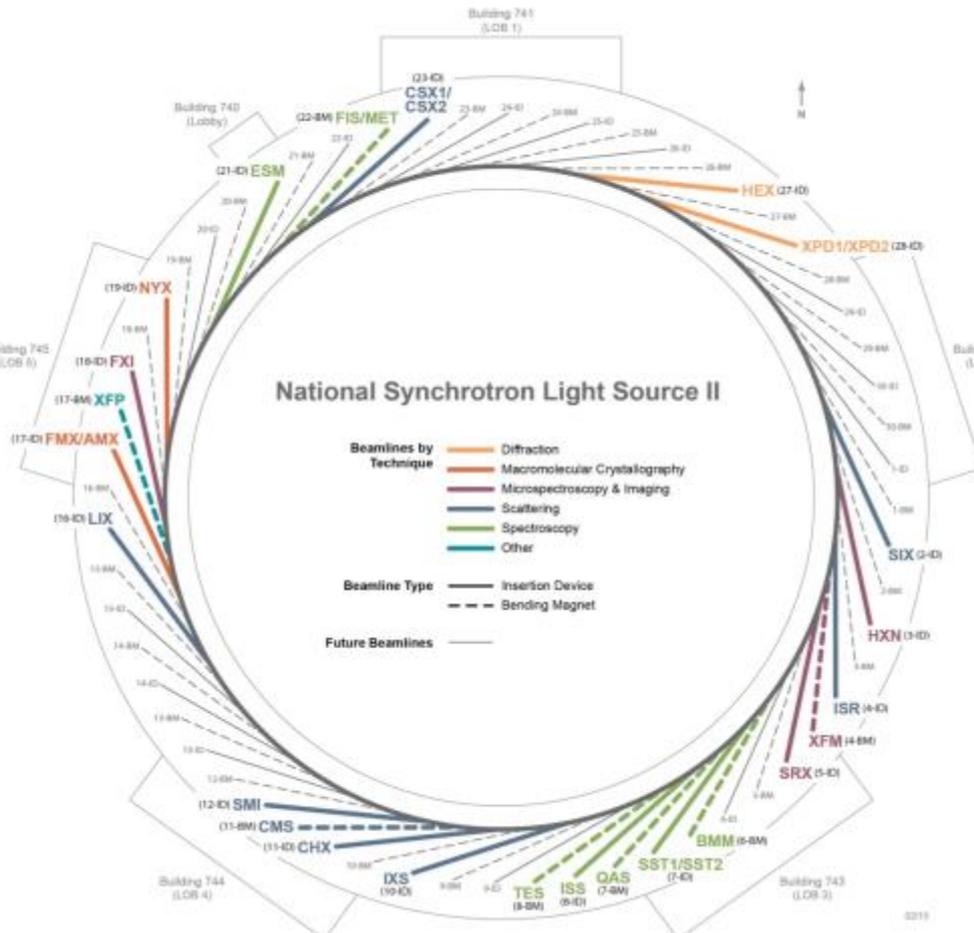
“First X-ray light” was observed at 23-ID beamline on the morning of Thursday, October 23, 2014

NSLS-II

Current Suite of Beamlines

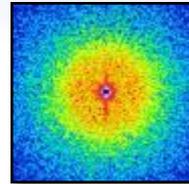
- 7 Operating
- 21 Under Development

<http://www.bnl.gov/ps/nsls2/beamlines/map.php>



Soft X-Ray Scattering & Spectroscopy

- 23-ID-1: Coherent Soft X-ray Scattering (2015)
- 23-ID-2: Soft X-ray Spectr & Polarization (2015)
- 21-ID: Photoemission-Microscopy Facility (2017)
- 2-ID: Soft Inelastic X-ray Scattering (2017)
- 22-BM: Magneto, Ellips, High-P Infrared (2018)



Complex Scattering

- 10-ID: Inelastic X-ray Scattering (2015)
- 11-ID: Coherent Hard X-ray Scattering (2015)
- 11-BM: Complex Materials Scattering (2016)
- 12-ID: Soft Matter Interfaces (2017)

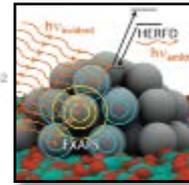


Diffraction & In Situ Scattering

- 28-ID-1: X-ray Powder Diffraction (2015)
- 28-ID-2: X-ray Powder Diffraction (2017)
- 4-ID: In-Situ & Resonant X-Ray Studies (2017)
- 27-ID: High Energy X-ray Diffraction (2020)

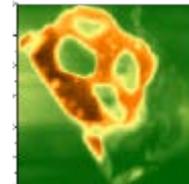
Hard X-Ray Spectroscopy

- 8-ID: Inner Shell Spectroscopy (2017)
- 7-BM: Quick X-ray Absorption and Scat (2016)
- 8-BM: Tender X-ray Absorption Spectr (2017)
- 7-ID-1: Spectroscopy Soft and Tender (2017)
- 7-ID-2: Spectroscopy Soft and Tender (2017)
- 6-BM: Beamline for Mater. Measurement (2017)



Imaging & Microscopy

- 3-ID: Hard X-ray Nanoprobe (2015)
- 5-ID: Sub-micron Resolution X-ray Spectr (2015)
- 4-BM: X-ray Fluorescence Microscopy (2017)
- 18-ID: Full-Field X-ray Imaging (2018)

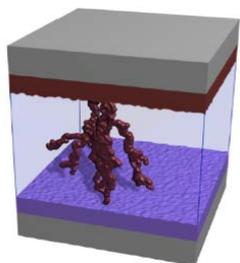


Structural Biology

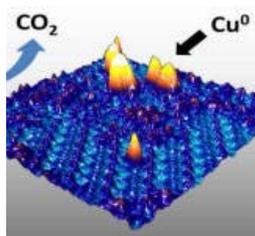
- 17-ID-1: Frontier Macromolec Cryst (2016)
- 17-ID-2: Flexible Access MacromolCryst (2016)
- 16-ID: X-ray Scattering for Biology (2016)
- 17-BM: X-ray Footprinting (2016)
- 19-ID: Microdiffraction Beamline (2017)



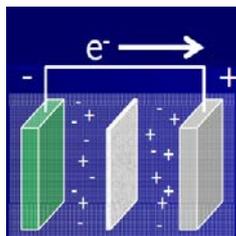
NSLS-II, as a Much Brighter Source Than NSLS, Provides New Enabling Tools for Materials Research



Nano-materials



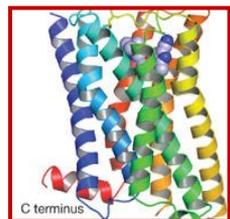
In-situ Catalysis



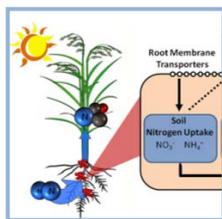
Energy Storage



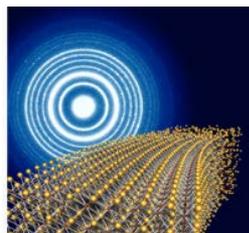
High Pressure Research



Protein Factory



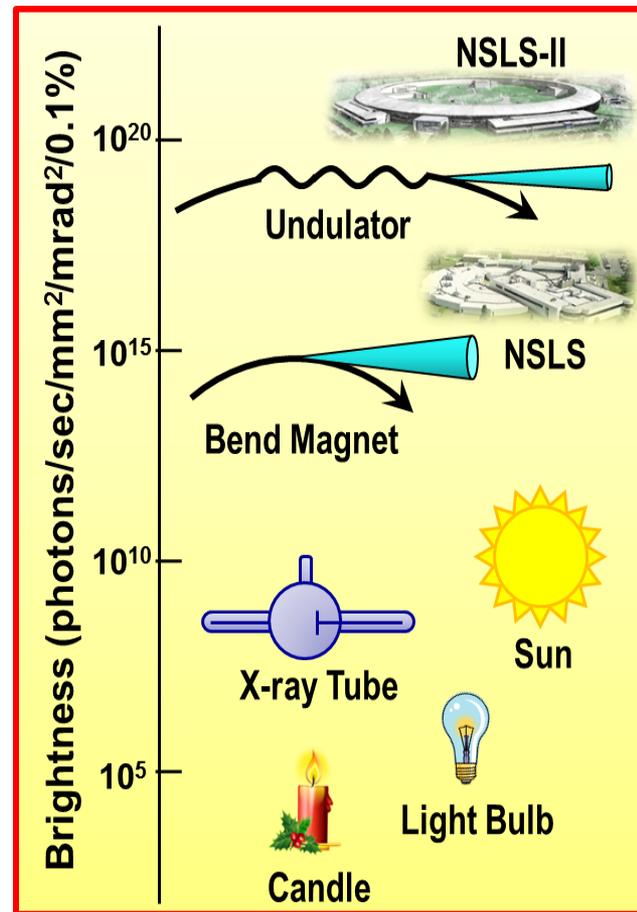
Mesoscale Bioscience



Polymer Research



Industry R&D



Today's Lecture

- Introduction to the Course
- About Brookhaven National Laboratory
- Overview of Synchrotron Sources and to NSLS-II
- X-ray Interactions with Matter
- Quick survey of synchrotron techniques

X-ray Interactions with Matter

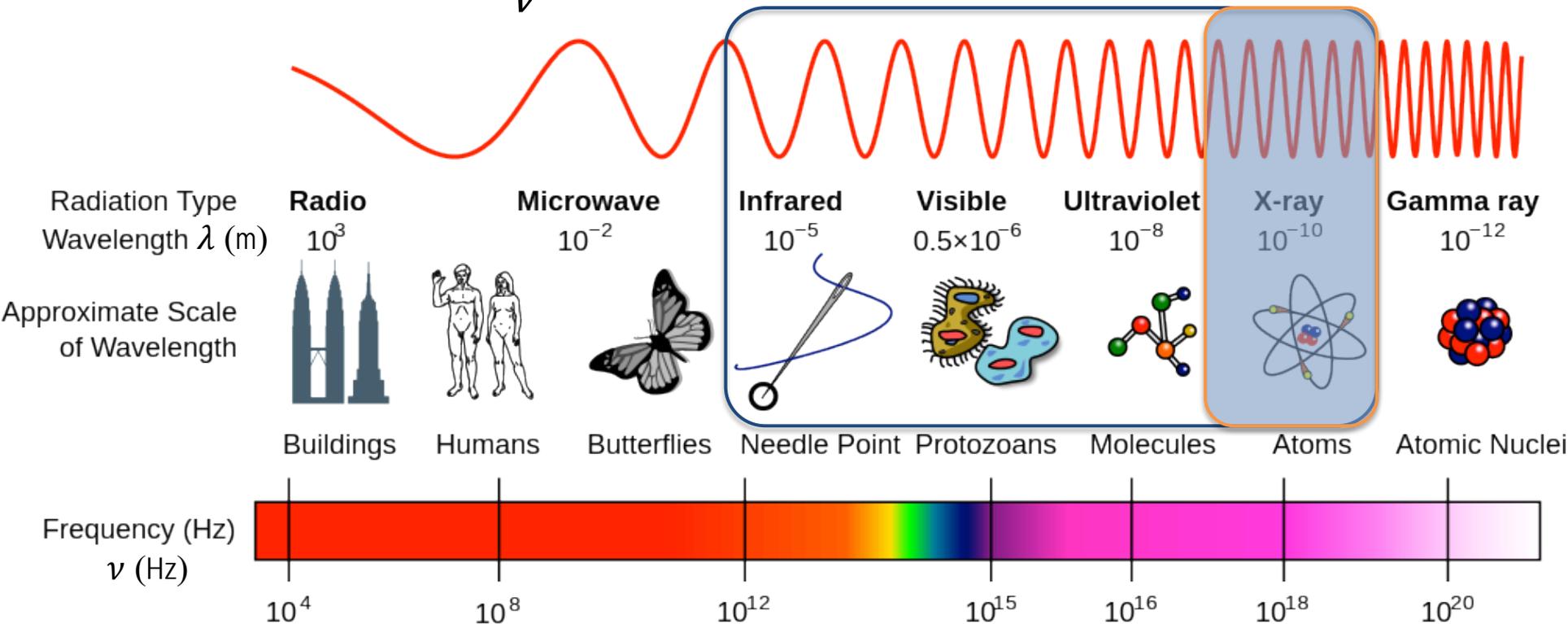
- X-ray as Electromagnetic Wave
- X-ray scattering by an Electron
- Dipole radiation

- Index of refraction
- Total external reflection
- Scattering cross-section

Synchrotron Light Covers a Broad Range of Electromagnetic Wave Spectrum

$$\lambda = \frac{c}{\nu}$$

Wavelength of Typical Synchrotron Light



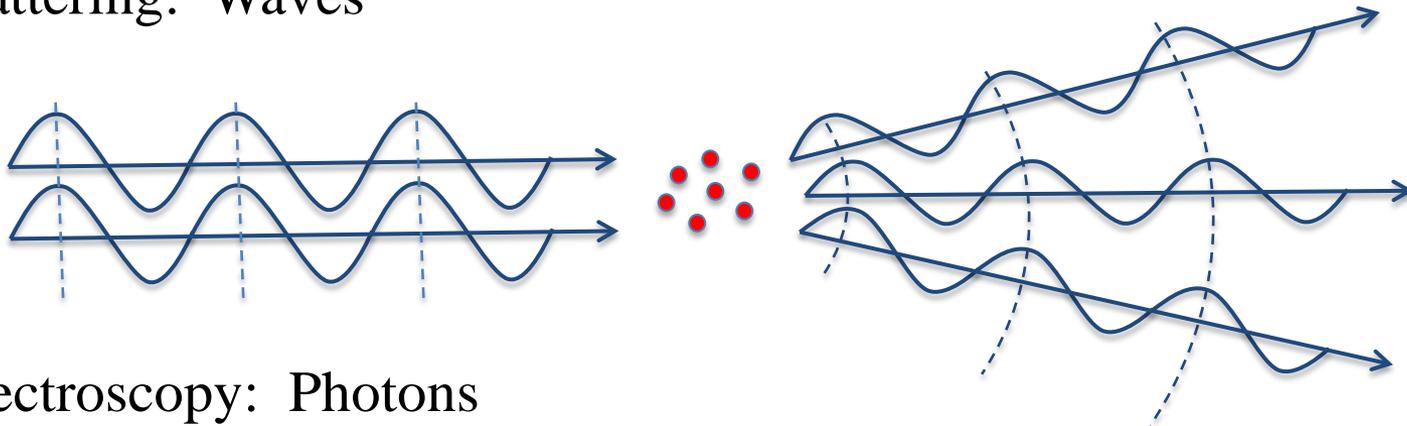
Wave-Particle Duality of Light or E-M Wave

- Light or electromagnetic wave can be viewed as an ensemble of elemental particles, much like electrons or neutrons
- The elemental particle, or ‘*quantum*’, of an electromagnetic wave is called ‘*photon*’
- For an electromagnetic wave of frequency ν , the energy of its photon is $E = h\nu$, where h is the Planck Constant $h = 6.626 \times 10^{-34}$ J-s
- The total energy carried by an electromagnetic wave is quantized to the energy of its photon $h\nu$: $E_{total} = n h\nu$.
- Since $E = h\nu$, and $\lambda = \frac{c}{\nu}$, we have $\lambda = \frac{hc}{E}$, or in practical units,

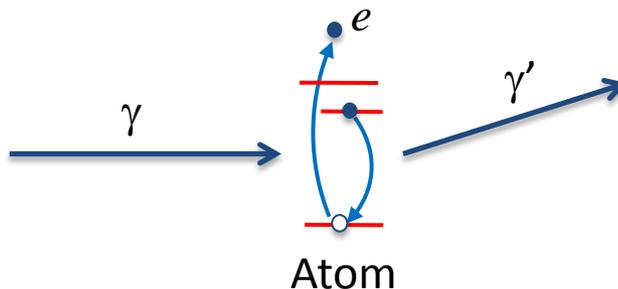
$$\lambda[\text{A}] = \frac{12.4}{E[\text{keV}]}$$

X-rays: Waves or Particles ?

- The fact that E-M waves can be described by either waves or by quantum particles is very useful materials applications, as it allows applying the most convenient theory to our experiments
- Scattering: Waves

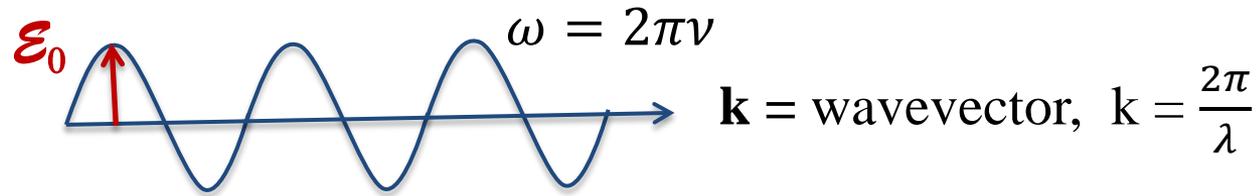


- Spectroscopy: Photons



X-ray Scattering by an Electron (1)

- X-rays or E-M wave interacts only with charged elementary particles – electrons and protons



- In classical electrodynamics, the interaction between E-M wave with electric wave field $\mathcal{E}(\mathbf{x}, t) = \mathcal{E}_0 e^{-i(\mathbf{k}\cdot\mathbf{x} - \omega t)}$ and a particle with mass m and charge q , is governed by Newton's second law of motion via Lorentz force:

$$m\ddot{\mathbf{x}} = \mathbf{F} = q\mathcal{E}(\mathbf{x}, t) \quad \text{where } \ddot{\mathbf{x}} = \left(\frac{d^2\mathbf{x}}{dt^2} \right)$$

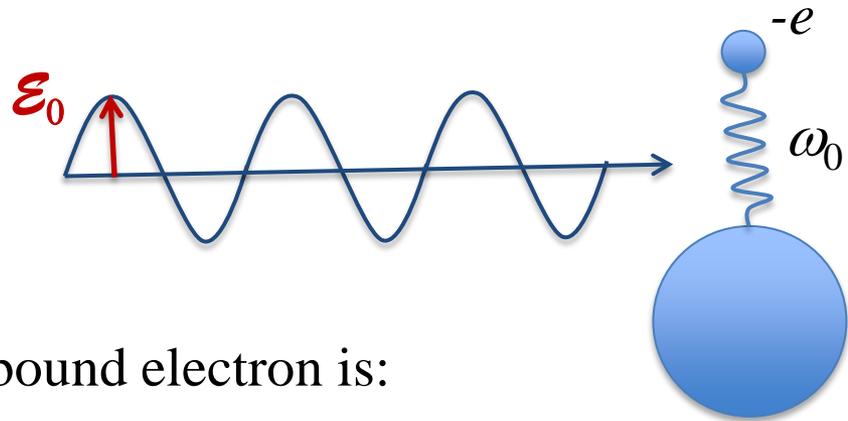
or

$$\ddot{\mathbf{x}} = \frac{q}{m}\mathcal{E}(\mathbf{x}, t)$$

- Proton has the same charge e as an electron, but its mass is 1836 times greater than electron mass. Therefore E-M waves and X-rays interact with mainly electrons in atoms

X-ray Scattering by an Electron (2)

- Assuming an electron is bound to atomic nuclei with an intrinsic 'binding' frequency ω_0 :



- The equation of motion for this bound electron is:

$$\ddot{\mathbf{x}} + \gamma\dot{\mathbf{x}} + \omega_0^2\mathbf{x} = \frac{-e}{m}\boldsymbol{\mathcal{E}}(\mathbf{x}, t) \quad \gamma = \text{damping loss factor}$$

- Solution is a forced oscillation along direction of $\boldsymbol{\mathcal{E}}_0$:

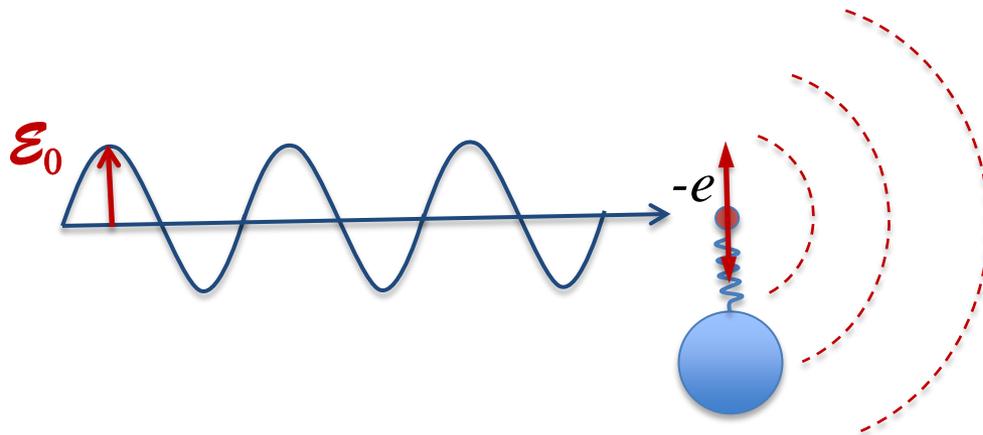
$$\mathbf{x}(t) = \frac{-e}{m} \frac{\boldsymbol{\mathcal{E}}_0 e^{i\omega t}}{(\omega_0^2 - \omega^2) + i\gamma\omega} \quad \leftarrow \text{dipole oscillator}$$

X-ray Scattering by an Electron (3)

- Induced dipole moment for this bound electron is:

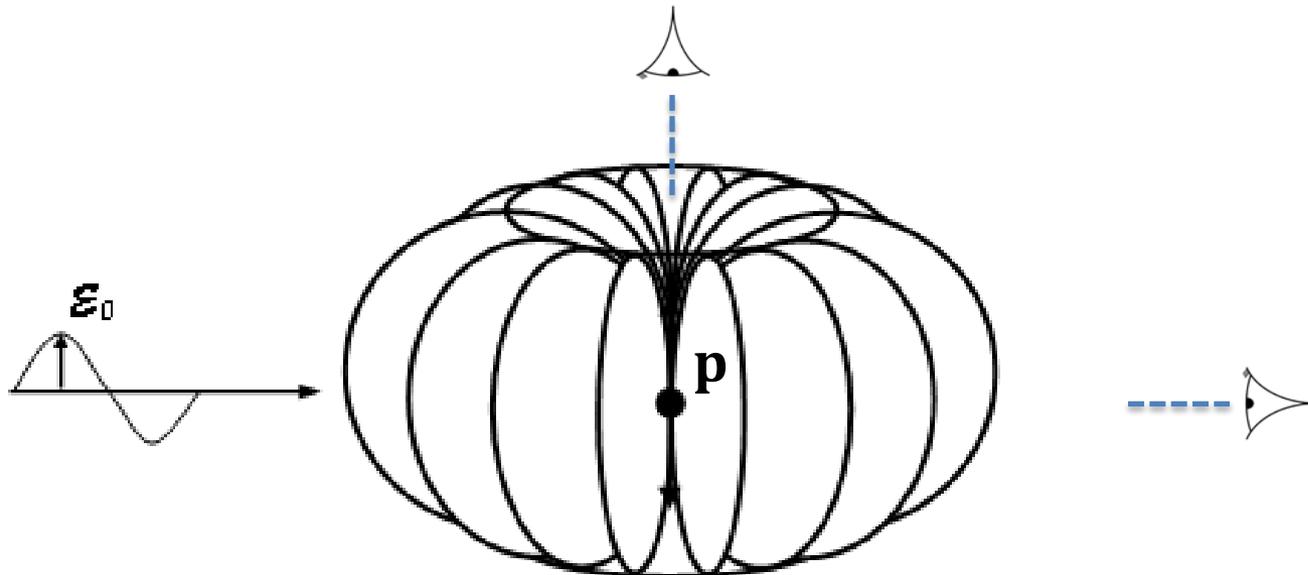
$$\mathbf{p} = -e\mathbf{x} = \frac{e^2}{m} \frac{\boldsymbol{\varepsilon}_0 e^{i\omega t}}{(\omega_0^2 - \omega^2) + i\gamma\omega}$$

- We see that an incident E-M wave forces the electron to oscillate or accelerate and decelerate repeatedly
- Any accelerating or decelerating electron (or any charge particle) will emit E-M radiation, much like an antenna



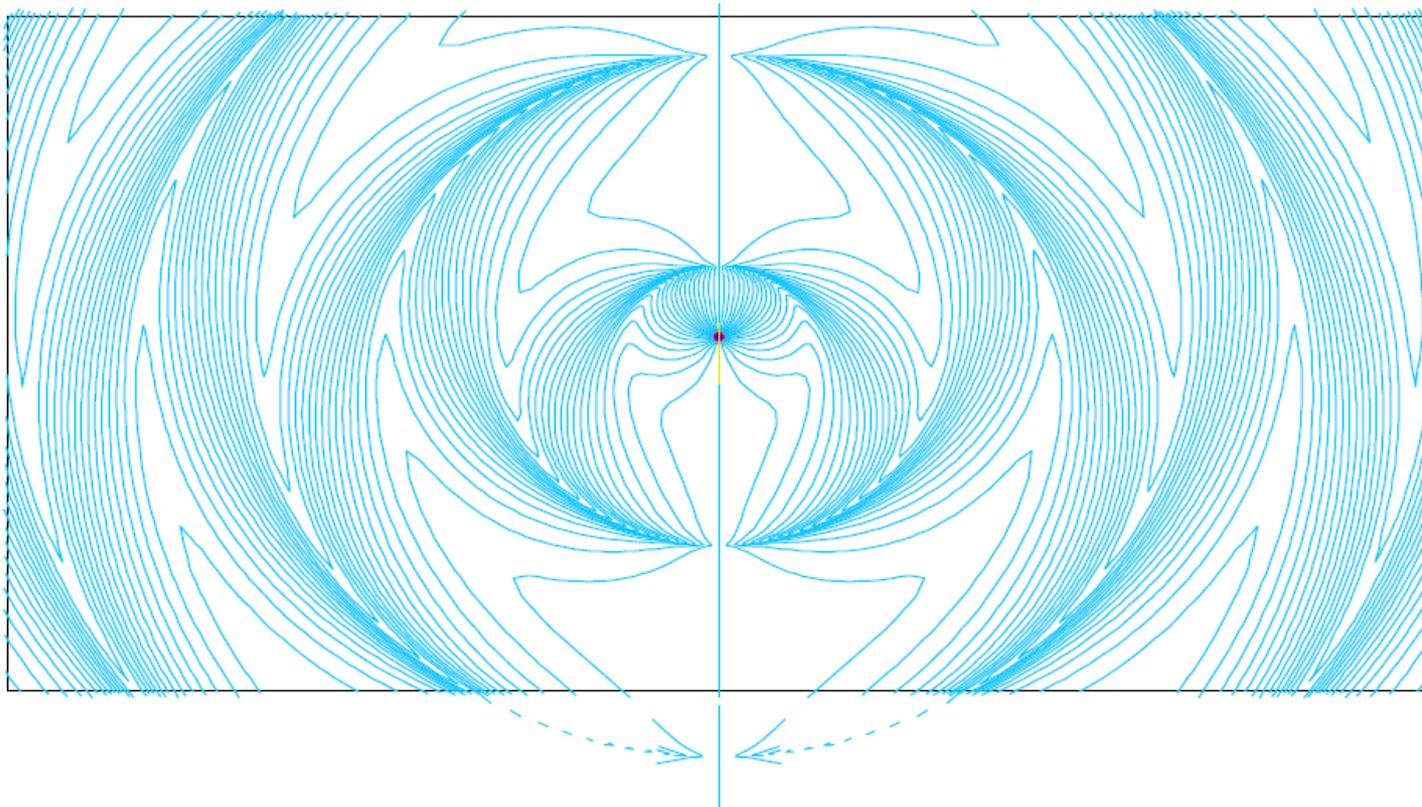
Irradiated Wave Field by Oscillating Electron

- Dipole irradiated wave field is anisotropic – strength of radiation is strongest along the equator and approaches zero at the poles (assuming the poles line up with the induced dipole moment \mathbf{p})
- This property of dipole radiation is very useful in designing your experiments at synchrotrons, as synchrotron radiation is typically linearly polarized in the horizontal plane



X-ray Scattering by an Electron

- Dipole oscillator emits E-M waves



Courtesy of Prof. Shintake:

<http://www.shintakelab.com/en/enEducationalSoft.htm>

X-ray Interactions with Matter

- X-ray as Electromagnetic Wave
- X-ray scattering by an Electron
- Dipole radiation

- Index of refraction
- Total external reflection
- Scattering cross-section

Induced Dipole Moment for N Atoms

- For an atom with Z electrons, the induced dipole moment for the whole atom is the sum of the dipole moments of all Z electrons, each may have different binding energy ω_j ($j = 1, 2, \dots, Z$):

$$\bar{\mathbf{p}} = \frac{e^2}{m} \sum_{j=1}^Z \frac{\boldsymbol{\varepsilon}_0 e^{i\omega t}}{(\omega_j^2 - \omega^2) + i\gamma_j \omega}$$

- For a specimen with N such atoms per unit volume, the total dipole moment per unit volume is:

$$\mathbf{P} = N\bar{\mathbf{p}} = \frac{Ne^2}{m} \sum_{j=1}^Z \frac{\boldsymbol{\varepsilon}_0 e^{i\omega t}}{(\omega_j^2 - \omega^2) + i\gamma_j \omega}$$

Index of Refraction for X-rays (1)

- Dielectric constant ϵ is defined as $\mathbf{D} = \epsilon \mathbf{E} = \mathbf{E} + 4\pi\mathbf{P}$, therefore:

$$\epsilon = 1 + \frac{4\pi N e^2}{m} \sum_{j=1}^Z \frac{1}{(\omega_j^2 - \omega^2) + i\gamma_j \omega}$$

- For X-rays, $\omega \gg \omega_j$, sum over Z electrons becomes $\sim -Z/\omega^2$. Thus we have:

$$\epsilon = 1 - \frac{4\pi N Z e^2}{m \omega^2} = 1 - \frac{4\pi N Z e^2}{m \left(\frac{2\pi c}{\lambda}\right)^2}$$

or:

$$\epsilon = 1 - \frac{e^2}{m c^2} \frac{N Z \lambda^2}{\pi} = 1 - \frac{r_e N Z \lambda^2}{\pi}$$

where $r_e = \frac{e^2}{m c^2} = 2.82 \times 10^{-5} \text{ \AA}$ is the classical radius of electron.

Index of Refraction for X-rays (2)

- For typical materials, $N \sim 0.1 \text{ atom/\AA}^3$, $Z \sim 10$, $\lambda \sim 1 \text{ \AA}$, thus:

$$\varepsilon = 1 - \frac{r_e NZ\lambda^2}{\pi} \sim 1 - 10^{-5}$$

only slightly less than 1.

- Index of refraction is defined as $n = \sqrt{\varepsilon}$:

$$n = 1 - \frac{r_e NZ\lambda^2}{2\pi}$$

- For X-rays, we usually write $n = 1 - \delta - i\beta$, where β is related to *photoelectric absorption*, and

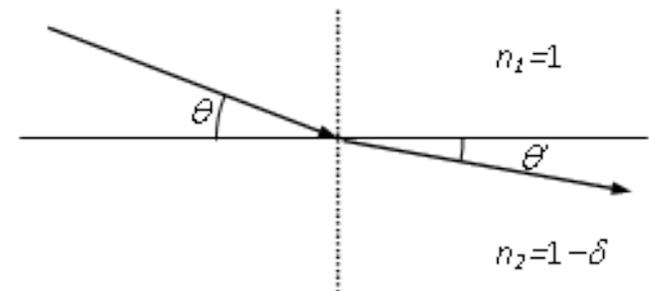
$$\delta = \frac{r_e NZ\lambda^2}{2\pi}$$

Index of Refraction for X-rays (3)

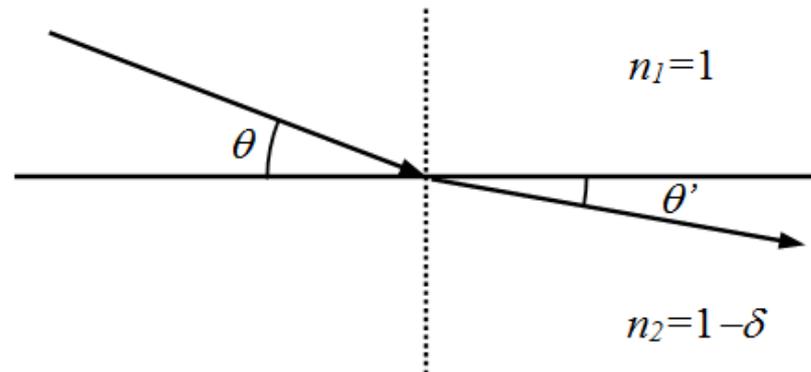
- Using $N = \rho NA/A$, where ρ = density, N_A = Avogadro number = $6.022 \times 10^{23}/\text{mol}$, A = molar mass, and $Z/A \sim 0.5$ for most elements, we get:

$$\delta = \frac{r_e NZ\lambda^2}{2\pi} = \frac{r_e N_A \lambda^2}{4\pi} \rho = 1.35 \times 10^{-6} \lambda [A]^2 \rho [g/cm^3]$$

- Conclusion: Index of refraction for X-rays is slightly less than unity, by about $\sim 10^{-5}$ - 10^{-6}
- Because $n < 1$ for X-rays, the refraction direction is opposite to that of visible light – instead of total internal reflection, we have total external reflection for X-rays
- Such property of X-rays may be used to increase surface sensitivity for X-rays at grazing incidence



Critical Angle & Total External Reflection



(i) Snell's law: $n_1 \cos \theta = n_2 \cos \theta'$

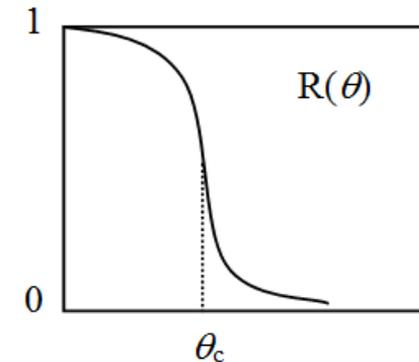
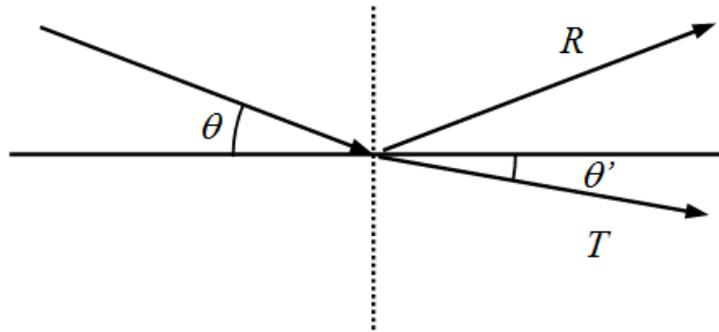
(ii) Critical angle: $\theta = \theta_c$ when $\theta' = 0 \quad \rightarrow \quad \cos \theta_c = 1 - \delta \approx 1 - \frac{\theta_c^2}{2}$

$\rightarrow \quad \theta_c = \sqrt{2\delta} \approx 0.00164 \lambda [A] \sqrt{\rho [g/cm^3]}$.

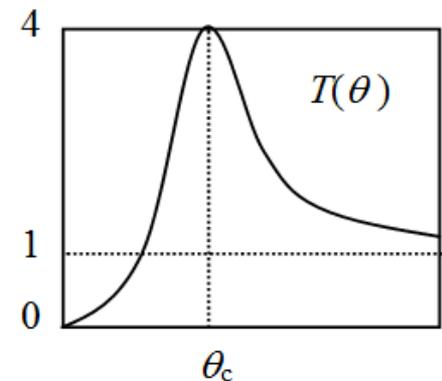
For Si, $\rho = 2.33 \text{ g/cm}^3$, take $\lambda = 1 \text{ A}$, we have: $\theta_c = 2.5 \text{ mrad} = 0.14^\circ$.

Critical Angle & Total External Reflection

(iii) Fresnel specular reflectivity:



$$R(\theta) = \left| \frac{\theta - \sqrt{\theta^2 - \theta_c^2}}{\theta + \sqrt{\theta^2 - \theta_c^2}} \right|^2, \quad T(\theta) = \left| \frac{2\theta}{\theta + \sqrt{\theta^2 - \theta_c^2}} \right|^2.$$



(iv) Evanescent wave at $\theta < \theta_c$: exponentially damped wave

Plot of $T(\theta)$: $T(\theta=0) = 0$, $T(\theta=\theta_c) = 2^2 = 4$, $T(\theta \gg \theta_c) = 1$.

- ⇒ surface sensitivity at $\theta = \theta_c$
- ⇒ total-reflection x-ray fluorescence (TXRF)
- ⇒ grazing incidence diffraction (GID)
- ⇒ penetration depth (skin depth): next page.

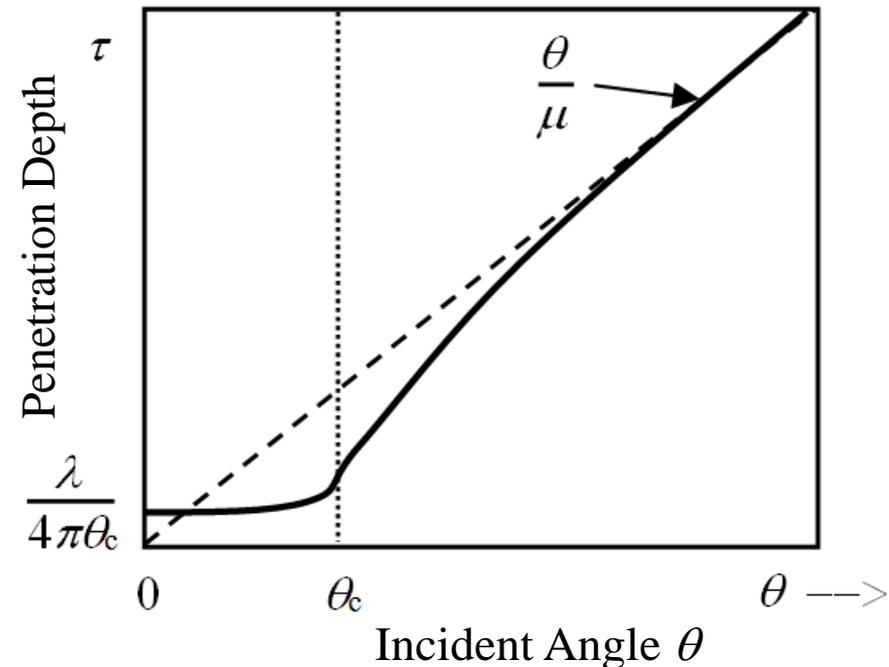
Critical Angle & Total External Reflection

(v) Penetration depth (skin depth) of the evanescent wave: at $\theta = 0$

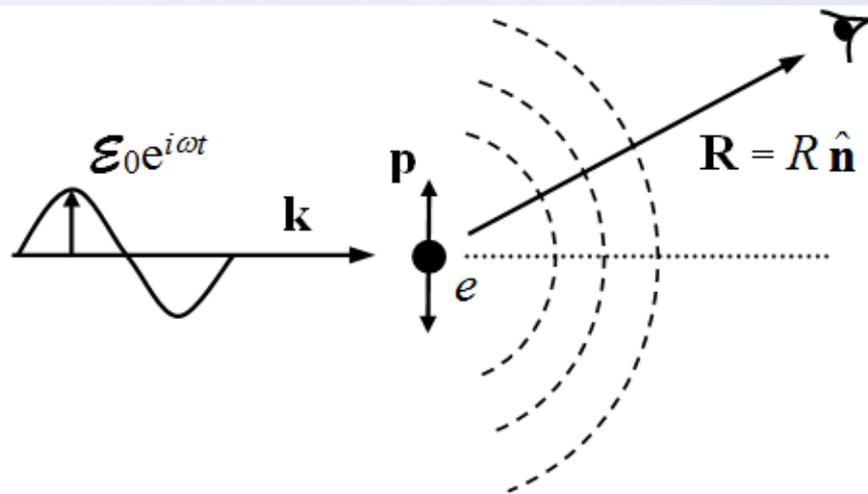
$$\tau = \frac{1}{2k_0\theta_c} = \frac{\lambda}{4\pi\theta_c}$$

Over the whole small angle region, τ looks like the curve at right, which asymptotically approaches θ/μ for larger angles.

μ = photo absorption length



Back to Scattering by an Electron



When an x-ray beam hits an electron, it forces the electron to oscillate along the direction of incident electric field, giving rise to an induced dipole moment \mathbf{p} (for $\omega \gg \omega_0$):

$$\mathbf{p} = -\frac{e^2 \boldsymbol{\mathcal{E}}_0}{m\omega^2}.$$

This oscillating dipole acts like an antenna, and emits radiation of the same oscillation frequency ω . The radiation field $\boldsymbol{\mathcal{E}}_e$ at position R along observation direction $\hat{\mathbf{n}}$ (= unit vector) is given by:

$$\boldsymbol{\mathcal{E}}_e = k^2 (\hat{\mathbf{n}} \times \mathbf{p}) \times \hat{\mathbf{n}} \frac{e^{-ikR}}{R}, \quad \text{with } k = \omega/c.$$

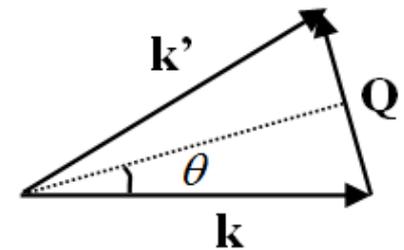
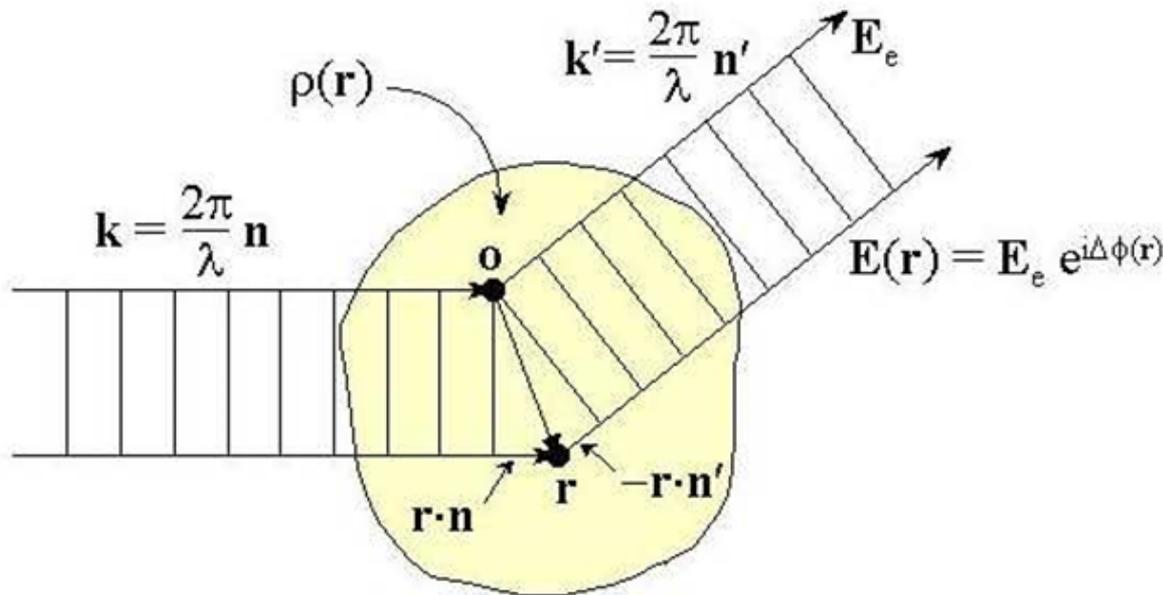
Putting in \mathbf{p} , we get:

$$\boldsymbol{\mathcal{E}}_e = r_e \hat{\mathbf{n}} \times (\hat{\mathbf{n}} \times \boldsymbol{\mathcal{E}}_0) \frac{e^{-ikR}}{R},$$

where r_e is the classical radius of electron defined earlier. This is the elastically scattered x-ray wave by an electron, so-called *Thomson Scattering*.

X-ray Scattering by an Atom (1)

To evaluate scattering by an ensemble of electrons with an electron density $\rho(\mathbf{r})$, we need to take proper account of the path length differences from different parts of the ensemble.



$$\Delta\phi(\mathbf{r}) = -\frac{2\pi}{\lambda} \mathbf{r} \cdot (\mathbf{n} - \mathbf{n}') = (\mathbf{k}' - \mathbf{k}) \cdot \mathbf{r} = \mathbf{Q} \cdot \mathbf{r}$$

$\mathbf{Q} = \mathbf{k}' - \mathbf{k}$ is called the *momentum transfer*. Its magnitude is $Q = 2k \sin\theta = 4\pi \sin\theta / \lambda$.

X-ray Scattering by an Atom (2)

Considering scattering from a volume element $\rho(\mathbf{r})d\mathbf{r}$ and integrating over the whole volume, we obtain the total scattered wave amplitude:

$$\mathcal{E} = \mathcal{E}_e \int e^{i\Delta\phi(\mathbf{r})} \rho(\mathbf{r})d\mathbf{r} = \mathcal{E}_e \int e^{i\mathbf{Q}\cdot\mathbf{r}} \rho(\mathbf{r})d\mathbf{r},$$

which is a Fourier transform of the charge density $\rho(\mathbf{r})$. This is a basic result for all scattering phenomenon based on single-scattering Born approximation.

Atomic scattering factor f :

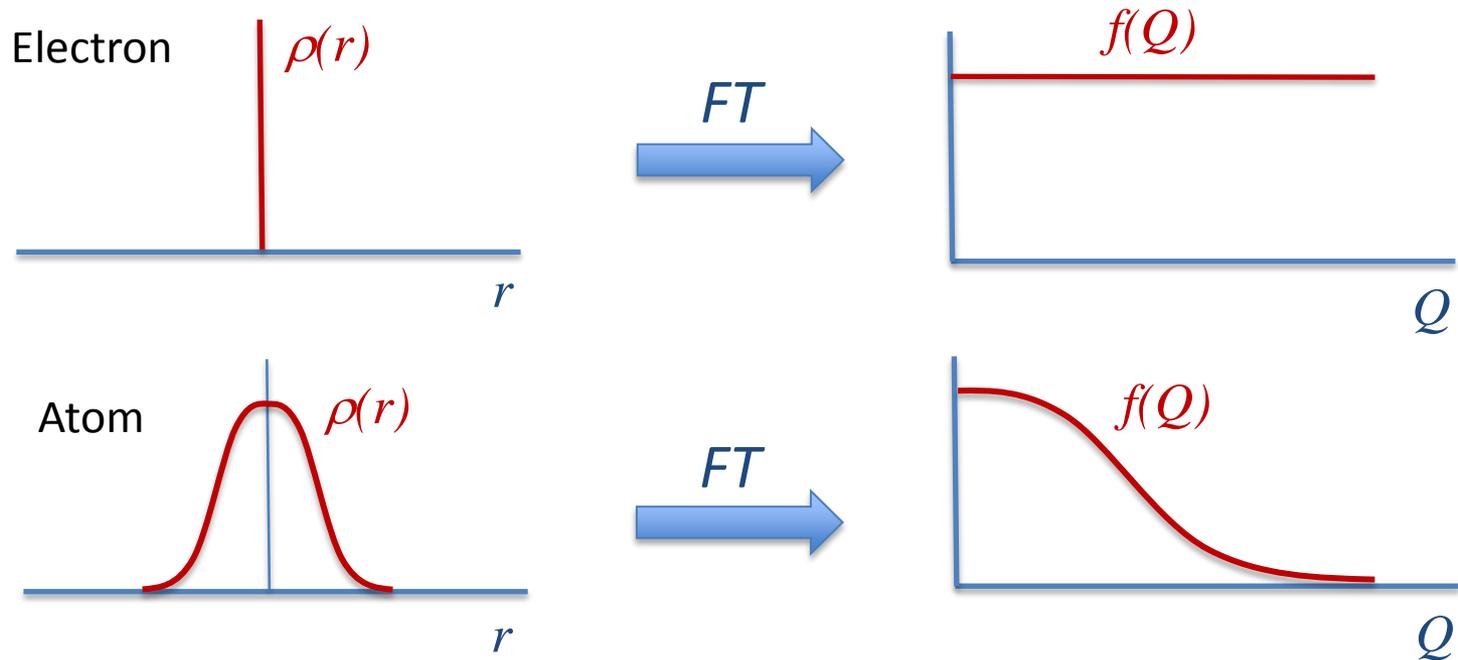
If $\rho(\mathbf{r}) =$ electron density for an atom, then the scattered amplitude is usually called the atomic scattering factor or atomic form factor f , which is normalized in such a way that the scattering amplitude from a single electron is unity (one). Thus,

$$f(\mathbf{Q}) = \int e^{i\mathbf{Q}\cdot\mathbf{r}} \rho(\mathbf{r})d\mathbf{r}.$$

And $f(Q = 0) = Z$. A conventional assumption is that $\rho(\mathbf{r})$ is spherical for an atom, therefore $f = f(Q)$ depends only on the length of momentum transfer Q .

X-ray Scattering by an Atom (3)

- How does the function $f(Q)$ look like? Consider properties of Fourier Transform:



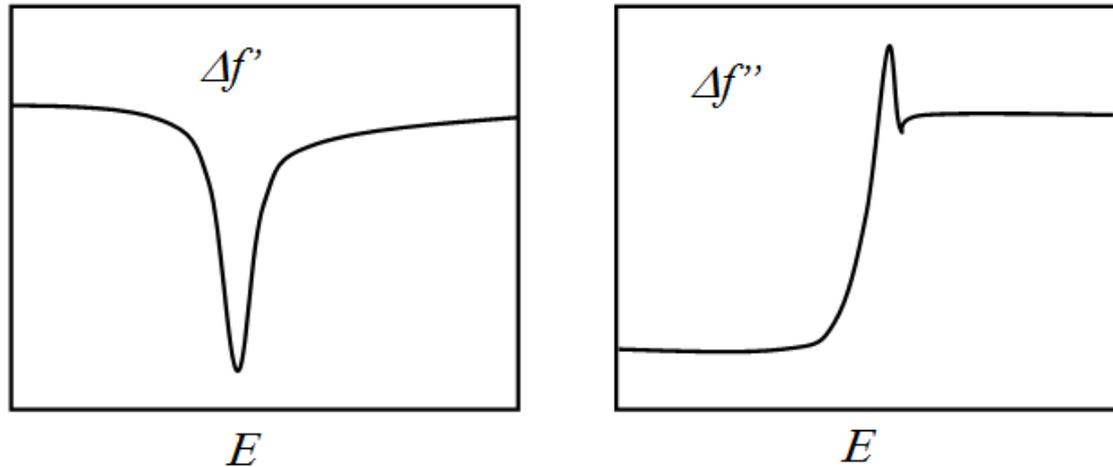
- In practice, atomic form factors can be calculated using tabulated values in International Tables for Crystallography, which are based on a 9-parameter empirical function of four Gaussians plus a constant

Anomalous Scattering Factors

When x-ray energy is close to an atomic absorption edge, it is necessary to include two correction terms in atomic scattering factor:

$$f \rightarrow f + \Delta f' + i\Delta f''.$$

Typical curves for $\Delta f'$ and $\Delta f''$ looks like the following.



$\Delta f'$ and $\Delta f''$ are related by Kramers-Kronig dispersion relation: $\Delta f' \sim -d\Delta f''/dE$.

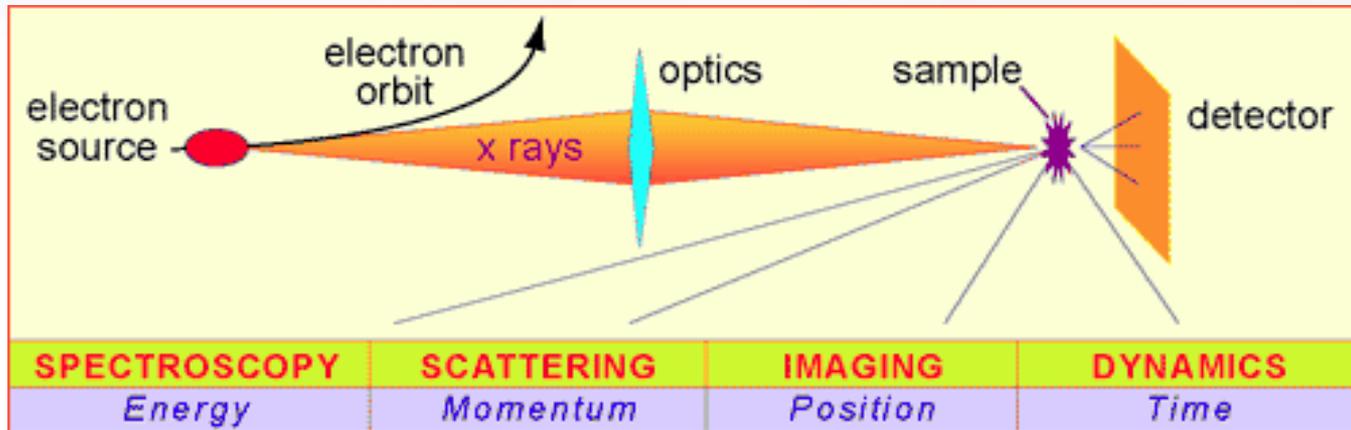
In practice, $\Delta f'$ and $\Delta f''$ values can be obtained on-line at

<http://www.cxro.lbl.gov/optical-constants/>.

Today's Lecture

- Introduction to the Course
- About Brookhaven National Laboratory
- Overview of Synchrotron Sources and to NSLS-II
- X-ray Interactions with Matter
- Quick survey of synchrotron techniques

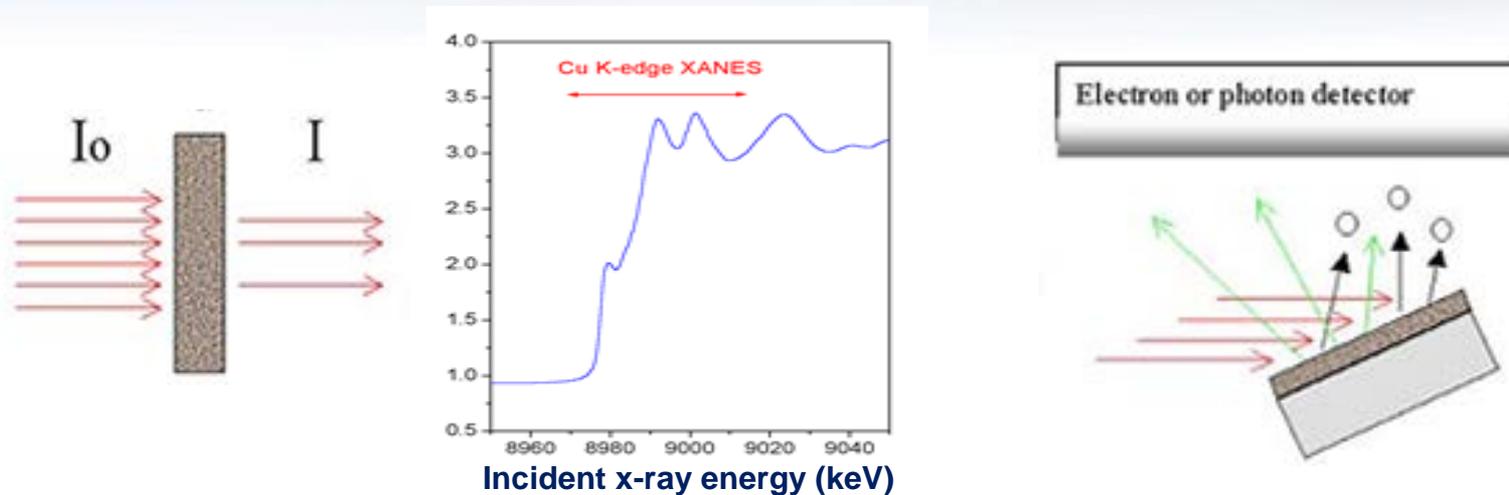
Synchrotron X-ray Techniques for Scientific Research



http://www.sc.doe.gov/bes/synchrotron_techniques/

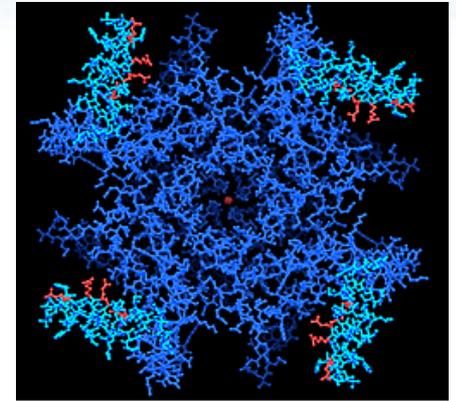
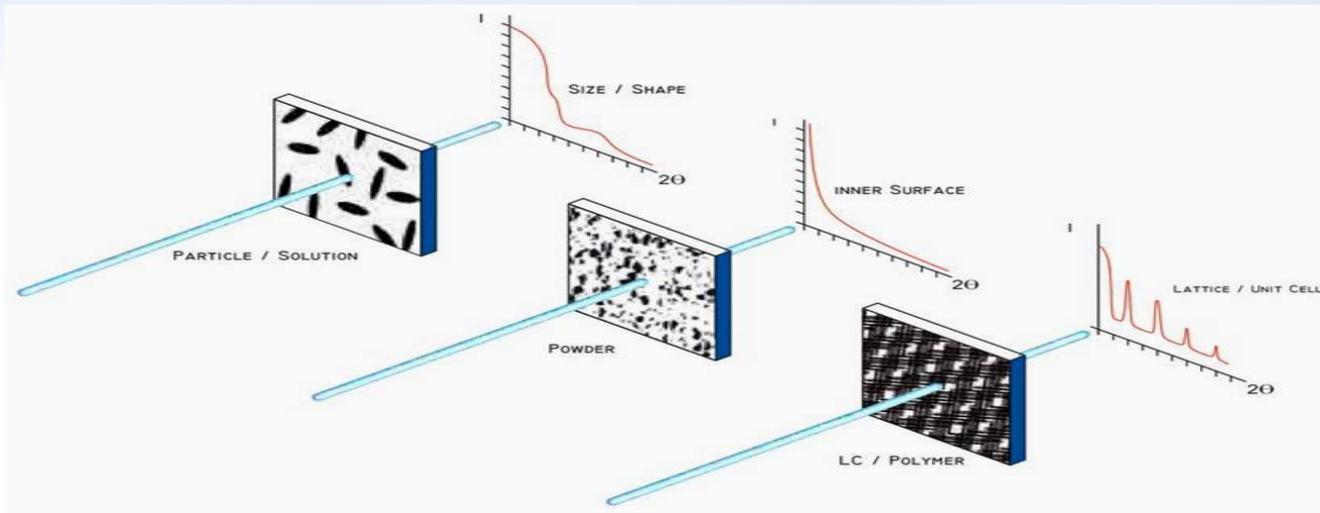
- **SPECTROSCOPY:** used to study the energy & the quantity of emitted particles when incident x-rays are absorbed by the sample → determine the characteristics of chemical bonding and electron energy band structure.
- **SCATTERING/diffraction:** make use of the patterns of scattered x-rays when incident x-rays are deflected by atoms in a sample → determine the structural arrangement of atoms in the sample.
- **IMAGING:** use the intense x-ray beam to obtain structural pictures of the sample with fine spatial resolution and chemical information → used in diverse research areas to image from biological cells to semiconductor chips and fuel cells.
- **Dynamics:** perform spectroscopy, scattering, & imaging measurements vs. time → used to study structural and electronic changes in the material.

Synchrotron X-ray Spectroscopy Techniques



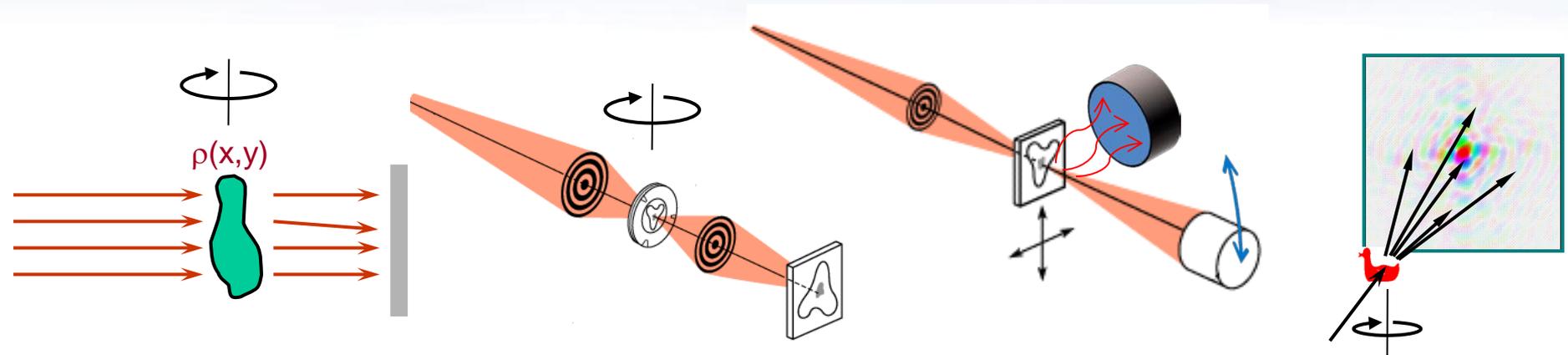
- **X-ray Absorption Spectroscopy (XAS):** measures the transmitted x-ray intensity through the sample as a function of incident x-ray energy → provide element specific chemical state information such as oxidation and bond characteristics.
- **X-ray Emission Spectroscopy (XES):** used to study the energy spectrum of emitted photons when incident x-rays are absorbed by the sample → provide information on the energy levels of the atoms in the sample.
- **Photoelectron Spectroscopy (PES):** used to study the energy spectrum of emitted electrons when incident x-rays are absorbed by the sample → determine the characteristics of collective electron motion and electron energy band structure.

Synchrotron X-ray Scattering & Diffraction



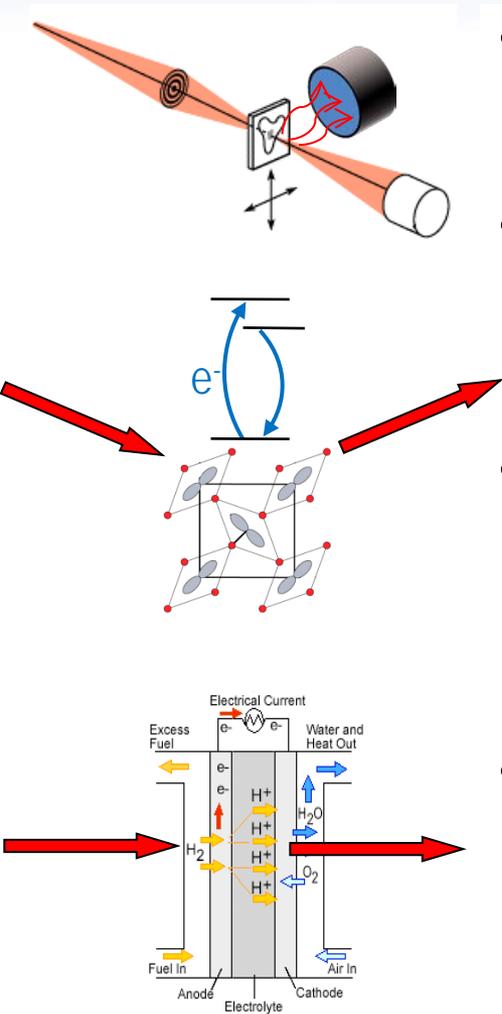
- **Single-Crystal/Powder X-ray Diffraction (XRD):** measures intensities of diffraction peaks in crystalline materials → provide high-resolution atomic-scale image of the molecular structure.
- **Macromolecular Crystallography (MX):** specialized XRD technique tailored for biological macromolecular crystallography.
- **Pair-Distribution Function (PDF):** studies diffuse scattering around diffraction peaks in polycrystalline (powder) materials → provide information on local atomic displacement (e.g. relaxation in nanoparticles) from the perfect crystal lattice.
- **Small-Angle/Wide-Angle X-ray Scattering (SAXS/WAXS):** studies diffuse scattering patterns from the sample → determine characteristic size distributions of particles and their correlated structural arrangements.

Synchrotron X-ray Imaging Techniques

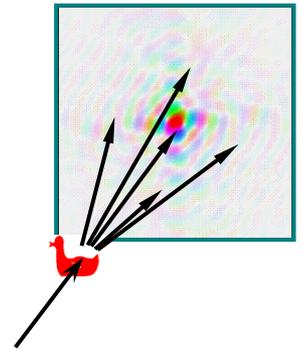


- **X-ray Tomography (xCT):** images internal structures in 3D → very much like clinical x-ray CT but with both absorption and phase contrasts, and with $\sim 1 \mu\text{m}$ resolution.
- **Transmission X-ray Microscopy (TXM):** applies an x-ray lens as objective to obtain high resolution image of internal structures in 3D → provides much larger depth penetration than TEM, ideal for in-situ studies of materials in real conditions.
- **Scanning X-ray Microscopy (SXM):** applies an x-ray lens to focused x-ray spot and measures transmitted, fluorescence, and/or diffracted signals as function of raster scan position on specimen → image heterogeneities in sample.
- **Coherent Diffraction Imaging (CDI):** measures x-ray diffraction pattern from non-crystalline specimens → applies phase retrieval to obtain real-space image.

Enhanced and New Capabilities at NSLS-II



- High brightness & small source size enables development of **nanometer sized** x-ray beams → Opens up new opportunities for structural & spectroscopic materials studies at nanoscales
- High brightness & high angular definition enables development of **high energy-resolution** x-rays → Opens up new possibilities for structural dynamic and spectroscopic studies based on inelastic processes
- High brightness & high coherence enables **coherence-based imaging** capabilities → Opens up new imaging modalities for structural studies of noncrystalline materials and amorphous materials
- High brightness & high flux enables a broad range of **in-situ** and **real-time** capabilities → Opens up new opportunities for to study materials structure and process under realistic conditions and in functional environment (buried structures, reaction, ...)



Today's Homework

MSAE E8235x

Homework #1

September 9, 2015

A focused monochromatic X-ray beam with an intensity of 5×10^{12} photons/sec and wavelength of 1.2 Angstroms is incident onto a silicon specimen with a density of 2.33 grams/cm³ and volume of 10 um by 10 um by 10 um. An X-ray detector with an active area of 1 cm² located at 1 m from the Si specimen is used to measure the scattered X-rays close to the incident beam direction.

Assuming that (a) the incident X-ray beam is entirely focused onto the Si specimen, (b) atoms in the specimen are randomly distributed, and (c) absorption can be neglected, estimate the signal strength of the scattered X-rays as measured by the X-ray detector.