Physik und Anwendungen von weicher Röntgenstrahlung I
(Physics and applications of soft X-rays I)

Sommersemester 2015

Veranstalter :
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Vorlesungstermine + Ort :
3 SWS (plus 1 SWS Laborbesichtigung) 6 ECTS Punkte
LMU Garching, Coulombwall 1
Mittwochs, 13:00 –16:00 Uhr, Seminarraum 224
(bis einschliesslich 3.6.) mündliche Abschlussprüfung

Vorlesungsinfos : www.xray.physik.uni-muenchen.de

Literatur:

Eberhard Spiller: Soft X-ray Optics / (SPIE Optical Engineering Press, Bellingham, Washington, ISBN 0-8184-1654-1)

A. Michette : X-ray Optics

D.T. Attwood: Soft X-ray and Extreme Ultraviolet Radiation (Cambridge Univ. Press, ISBN 0-521-65214-6)

Sowie aktuelle Wissenschaftspublikationen…

Begleitendes Seminar :

Studentische Vorträge zu aktuellen Forschungsarbeiten
(z.B. Röntgenmikroskopie, EUV Lithographie, Röntgenlaser, …)
Ort und Zeit : Mittwochs 16 c.t – 18 Uhr, Seminarraum 219

Outline :

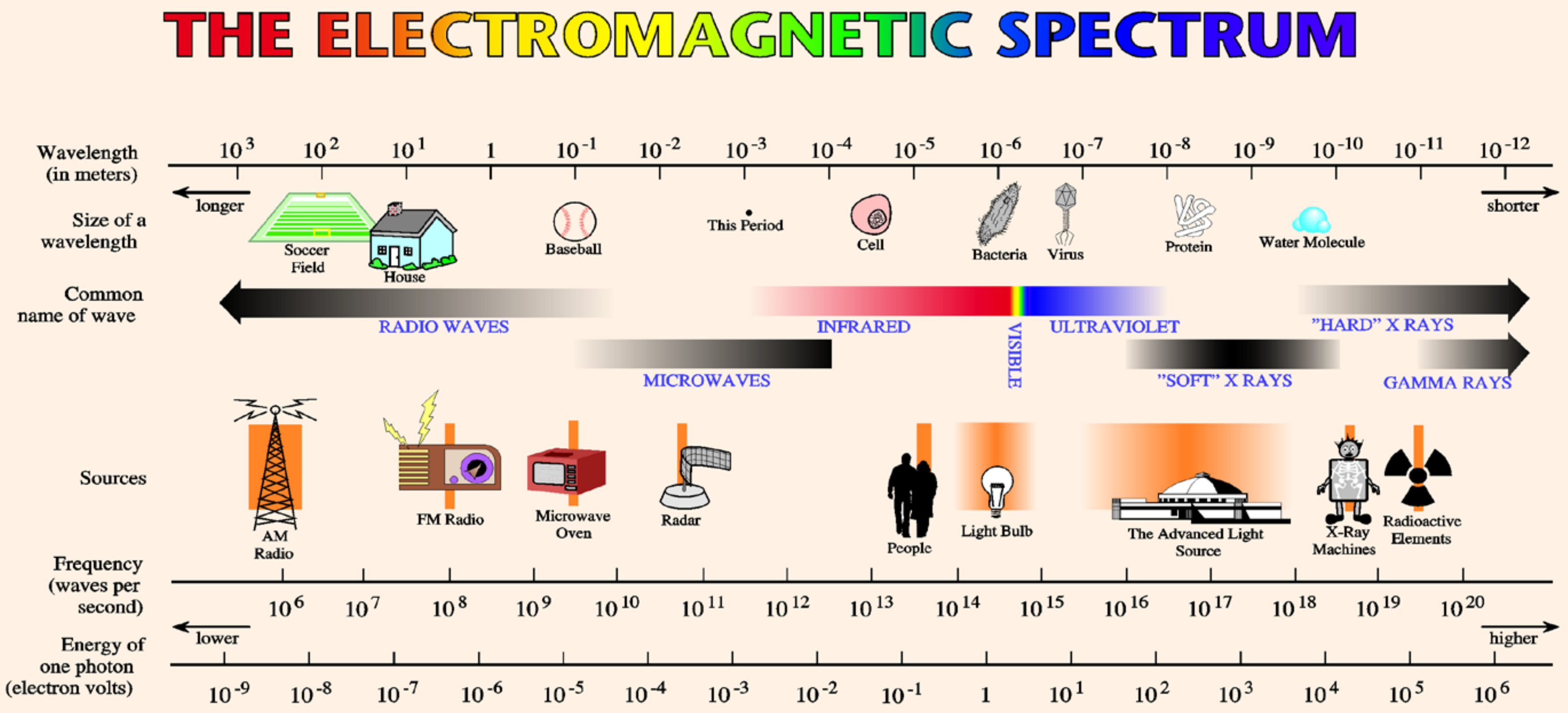
- **Basics :**
- Introduction to physics in the soft X-ray range
- Basic processes, emission and absorption
- Maxwell-equations, wave equation
- Scattering by free and bound electron
- Scattering by multiple electron atom, atomic scattering factor
- Complex refraction index, wave propagation in media
- **Thin films optics :**
- Interfaces, Fresnel-equations, total external reflection, Brewster angle
- Multilayer-Optics, basics, theory and technology
- **Sources :**
- Introduction to Synchrotron Radiation, Wigglers and Undulators
- Basics of the Free Electron Laser (FEL)
- Laser Plasma (LIP) and discharge plasma (DPP) sources
- X-ray lasers, High Harmonics
- **Nanooptics and diffractive optics**
- Diffractive optics, amplitude and phase gratings
- Zoneplates and refractive optics
- Waveguides and capillary optics
- **Detectors for soft X-rays**
- CCD, photodiode, DLD detector

Technology and applications :

- Soft X-ray microscopy and micro-spectroscopy
- Diffractive Imaging and Holography
- Extreme Ultraviolet Lithography
- Attosecond electron spectroscopy and microscopy
- Solar astronomy

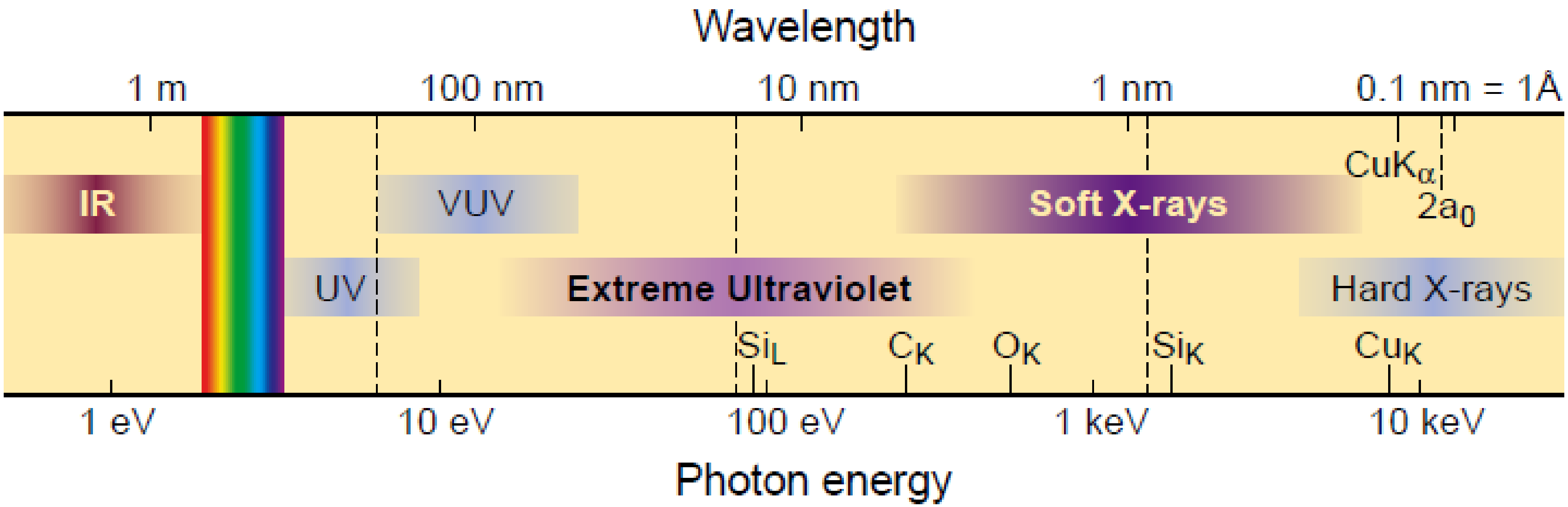
- ….

From radio waves to gamma rays



jc.fs/emspectrum/9-96

What is specific about the soft X-ray range ?



Short wavelength ~ 1 nm > see smaller features
> write smaller features

Core level electron energies > element specificity
> chemical specificity

Single cycle period sub-fsec > shortest electromagnetic pulses
> attosecond physics of e-dynamics

Resolution

How to determine the resolution of an optimal instrument / microscope ?

- Rayleigh-criterion:

$$d = \frac{0{,}61 * \lambda}{NA}$$

with λ = wavelength
NA = numerical Aperture

NA Animation : NA

http://micro.magnet.fsu.edu/primer/java/nuaperture/index.html

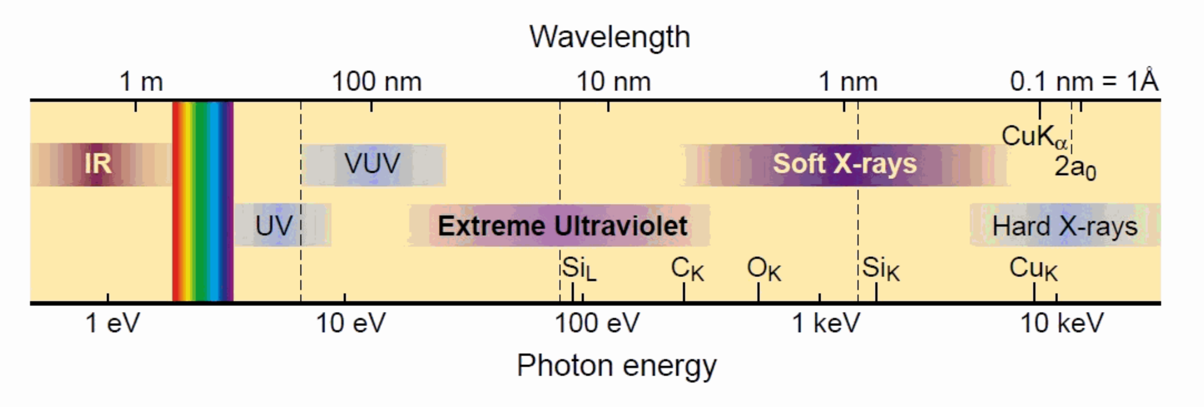
NA Immersion : NA Immersion

http://micro.magnet.fsu.edu/primer/java/microscopy/immersion/index.html

Rayleigh: Resolution

http://micro.magnet.fsu.edu/primer/java/imageformation/rayleighdisks/index.html

See smaller features with smaller wavelength !



X-ray microscopy in the water window

- Between the K-edge of carbon and oxygen

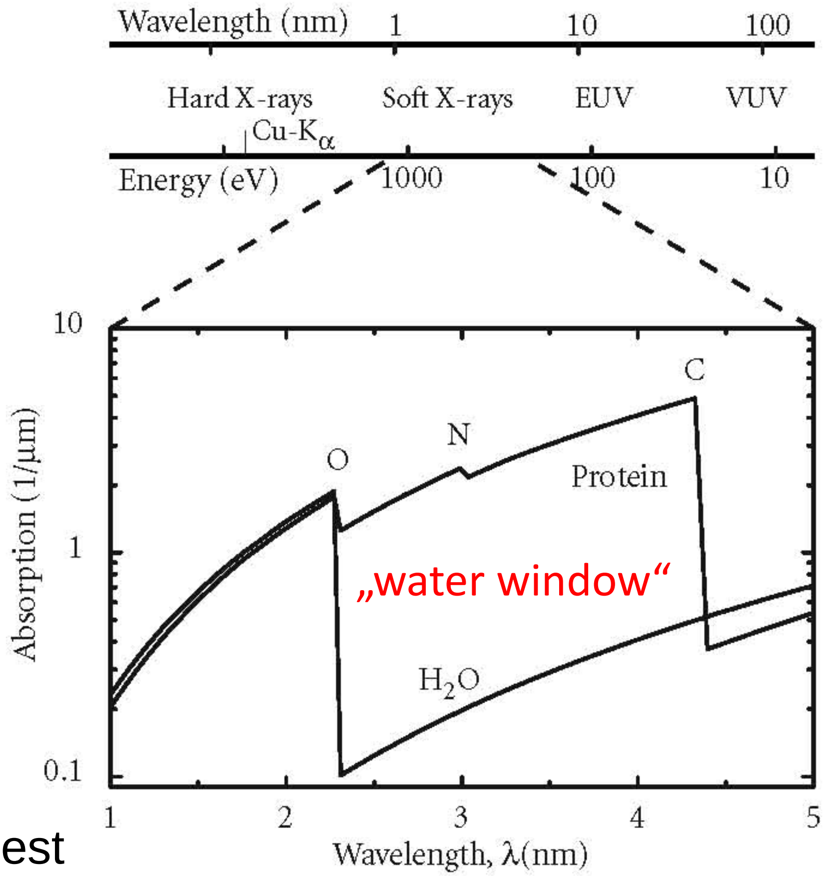
  K-absorption edge O_2 : 2.28 nm = 543.1 eV

  K-absorption edge C : 4.36 nm = 284.2 eV

- Natural contrast between materials containing carbon and water

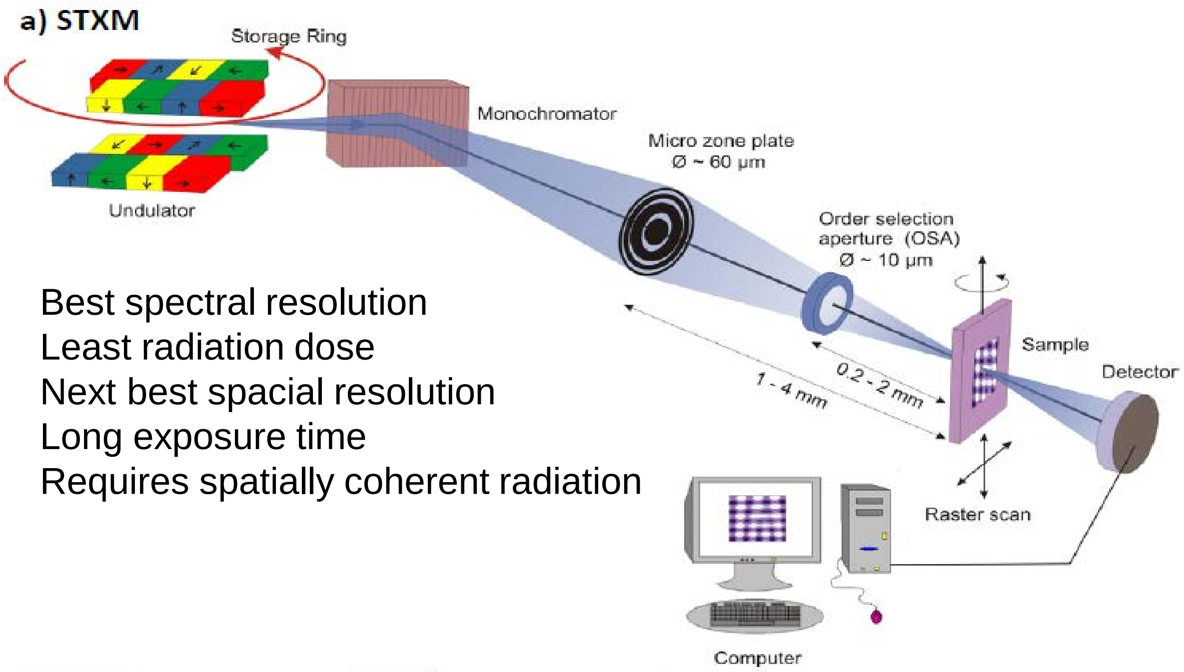
- In-Vivo image of biological objects with high resolution

➢ Of high microscopic and spectroscopic interest



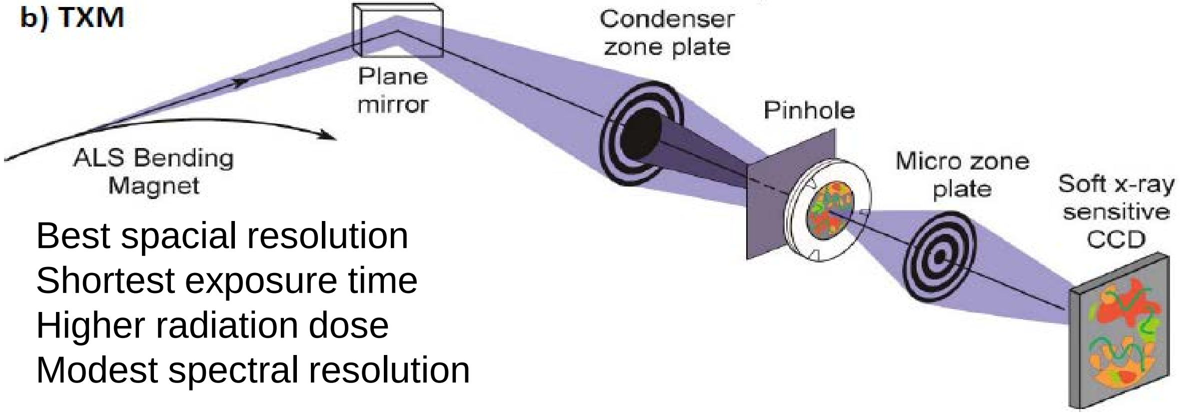
X-ray microscopy methods

a) STXM



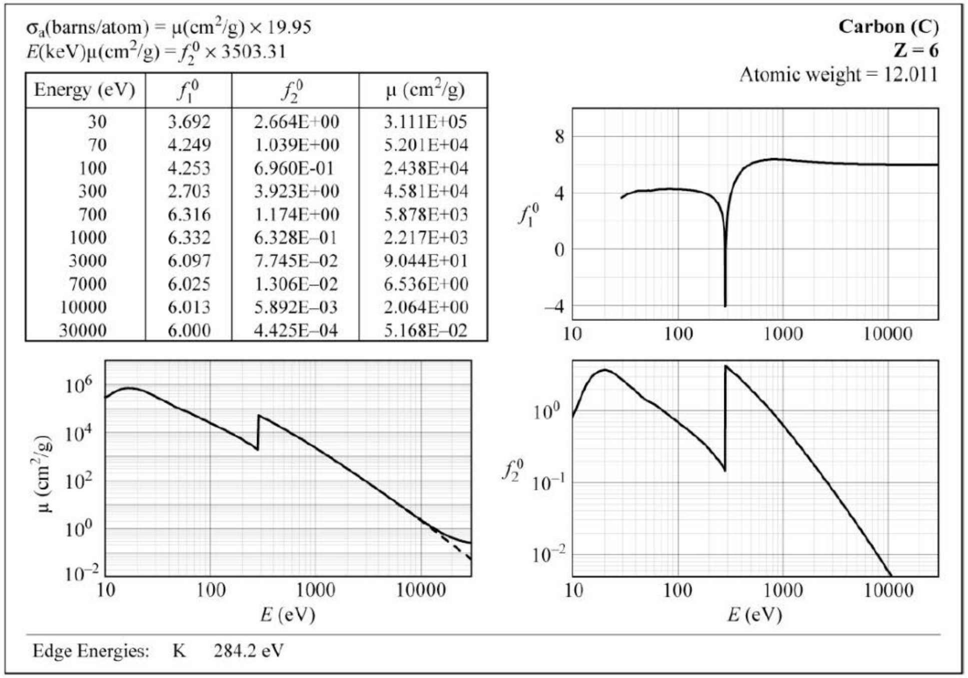
Best spectral resolution
Least radiation dose
Next best spacial resolution
Long exposure time
Requires spatially coherent radiation

b) TXM



Best spacial resolution
Shortest exposure time
Higher radiation dose
Modest spectral resolution

Refractive index, X-ray optics



σ_a(barns/atom) = μ(cm^2/g) × 19.95
E(keV)μ(cm^2/g) = f_2^0 × 3503.31

Carbon (C)
Z = 6
Atomic weight = 12.011

Energy (eV)	f_1^0	f_2^0	μ (cm^2/g)
30	3.692	2.664E+00	3.111E+05
70	4.249	1.039E+00	5.201E+04
100	4.253	6.960E−01	2.438E+04
300	2.703	3.923E+00	4.581E+04
700	6.316	1.174E+00	5.878E+03
1000	6.332	6.328E−01	2.217E+03
3000	6.097	7.745E−02	9.044E+01
7000	6.025	1.306E−02	6.536E+00
10000	6.013	5.892E−03	2.064E+00
30000	6.000	4.425E−04	5.168E−02

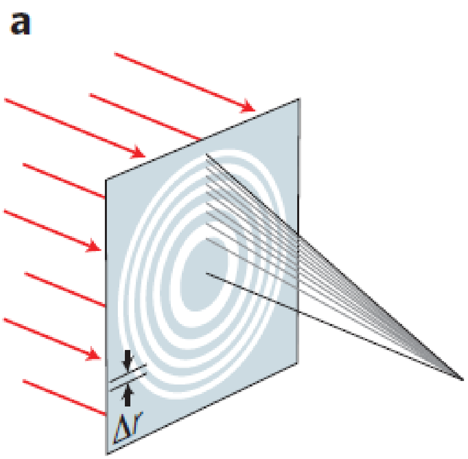
Edge Energies: K 284.2 eV

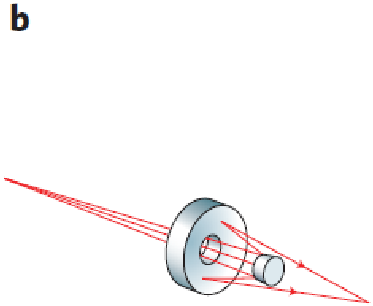
(Henke and Gullikson; www-cxro.LBL.gov)

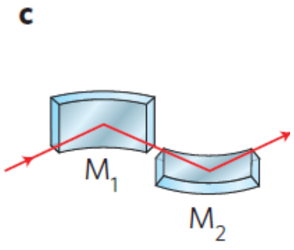
Ch02_F13VG.ai

Four common X-ray microscopy optics:

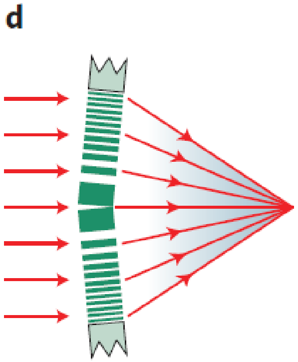
a) Zone plate
b) Schwarzschild optics
c) Kirkpatrick-Baez mirror pair
d) Laue lens



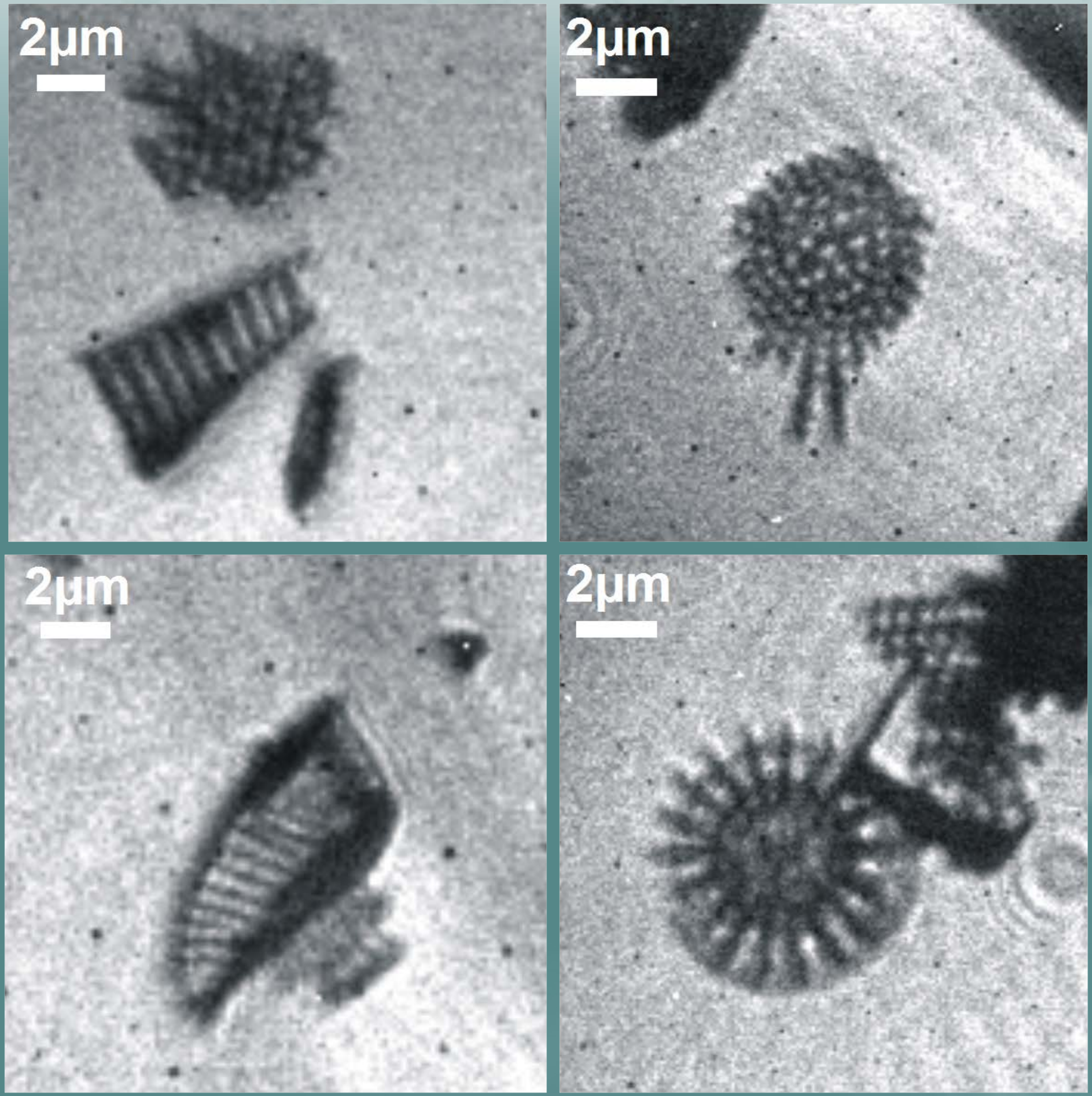




$$\theta_c = \sqrt{2\delta}$$



See smaller features : soft X-ray microscopy

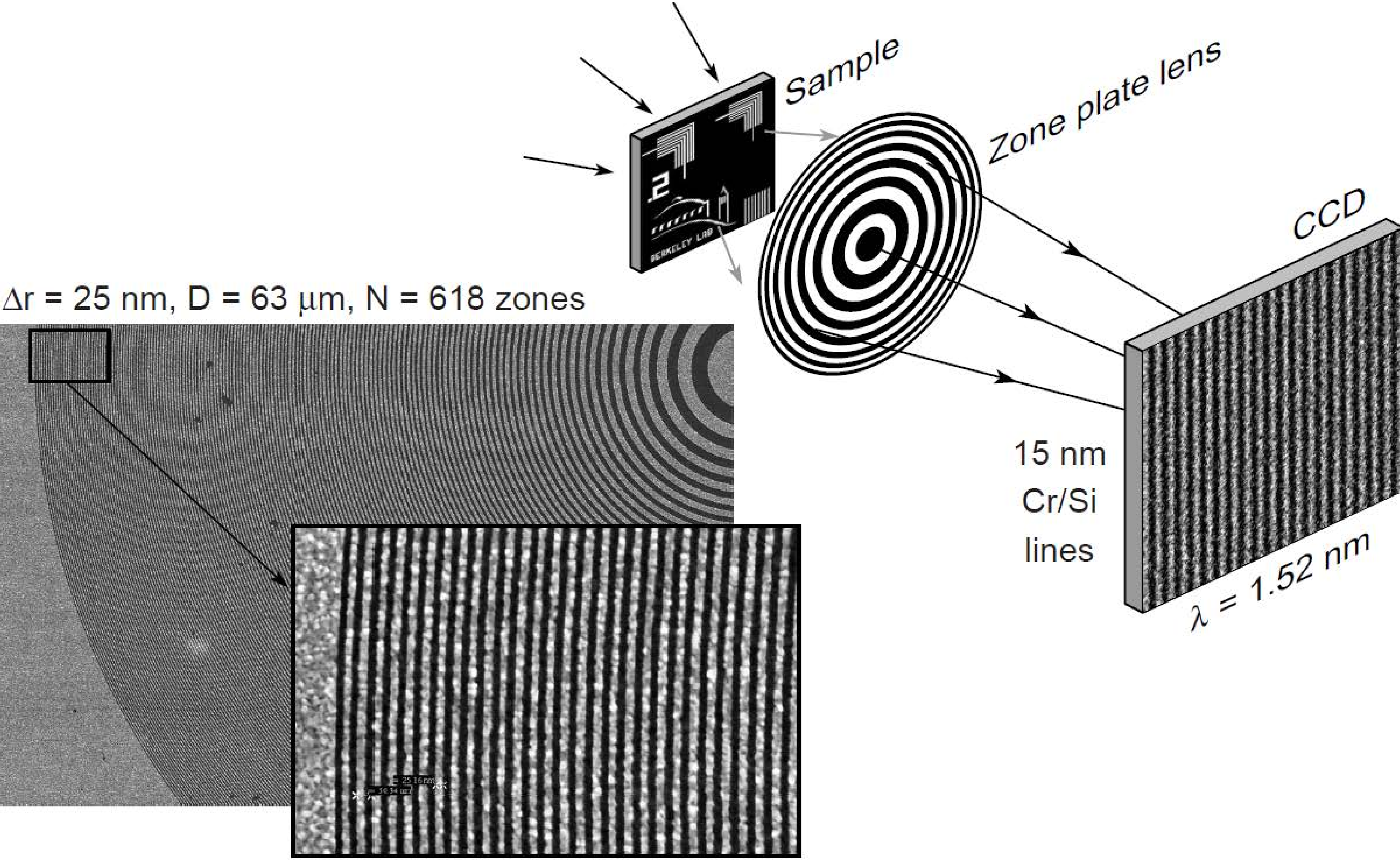


Soft X-ray microscopy
on diatoms (silica algae)

Eph = 97 eV

Lateral resolution :
< 200 nm

Soft X-Ray Microscopy at the ALS



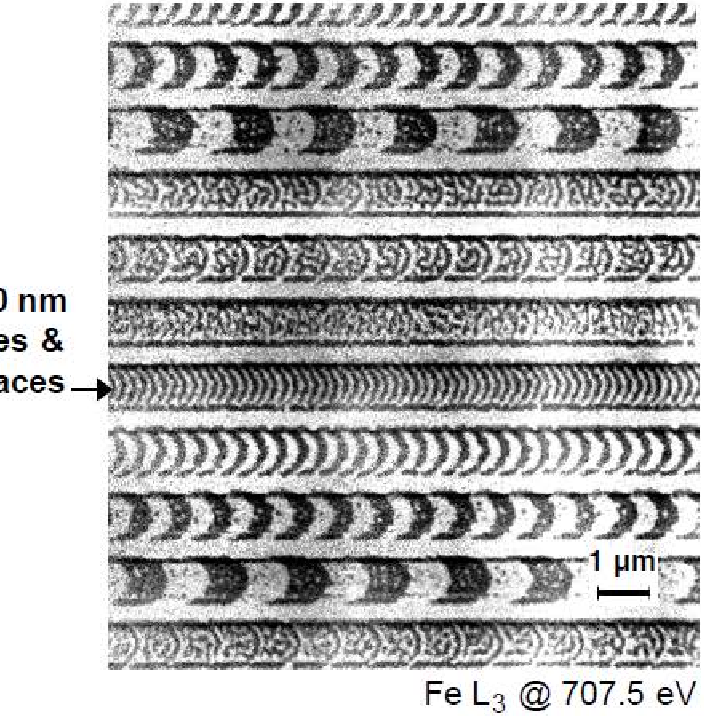
Δr = 25 nm, D = 63 μm, N = 618 zones

Courtesy of E. Anderson and W. Chao (CXRO/LBNL)

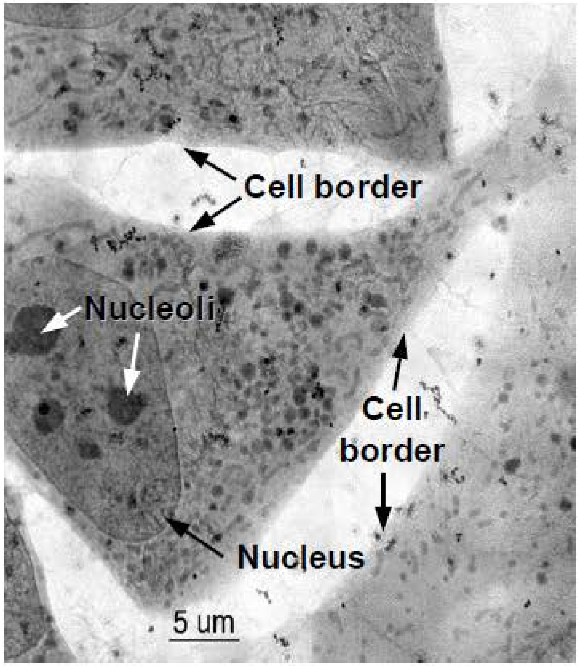
Applications of Soft X-Ray Microscopy

Magnetic Recording Materials

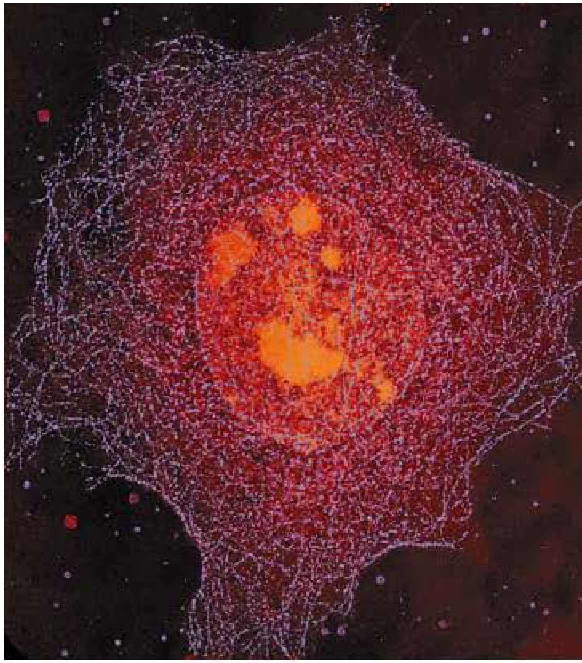
Cryo Microscopy for the Life Sciences



FeTbCo Multilayer
with AL Capping Layer



Cryo X-Ray Microscopy
of 3T3 Fibroblast Cells



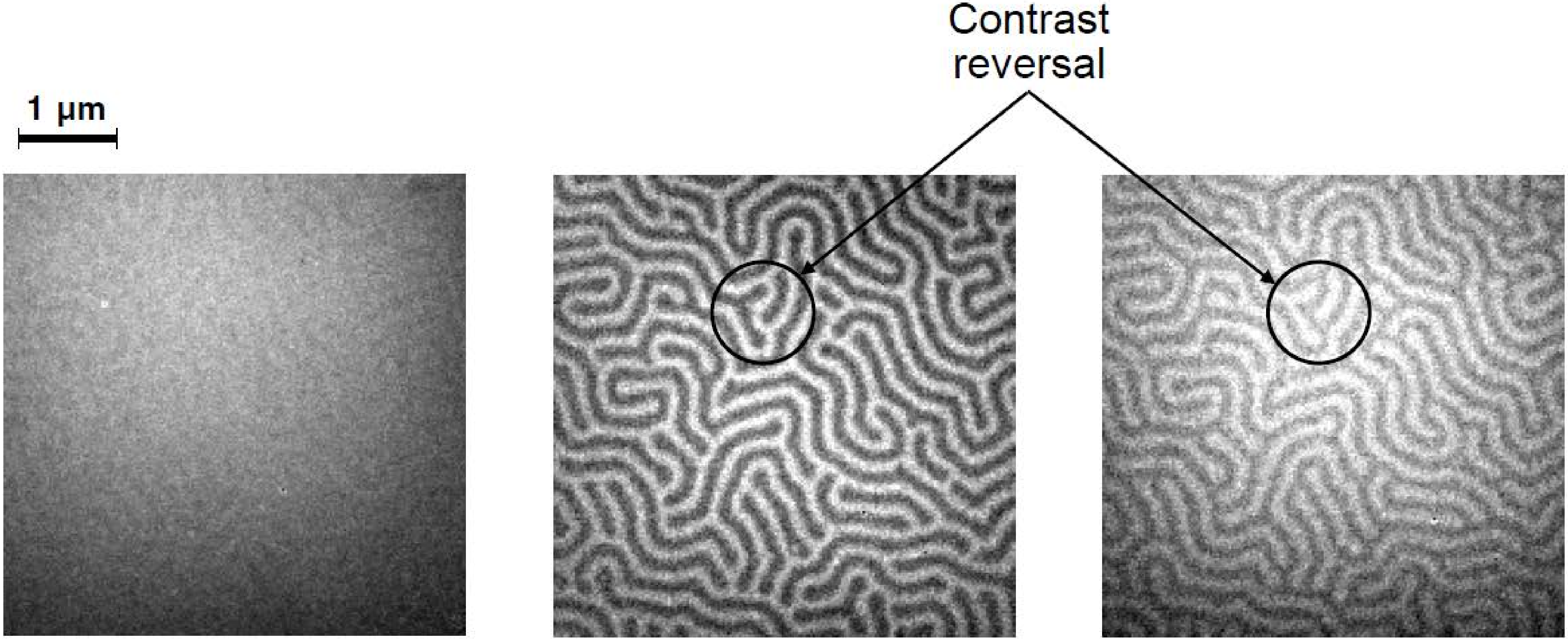
Protein Labeled
Microtubule Network

Courtesy of P. Fischer, Wuerzberg
and G.Denbeaux, CXRO/LBNL

Courtesy of C. Larabell, UCSF
and W. Meyer-Ilse, CXRO/LBNL

Different Photons Energies

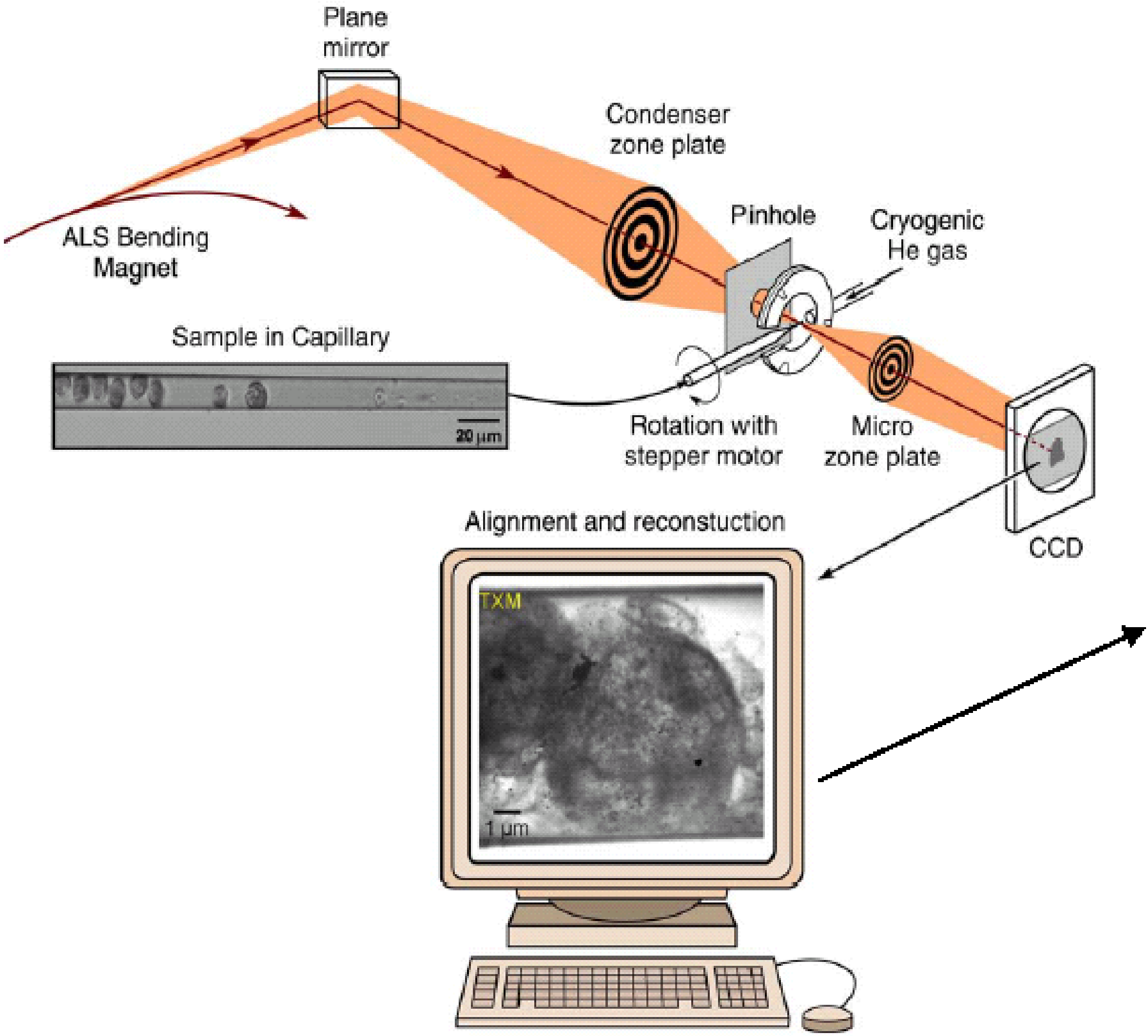
FeGd Multilayer

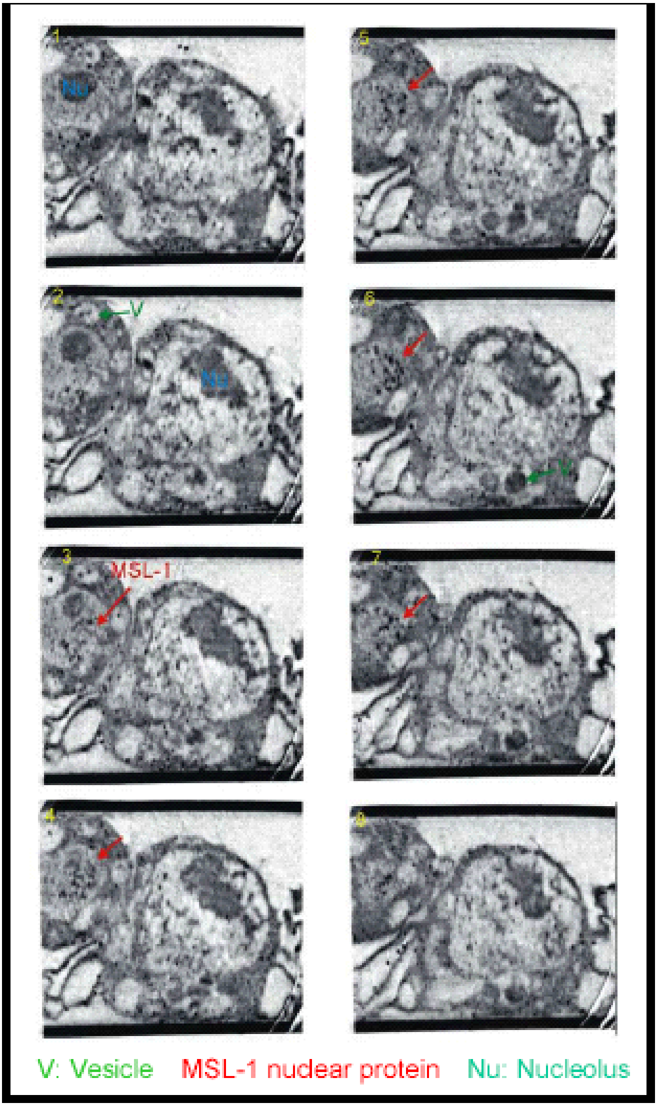


$\hbar\omega$ = 704 eV
below Fe L-edges

$\hbar\omega$ = 707.5 eV
Fe L_3-edge

$\hbar\omega$ = 720.5 eV
Fe L_2-edge

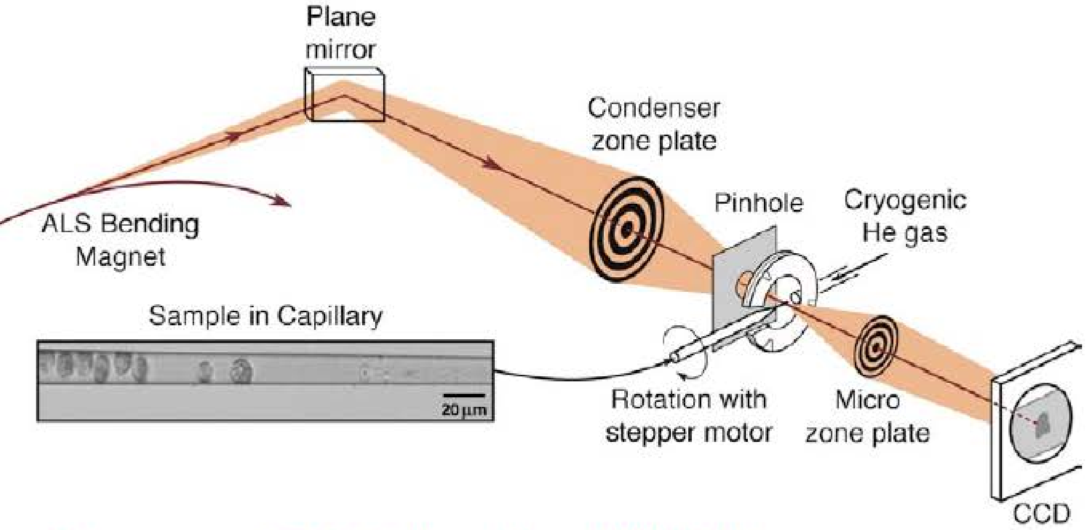




150 nm thick slices through the volume

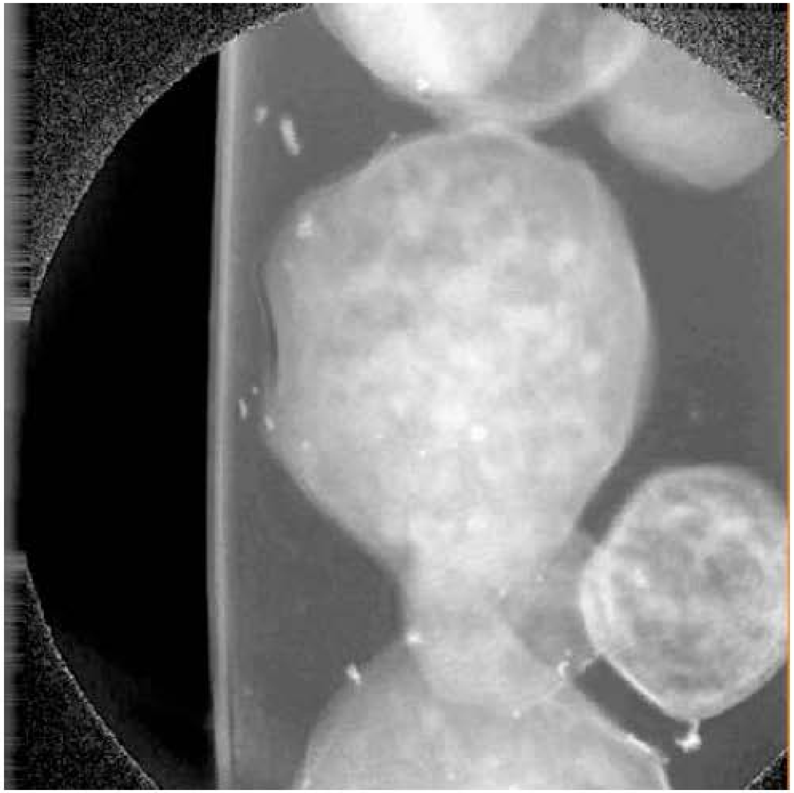
Bio-Nanotomography for 3D Imaging of Cells

Nanotomography of Cryogenic Fixed Cells



Courtesy of G. Schneider (BESSY)
Surf. Rev. Lett. 9, 177 (2002)

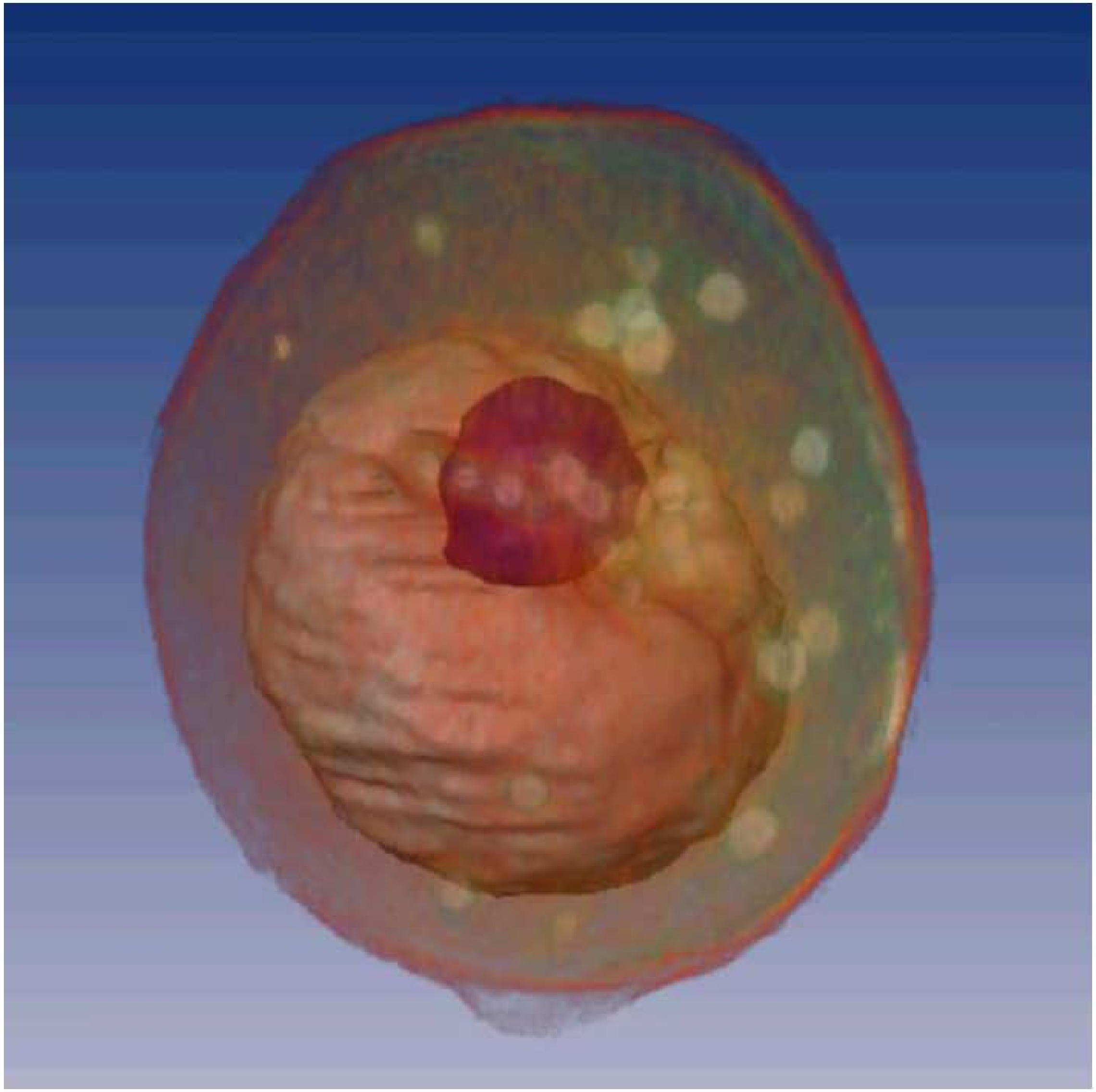
Soft X-Ray Nanotomography of a Yeast Cell



λ = 2.5 nm

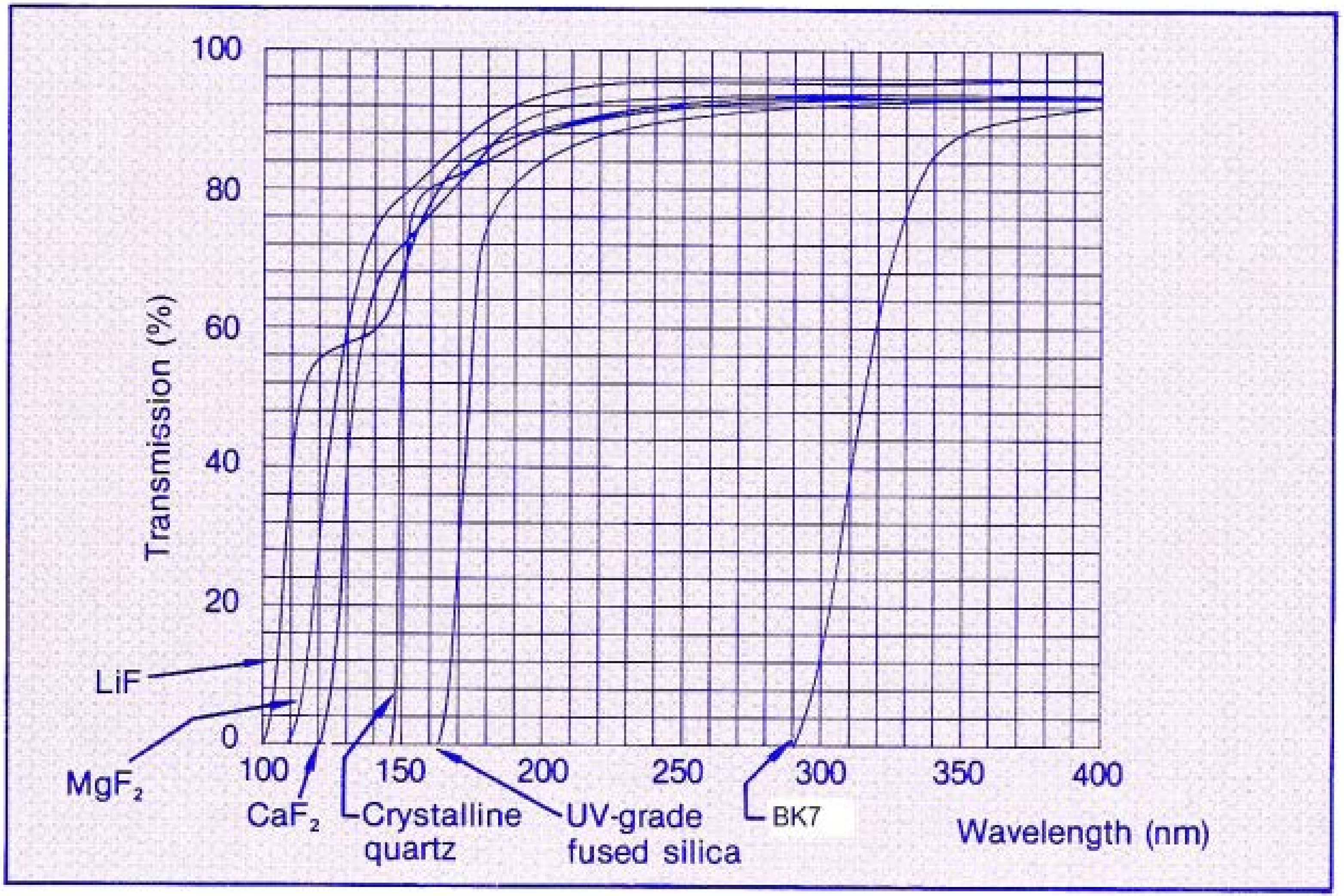
Courtesy of C. Larabell (UCSF & LBNL)
and M. LeGros (LBNL)

Soft X-Ray Nano Tomography of a Yeast Cell



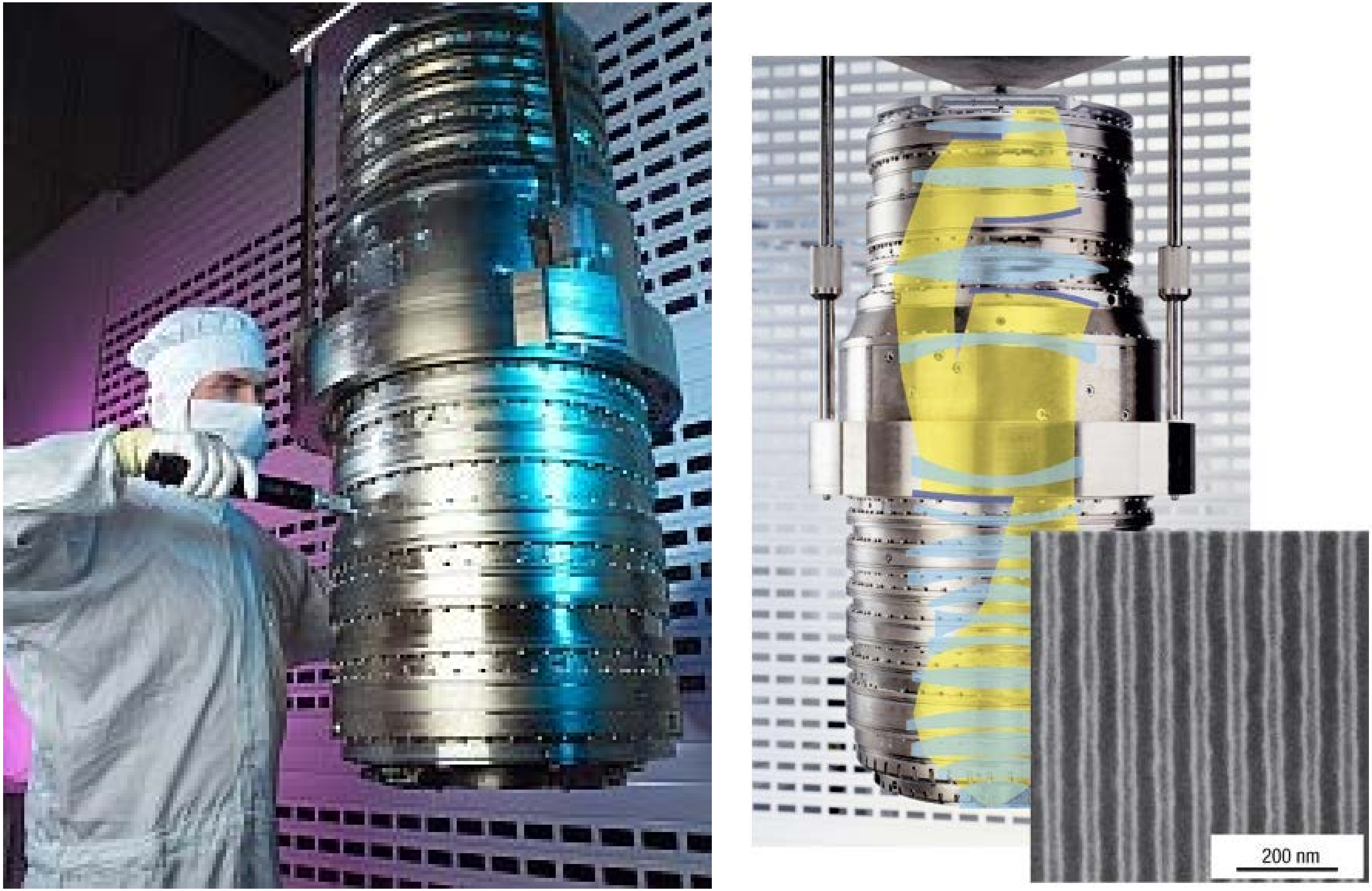
Courtesy of C. Larabell / UCSF & LBNL, and M. LeGros / LBNL

Transmission of fluoride materials in the DUV



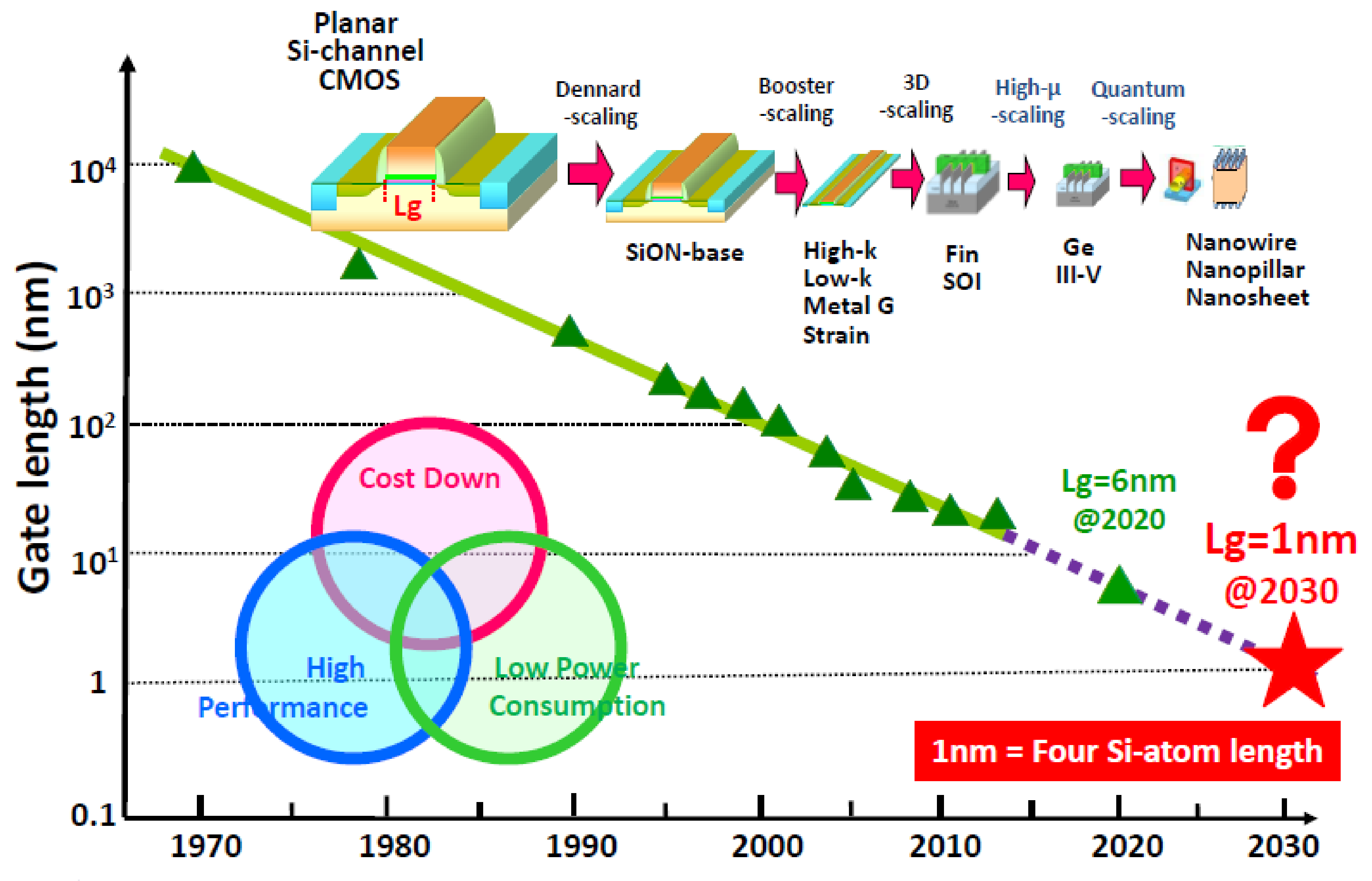
- ➢ No window materials below 110 nm wavelength
- ➢ No conventional transmission lenses possible !

193 nm DUV lithography objective (Zeiss)



> CaF aspherical lense optics

Write smaller features : Extreme Ultraviolet Lithography

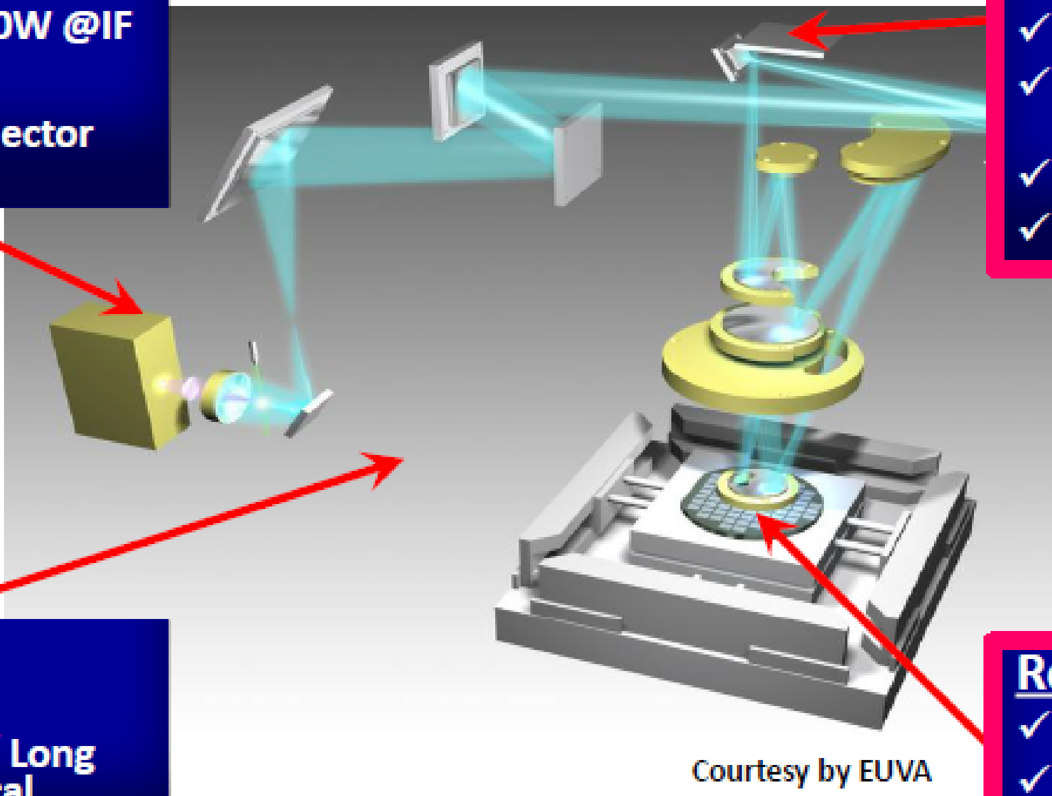


Challenges of Extreme Ultraviolet Lithography

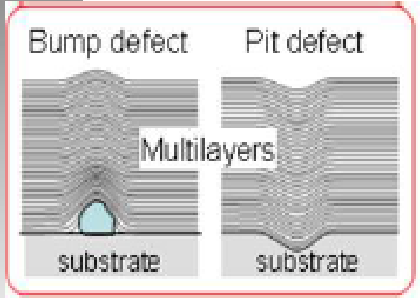
Source
- ✓ High power: 250W @IF
- ✓ Stability
- ✓ Long Life of Collector Mirror

Scanner
- ✓ Field data
- ✓ Higher quality / Long lifetime of optical components

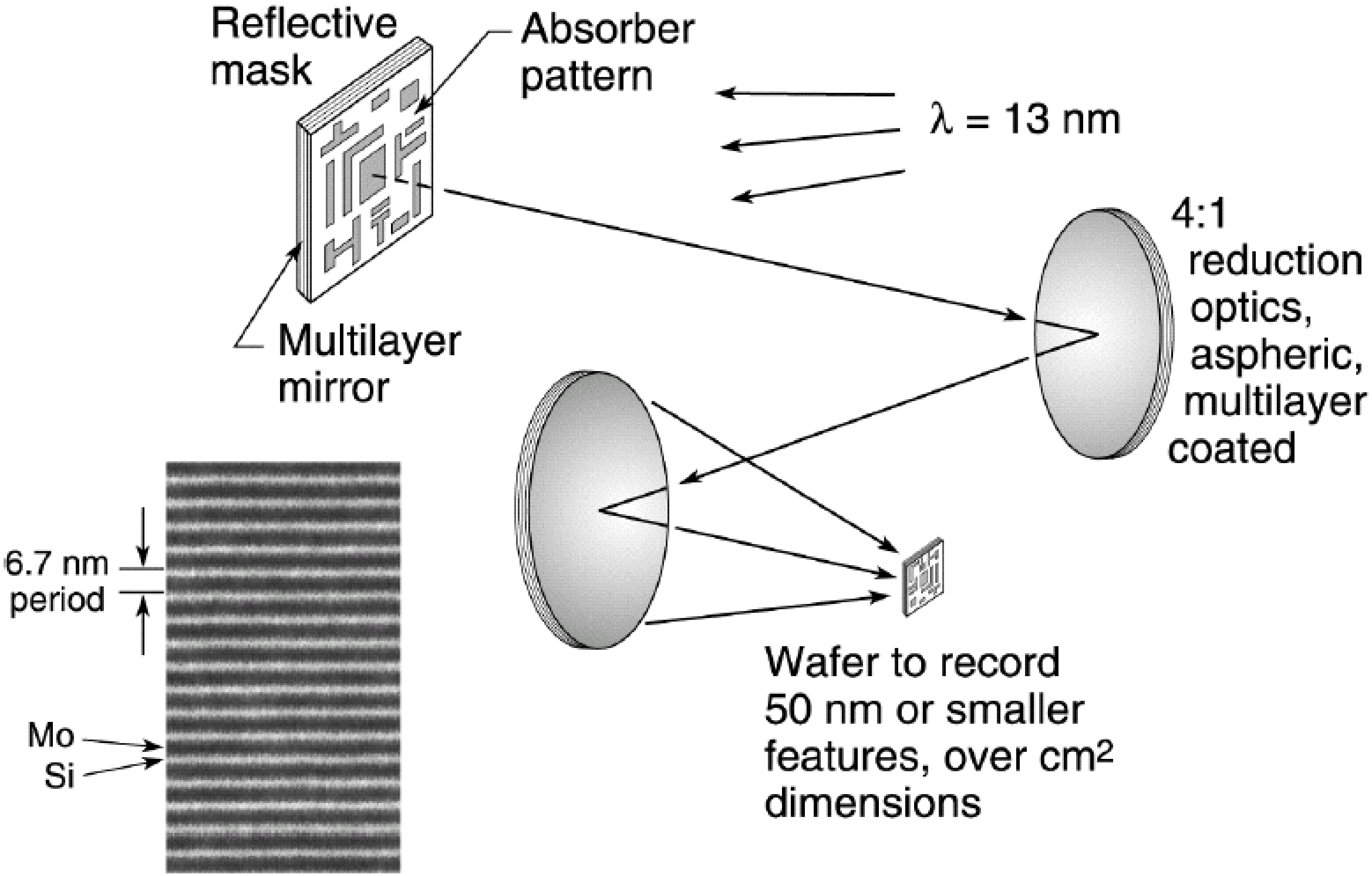
Mask
- ✓ Blank Inspection
- ✓ Patterned Mask Inspection
- ✓ Defect Review System
- ✓ Particle Free Handling

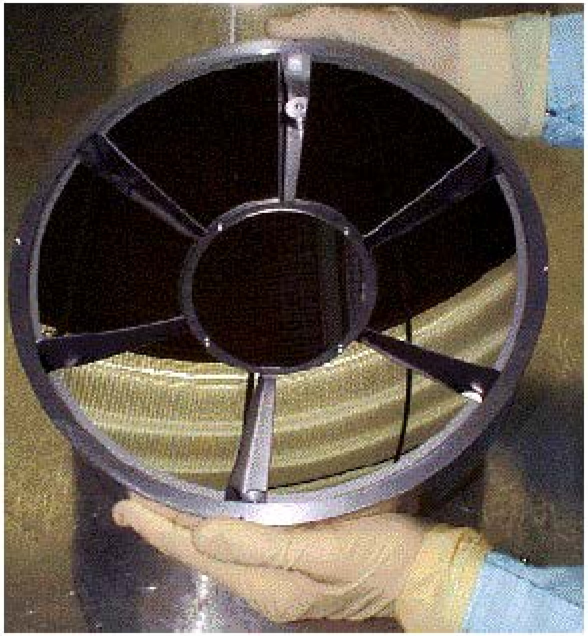


Courtesy by EUVA



Resist
- ✓ Resolution < 20nmHP
- ✓ Sensitivity < $10 mJ/cm^2$
- ✓ LER < 2nm
- ✓ Lower outgassing

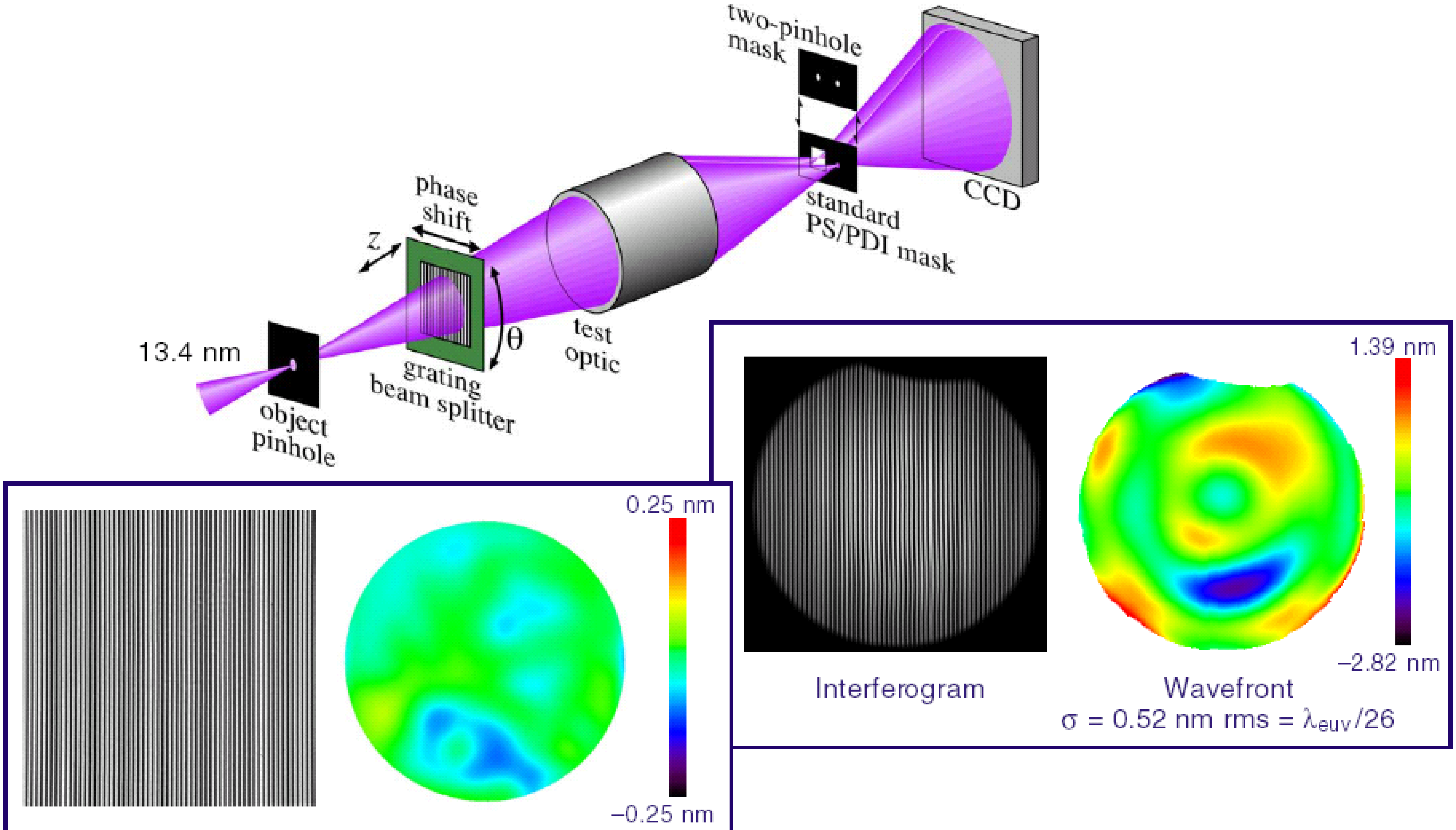

Reflective mask
Absorber pattern
λ = 13 nm
Multilayer mirror
4:1 reduction optics, aspheric, multilayer coated
6.7 nm period
Mo
Si
Wafer to record 50 nm or smaller features, over cm2 dimensions



Condenser optic

Projection optic

Courtesy of J. Taylor and D. Sweeney / LLNL



Interferogram

Wavefront

$\sigma = 0.52$ nm rms $= \lambda_{euv}/26$

Null test interferogram

Reference wavefront

$\sigma = 0.044$ nm rms $= \lambda_{euv}/300$

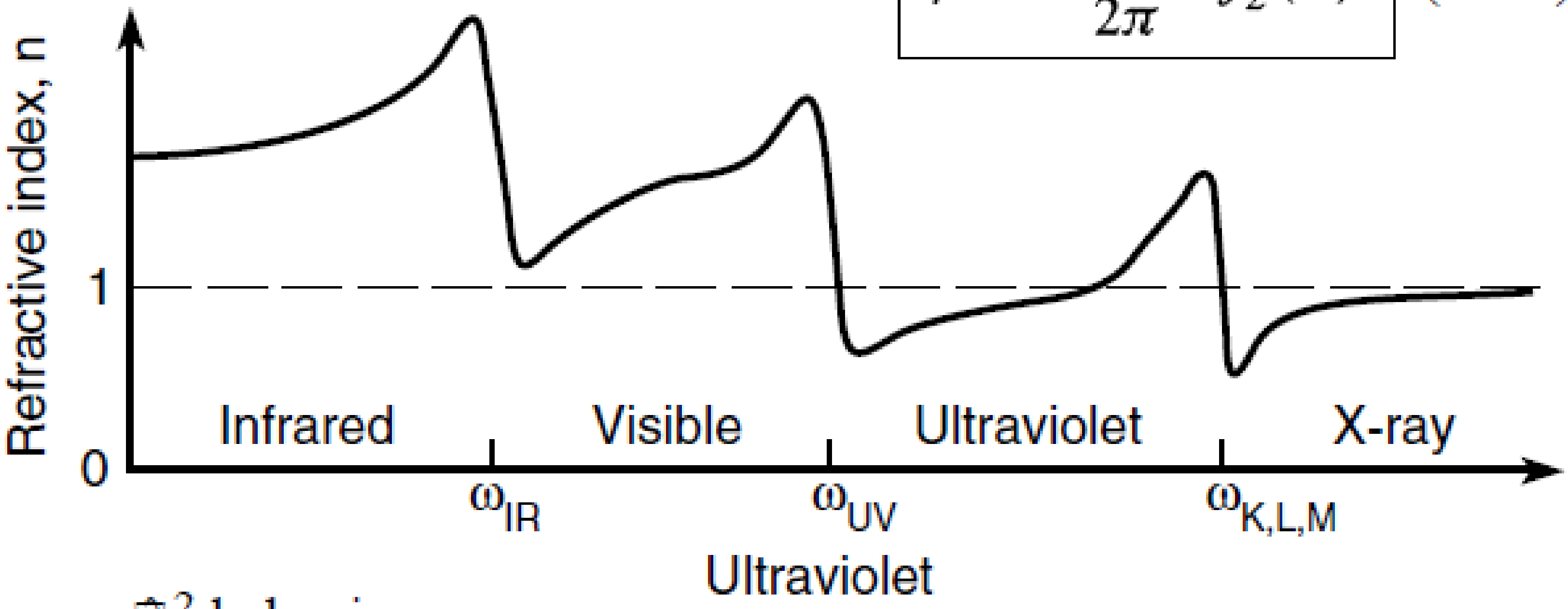
Courtesy of K. Goldberg, P. Naulleau, J. Bokor, et al., LBNL.

Complex index of refraction/atomic scattering factors

$$\boxed{n(\omega) = 1 - \delta + i\beta} \quad (3.12)$$

$$\delta = \frac{n_a r_e \lambda^2}{2\pi} f_1^0(\omega) \quad (3.13a)$$

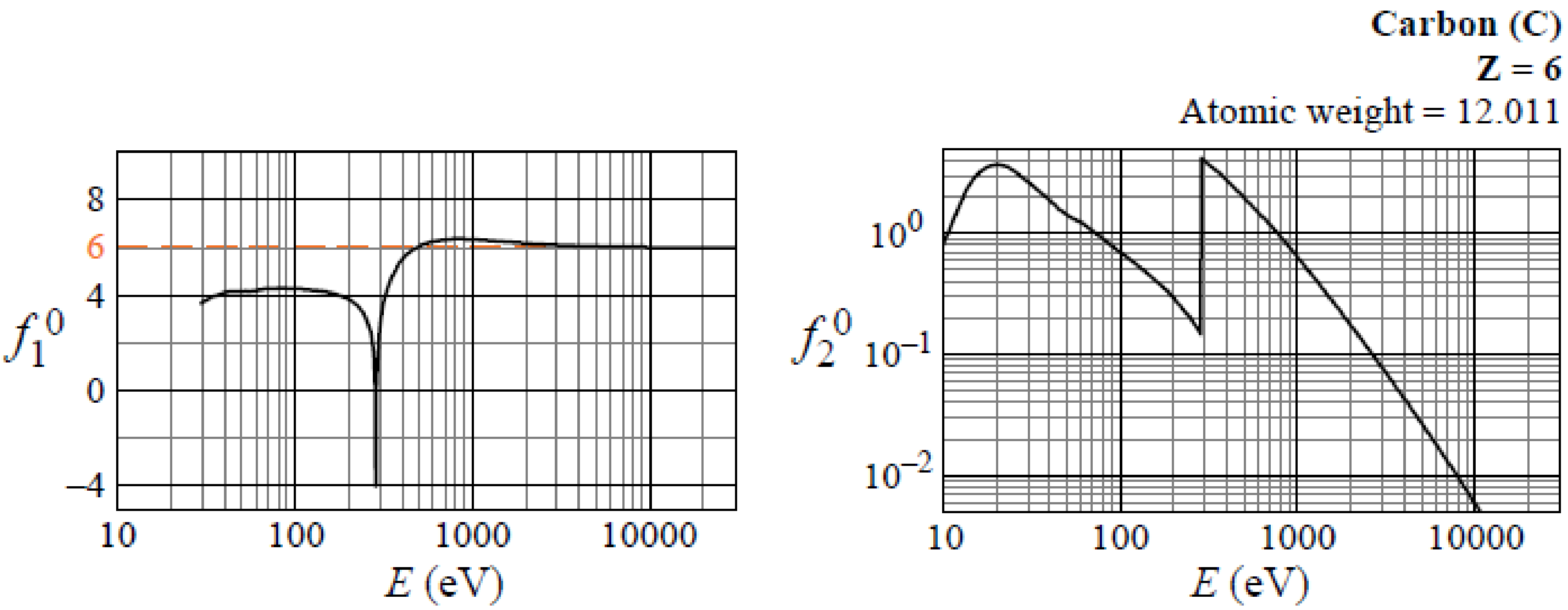
$$\beta = \frac{n_a r_e \lambda^2}{2\pi} f_2^0(\omega) \quad (3.13b)$$



- λ^2 behavior
- δ & β << 1
- δ-crossover

Complex atomic scattering factors

$$f^0(\omega) = f_1^0(\omega) - i f_2^0(\omega)$$



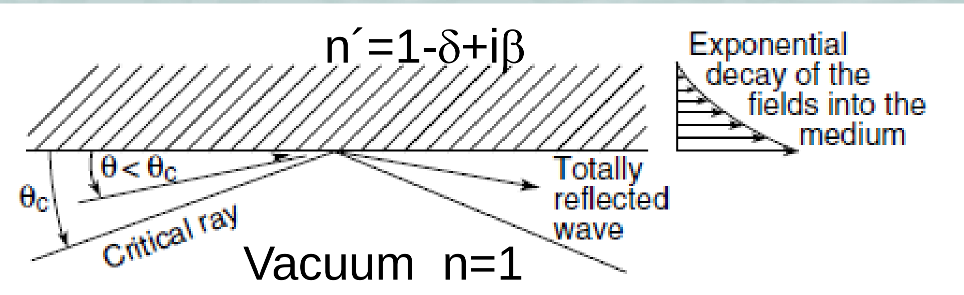
(Henke and Gullikson; www-cxro.LBL.gov)

valid only for : long wavelength $\lambda >> a_0$ (0.529 A) or forward scattering

f_1 equals Z for $\omega >> \omega_s$ all electrons scatter in phase !

Scattering cross section ~ Z^2

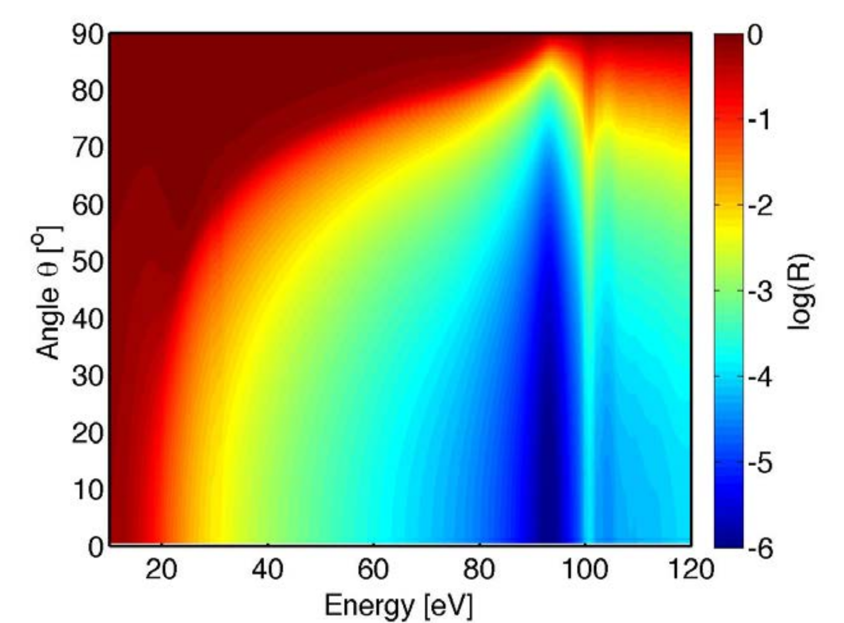
Single interface optics (example Si)

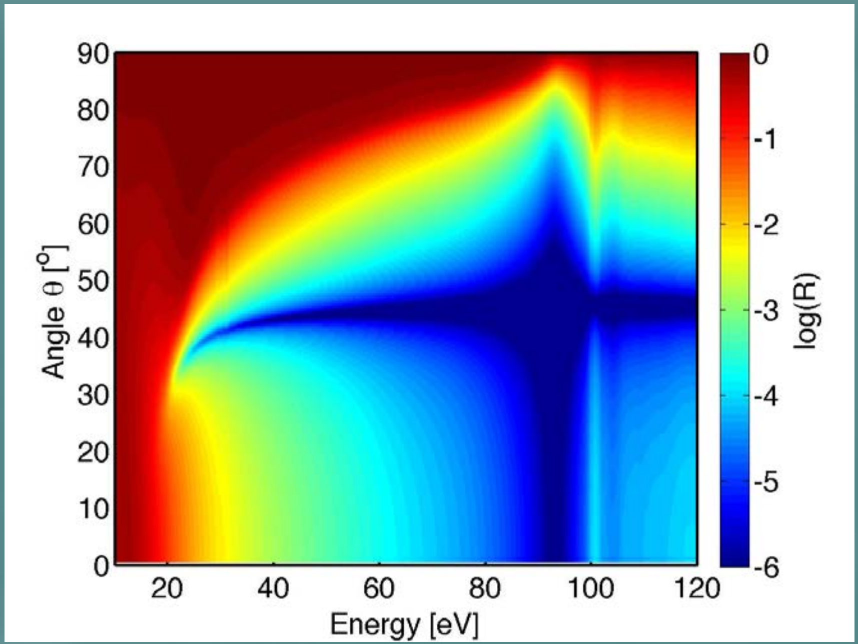


Snell´s law :
sin ϕ' = sin ϕ /n´
Critical angle : $\Theta_c = 2\delta^{1/2}$

S- polarisation

P- polarisation





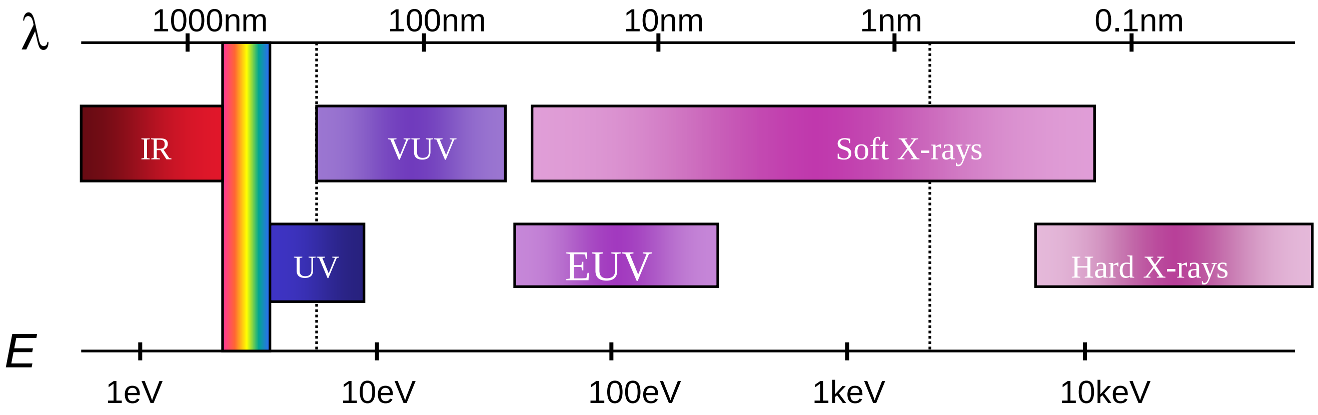
$$R_s = \frac{\left|\cos\phi - \sqrt{n^2 - \sin^2\phi}\right|^2}{\left|\cos\phi + \sqrt{n^2 - \sin^2\phi}\right|^2}$$

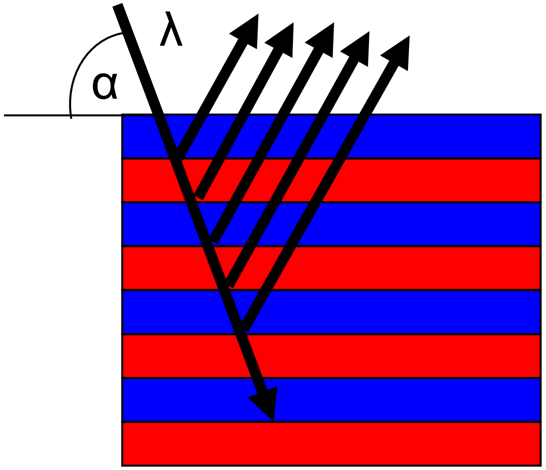
Fresnel Equations (s, p pol.)

$$R_p = \left|\frac{E_0''}{E_0}\right|^2 = \frac{\left|n^2\cos\phi - \sqrt{n^2 - \sin^2\phi}\right|^2}{\left|n^2\cos\phi + \sqrt{n^2 - \sin^2\phi}\right|^2}$$

$R_{perp} = (\delta^2 + \beta^2)/4$

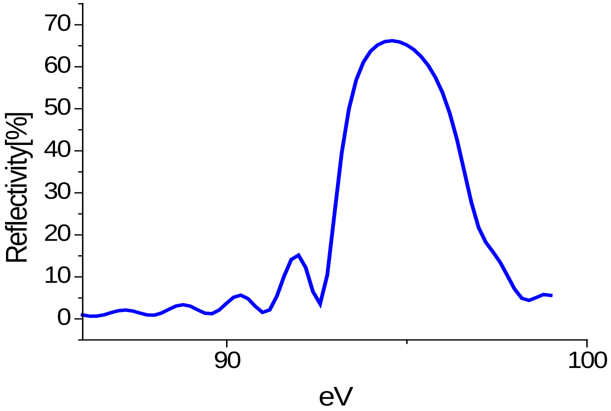
Principle of XUV multilayer mirrors at near normal incidence angles



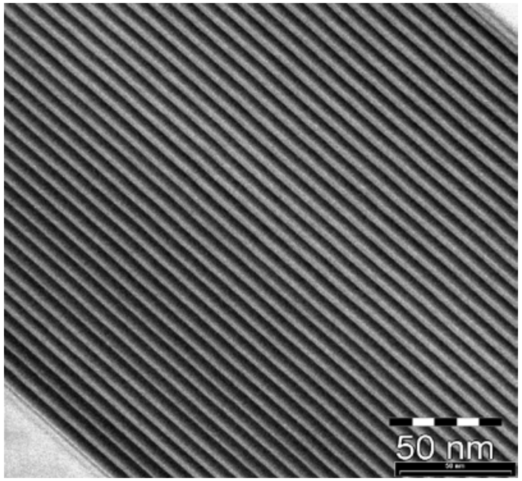


Principle of an XUV multilayer mirror

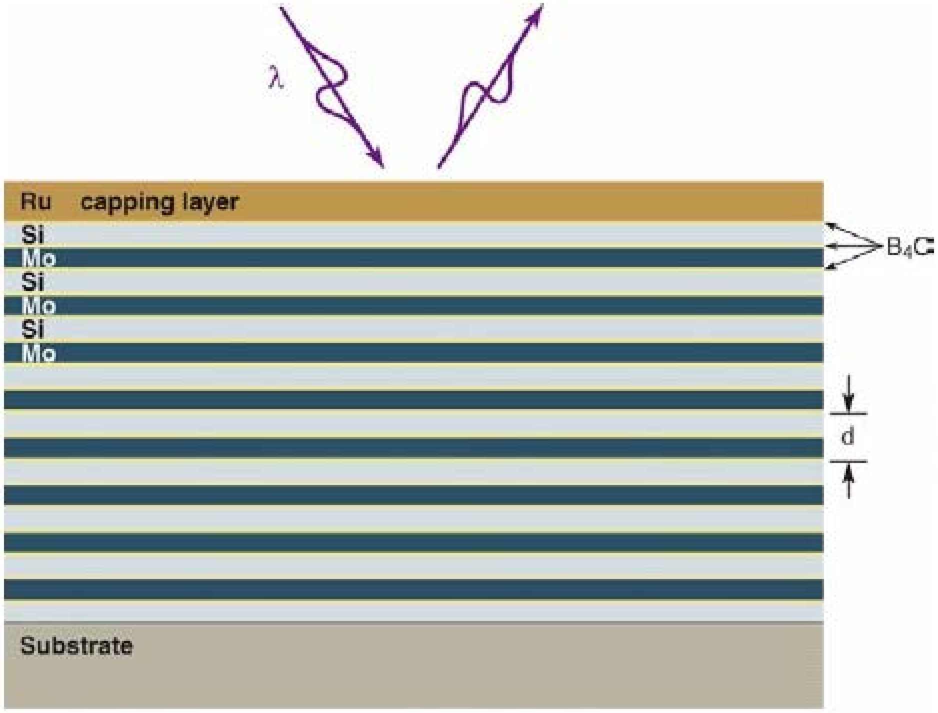
$$m\lambda = 2d\cos\alpha\sqrt{1-\frac{2\delta-\delta^2}{\cos^2\alpha}}$$



68% measured reflectivity of a MoSi multilayer mirror @ 93 eV



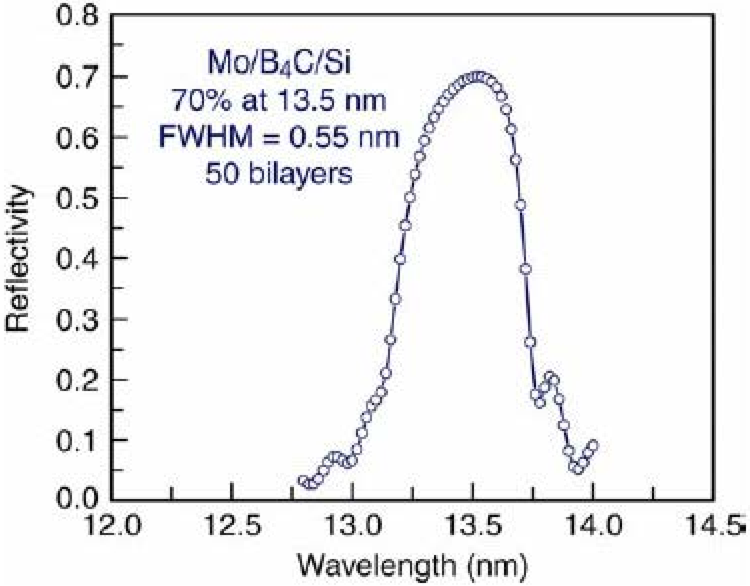
TEM image of a MoSi multilayer



λ = 13.4 nm

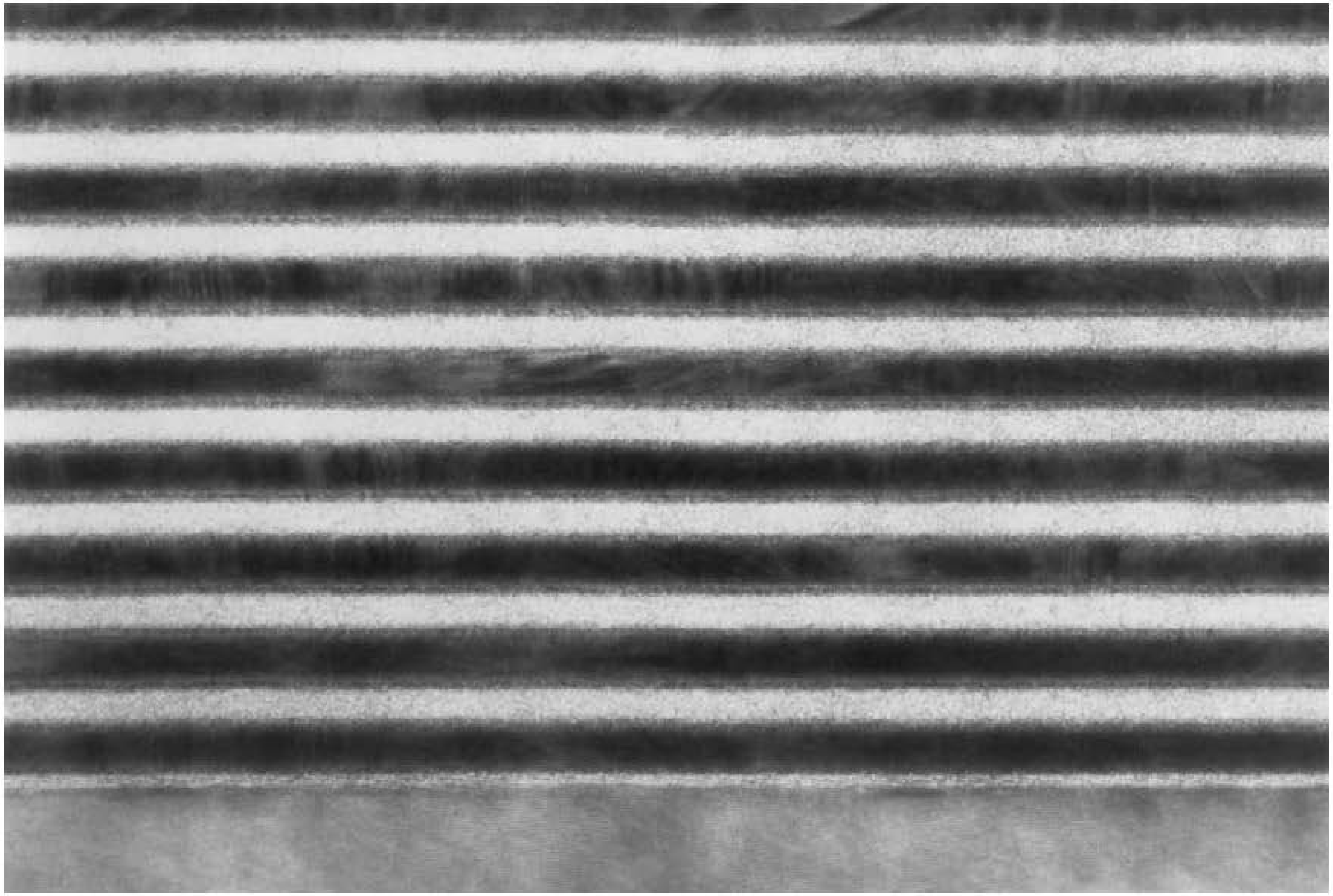
Ru (1.70 nm)
Si (4.14 nm)
B_4C (0.25 nm)
Mo (2.09 nm)
B_4C (0.40 nm)

d = 6.88 nm
Γ = 0.34



Courtesy of Saša Bajt / LLNL

Mo/Si Multilayer Coating

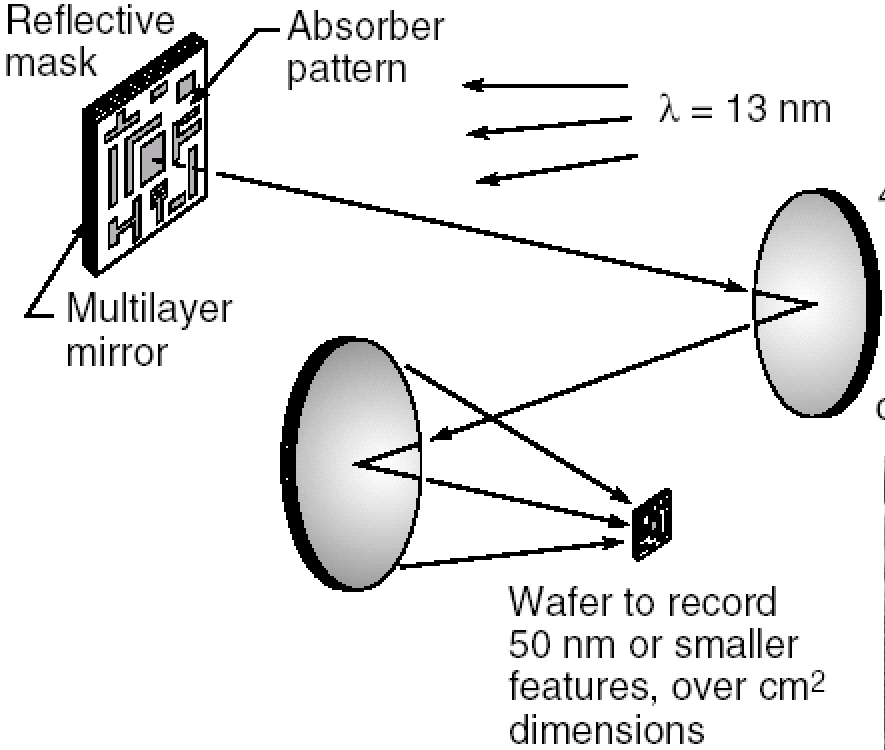


(T. Nguyen, CXRO/LBNL)

First year of volume production	**2001**	**2003*** ~~**2004**~~	**2005*** ~~**2007**~~	**2007*** ~~**2010**~~	**2009*** ~~**2013**~~	**2011*** ~~**2016**~~
Technology Generation (Dense lines, printed in resist)	130 nm	90 nm	65 nm	45 nm	32 nm	23 nm
Isolated Lines (in resist) [Physical gate, post-etch]	90 nm [65 nm]	53 nm [37 nm]	35 nm [25 nm]	25 nm [18 nm]	18 nm [13 nm]	13 nm [9 nm]
Chip Frequency	1.7 GHz	4.0 GHz	6.8 GHz	12 GHz	19 GHz	29 GHz
Transistors per chip (HV) (3 × for HP ; 5 × for ASICs)	100 M	190 M	390 M	780 M	1.5 B	3.1 B
DRAM Memory (bits)	510 M	1.1 G	4.3 G	8.6 G	34 G	69 G
Gate CD Control (3σ, post-etch)	5 nm	3 nm	2 nm	1.5 nm	1.1 nm	0.7 nm
Field Size (mm × mm)	25 × 32	25 × 32	22 × 26	22 × 26	22 × 26	22 × 26
Chip Size (mm) (2.2 × for HP ; to 4 × for ASIC)	140	140	140	140	140	140
Water Size (diameter)	300 mm	300 mm	300 mm	450 mm	450 mm	450 mm

*Semiconductor Industry Association (SIA), December 2001. ***Possible 2-year cycle.**

Extreme Ultraviolet (EUV) Lithography



Reflective mask

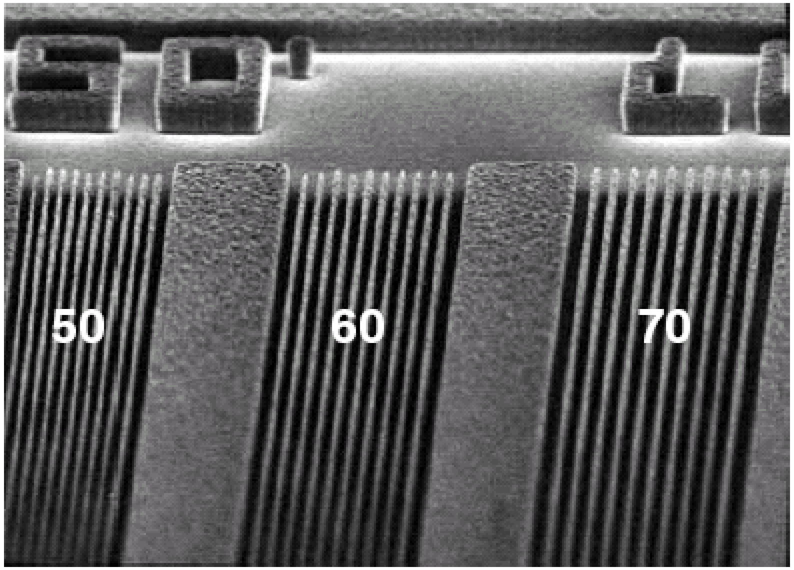
Absorber pattern

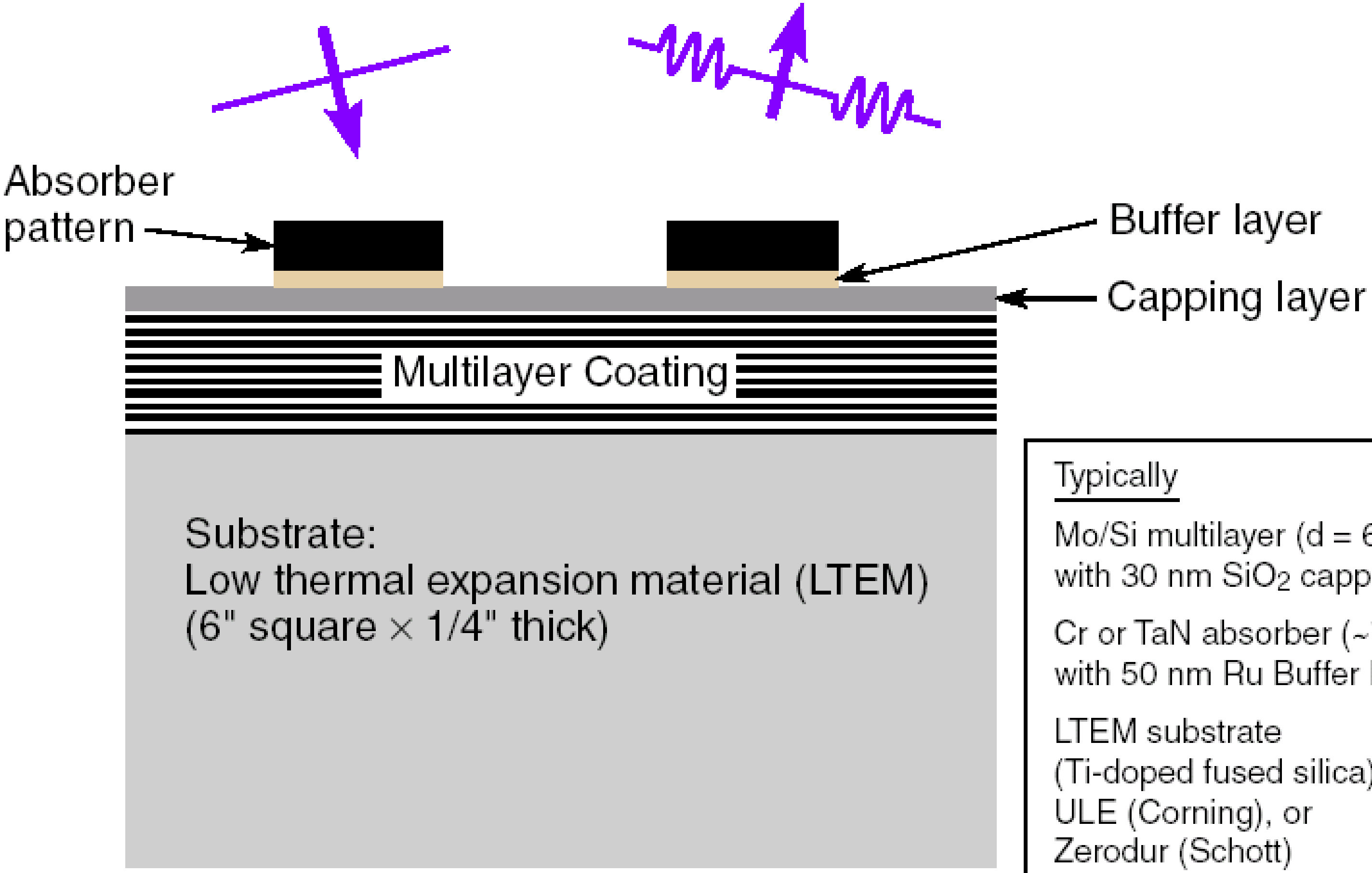
$\lambda = 13$ nm

Multilayer mirror

4:1 reduction optics, aspheric, multilayer coated

Wafer to record 50 nm or smaller features, over cm^2 dimensions





Absorber pattern

Buffer layer

Capping layer

Multilayer Coating

Substrate:
Low thermal expansion material (LTEM)
(6" square × 1/4" thick)

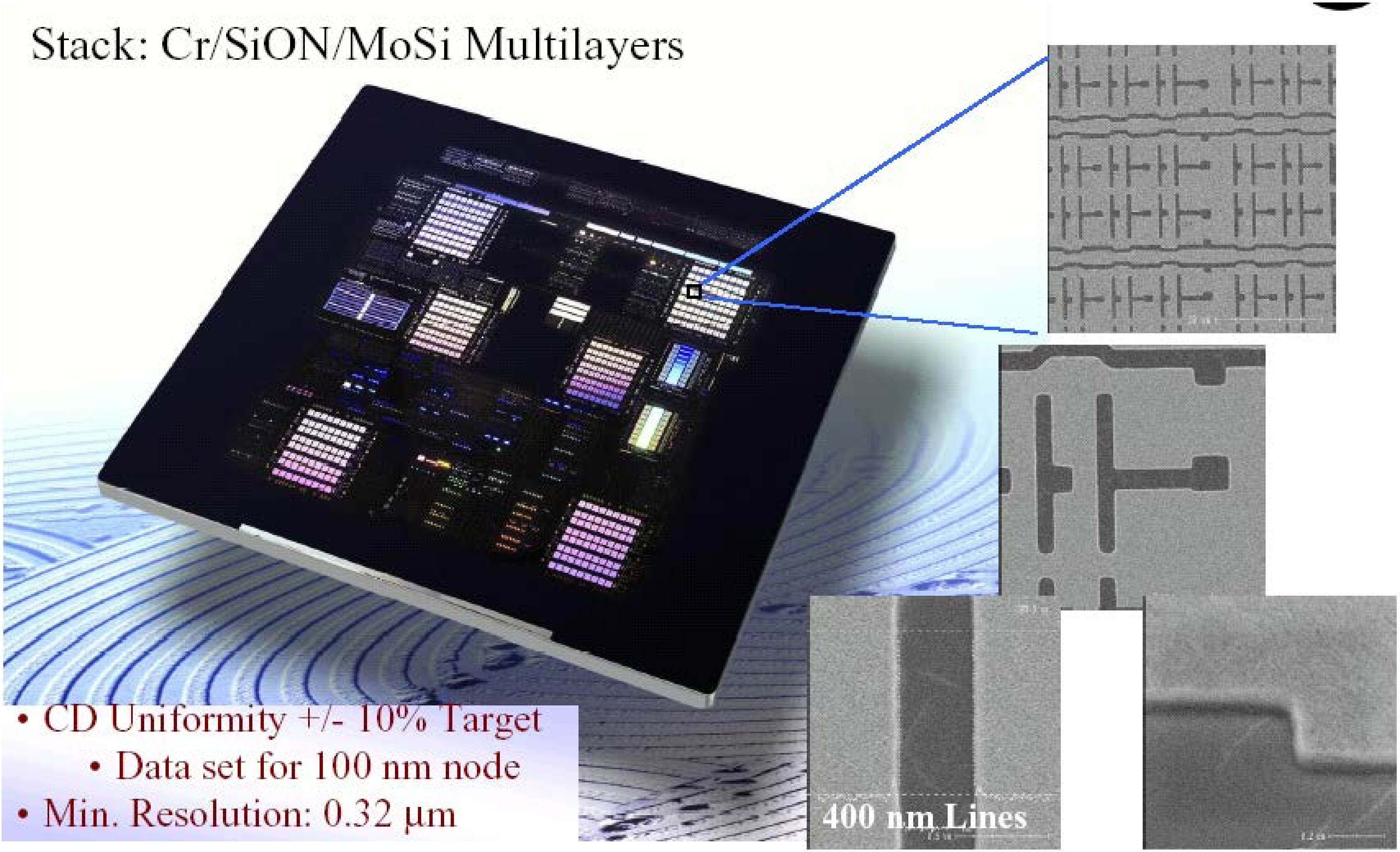
Typically

Mo/Si multilayer (d = 6.7 nm)
with 30 nm SiO$_2$ capping layer

Cr or TaN absorber (~70 nm)
with 50 nm Ru Buffer layer

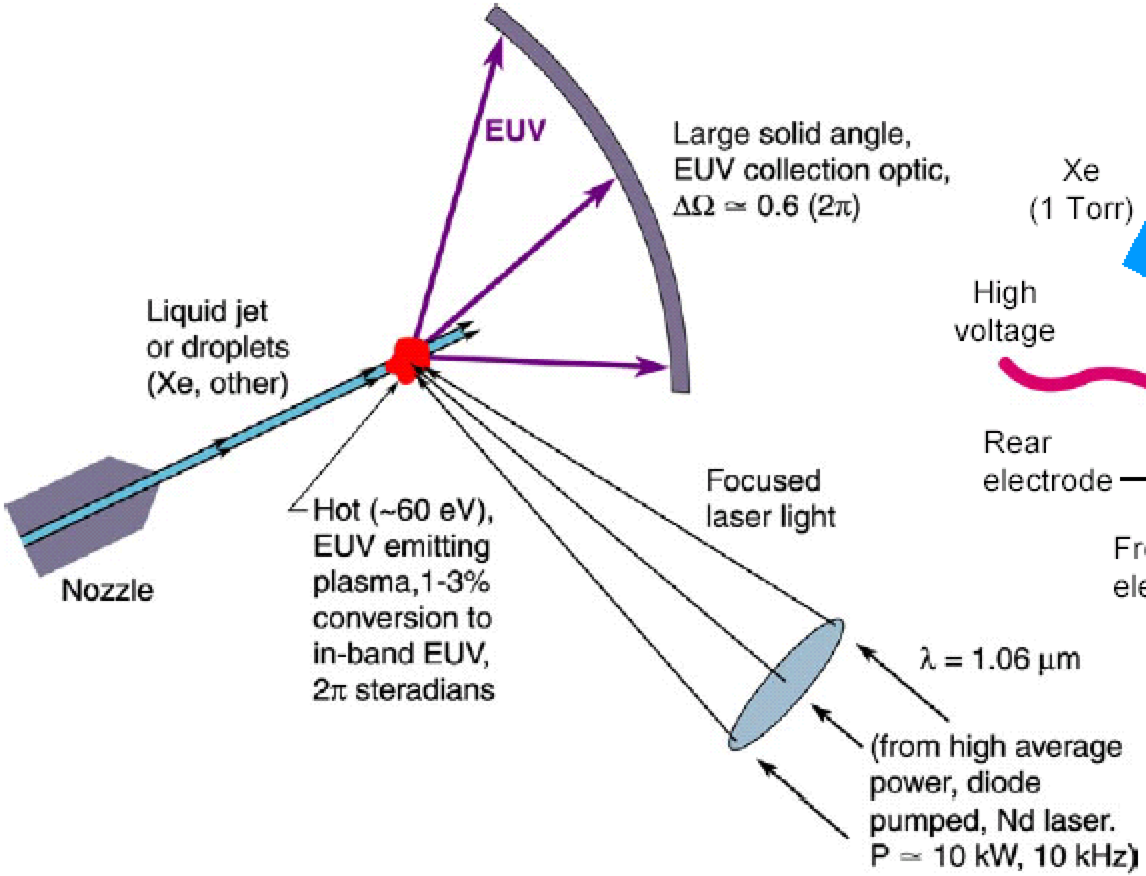
LTEM substrate
(Ti-doped fused silica)
ULE (Corning), or
Zerodur (Schott)

Stack: Cr/SiON/MoSi Multilayers

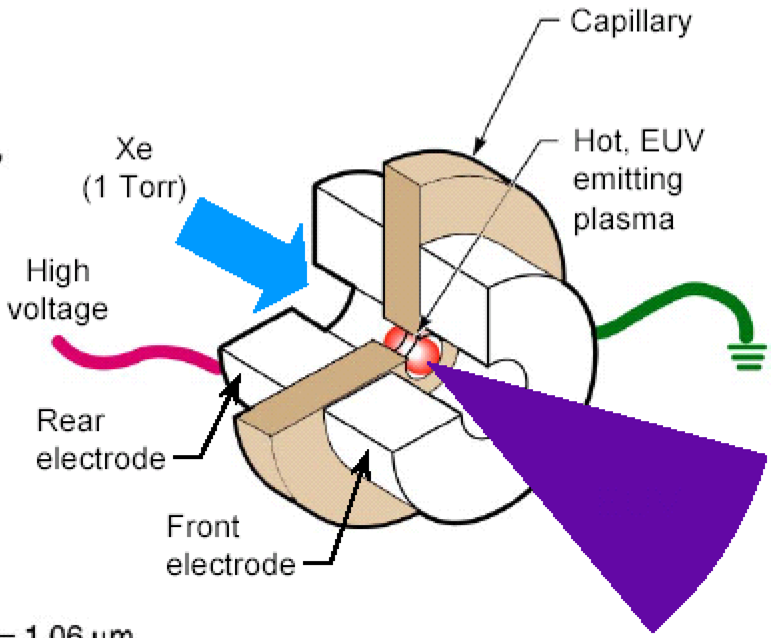


- CD Uniformity +/- 10% Target
  - Data set for 100 nm node
- Min. Resolution: 0.32 μm

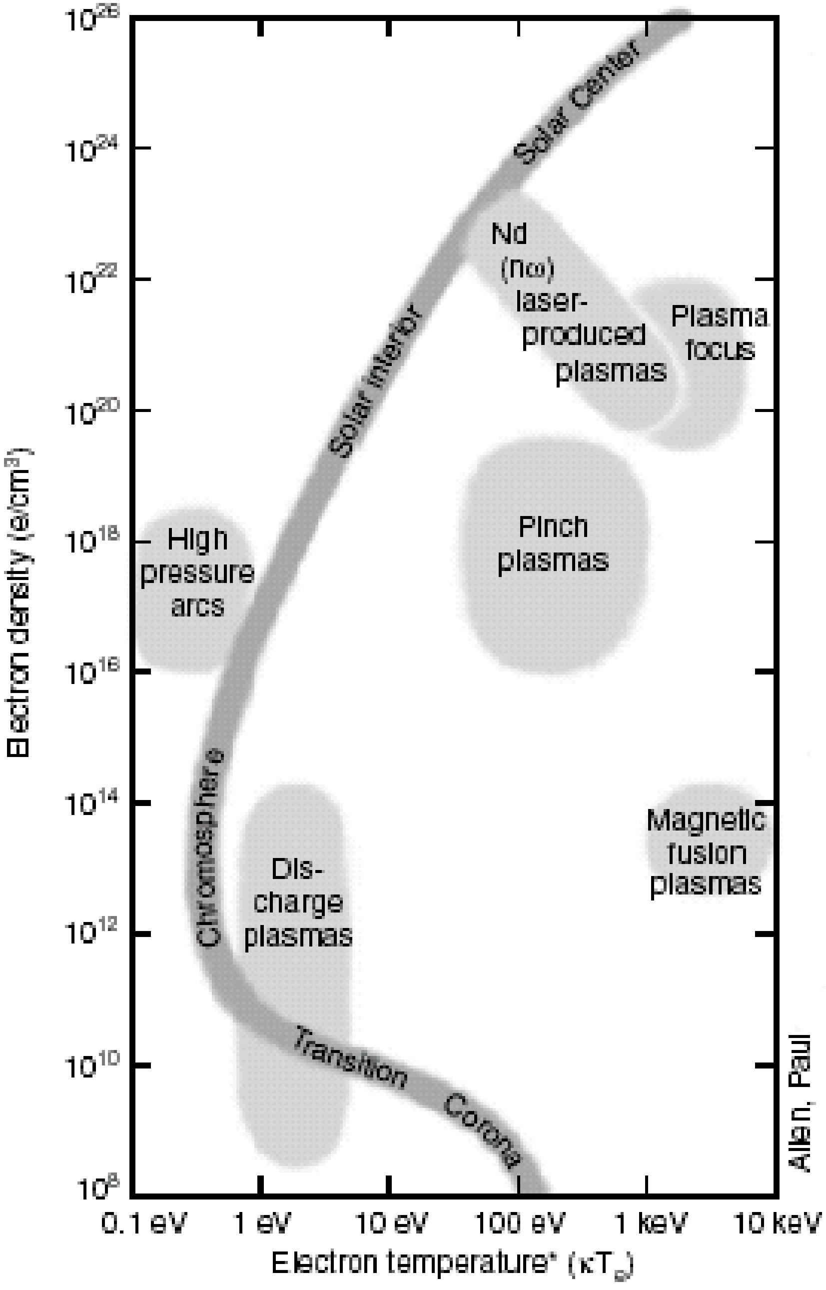
Laser Produced Plasma Source



Electrical Discharge Plasma Source

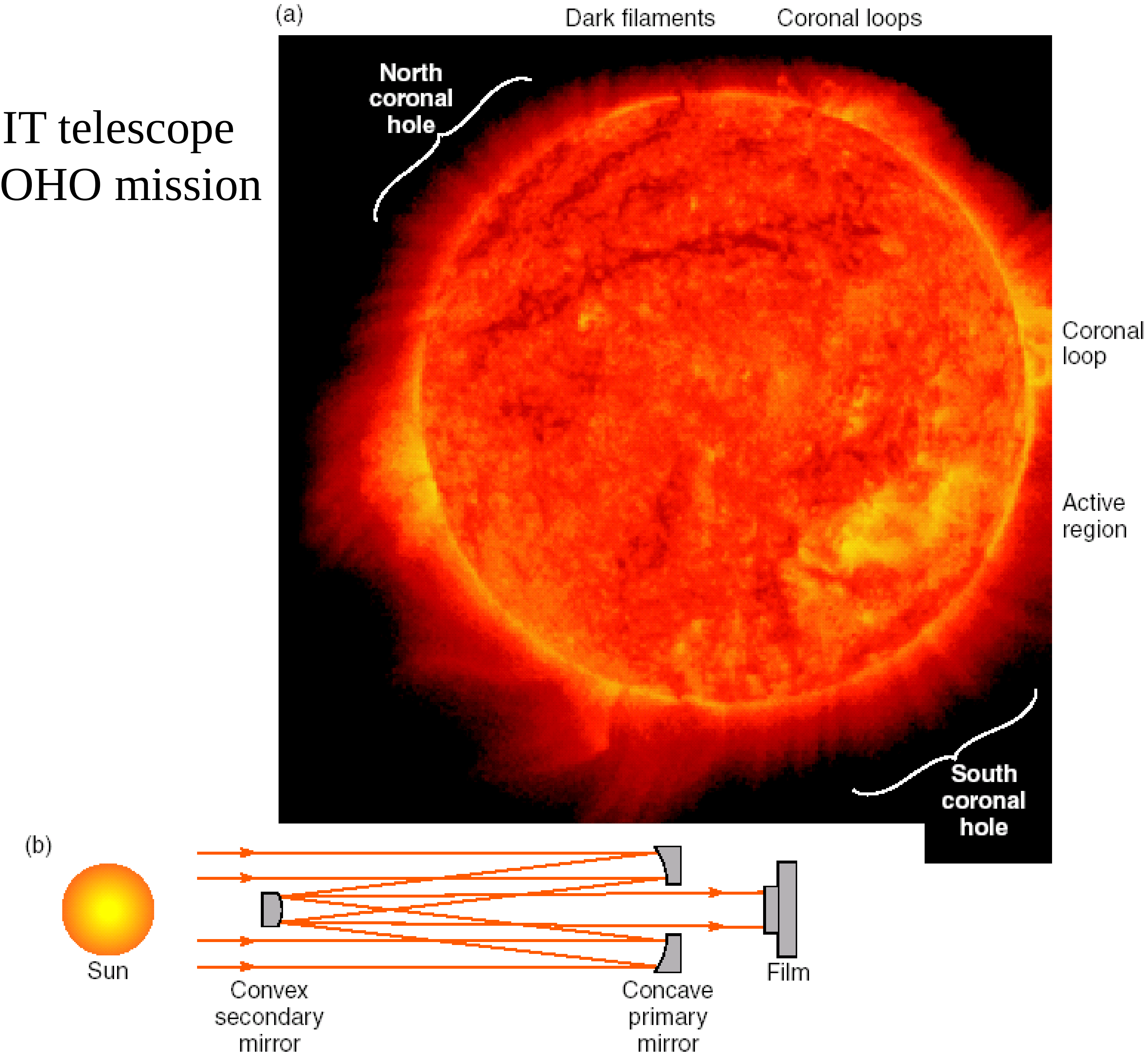


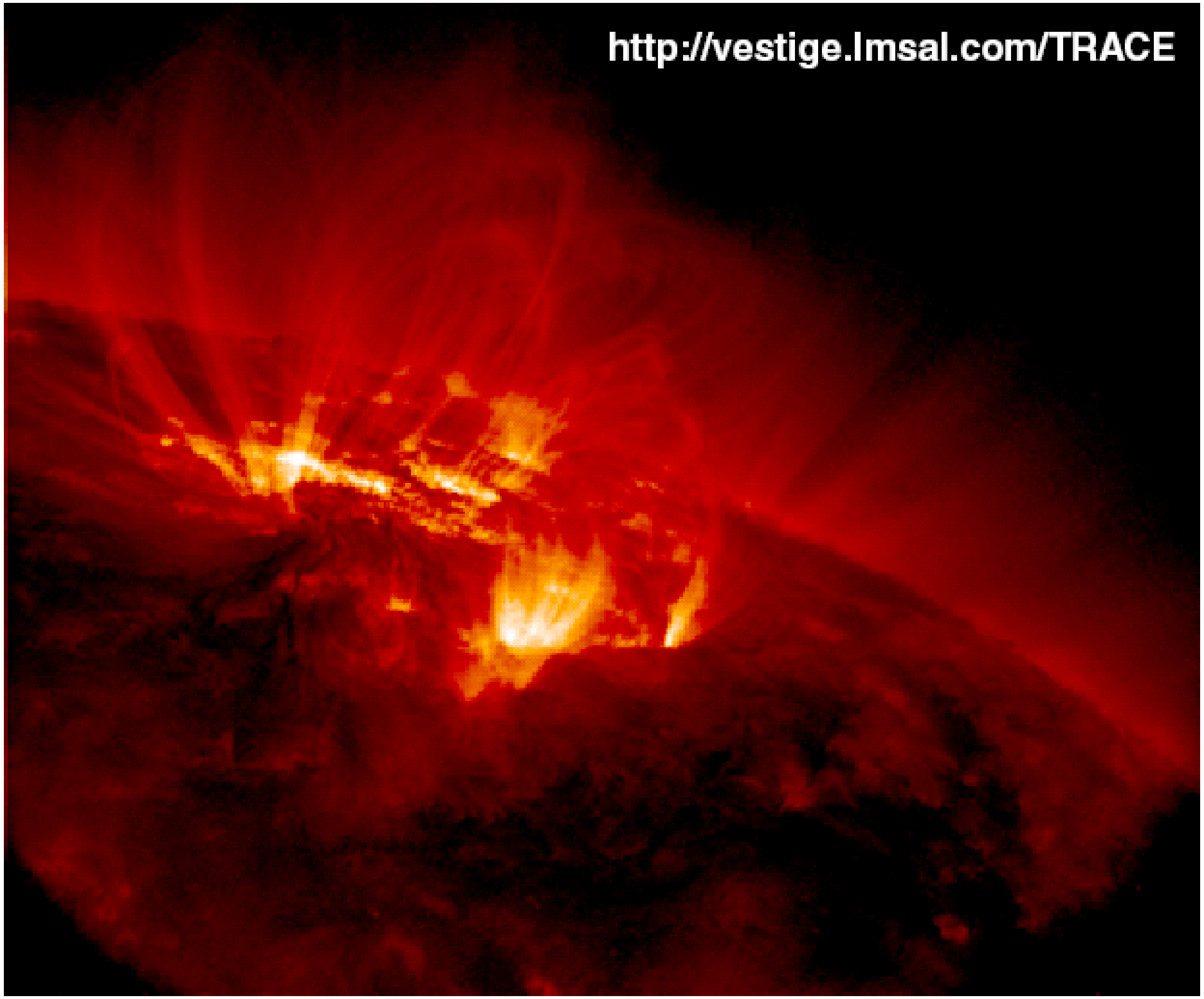
Courtesy of Neil Fornaciari
and Glenn Kubiak, Sandia.


10^26
10^24
10^22
10^20
10^18
10^16
10^14
10^12
10^10
10^8
Electron density (e/cm³)
0.1 eV
1 eV
10 eV
100 eV
1 keV
10 keV
Electron temperature* (κTₑ)
Solar Center
Solar interior
Chromosphere
Transition
Corona
Nd (nω) laser-produced plasmas
Plasma focus
High pressure arcs
Pinch plasmas
Dis-charge plasmas
Magnetic fusion plasmas

Allen, Paul

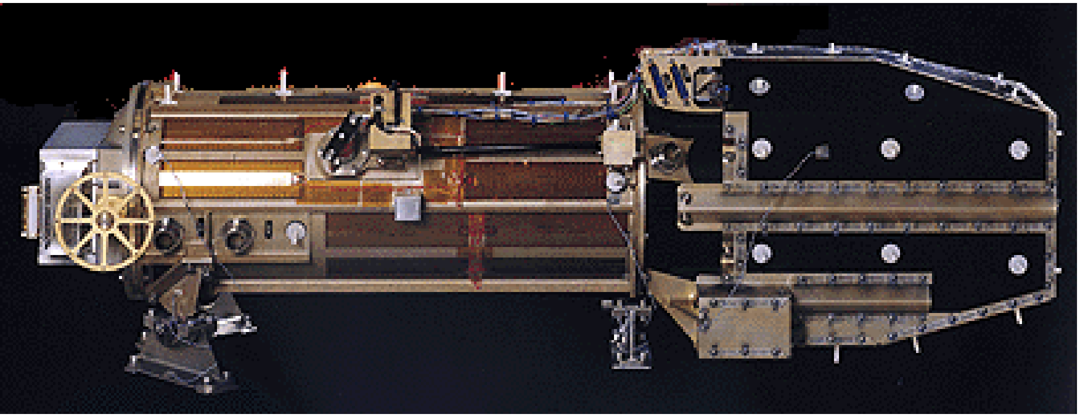
EIT telescope
SOHO mission

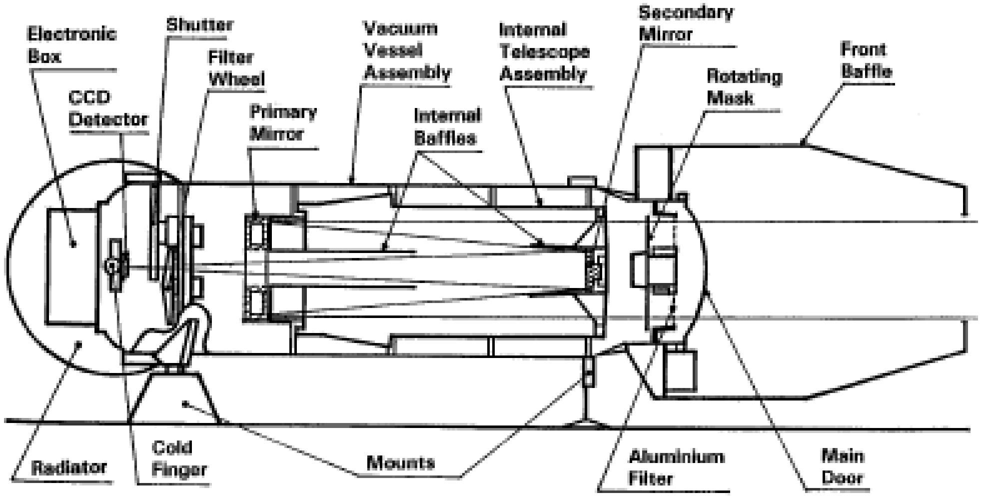




(Courtesy of L.Golub, Harvard-Smithsonian and T. Barbee, LLNL)

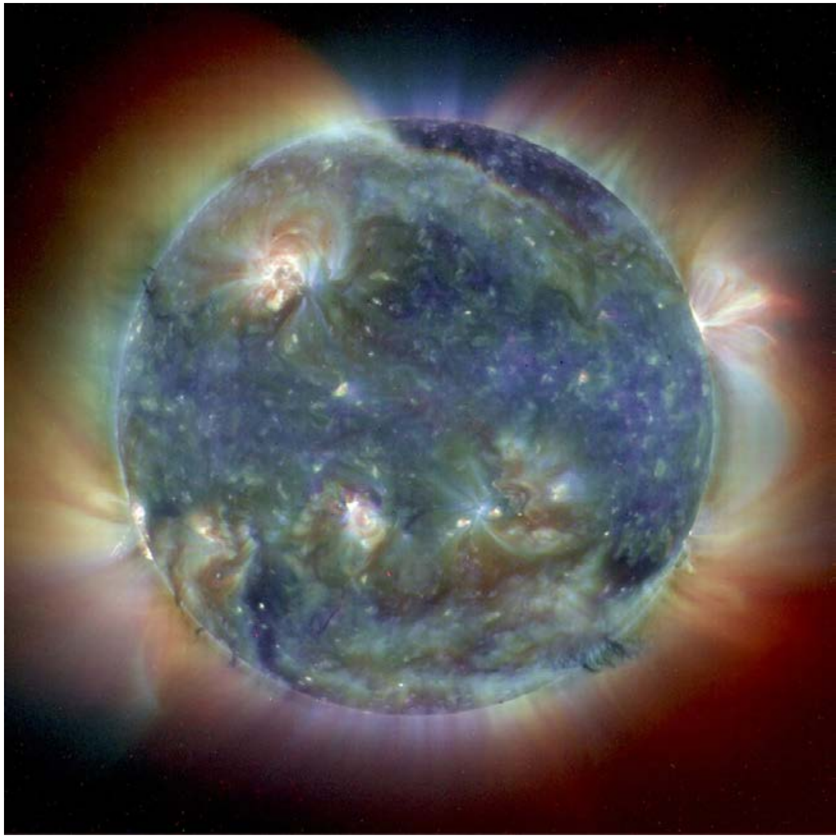
The Extreme Ultraviolet Imaging Telescope (EIT)





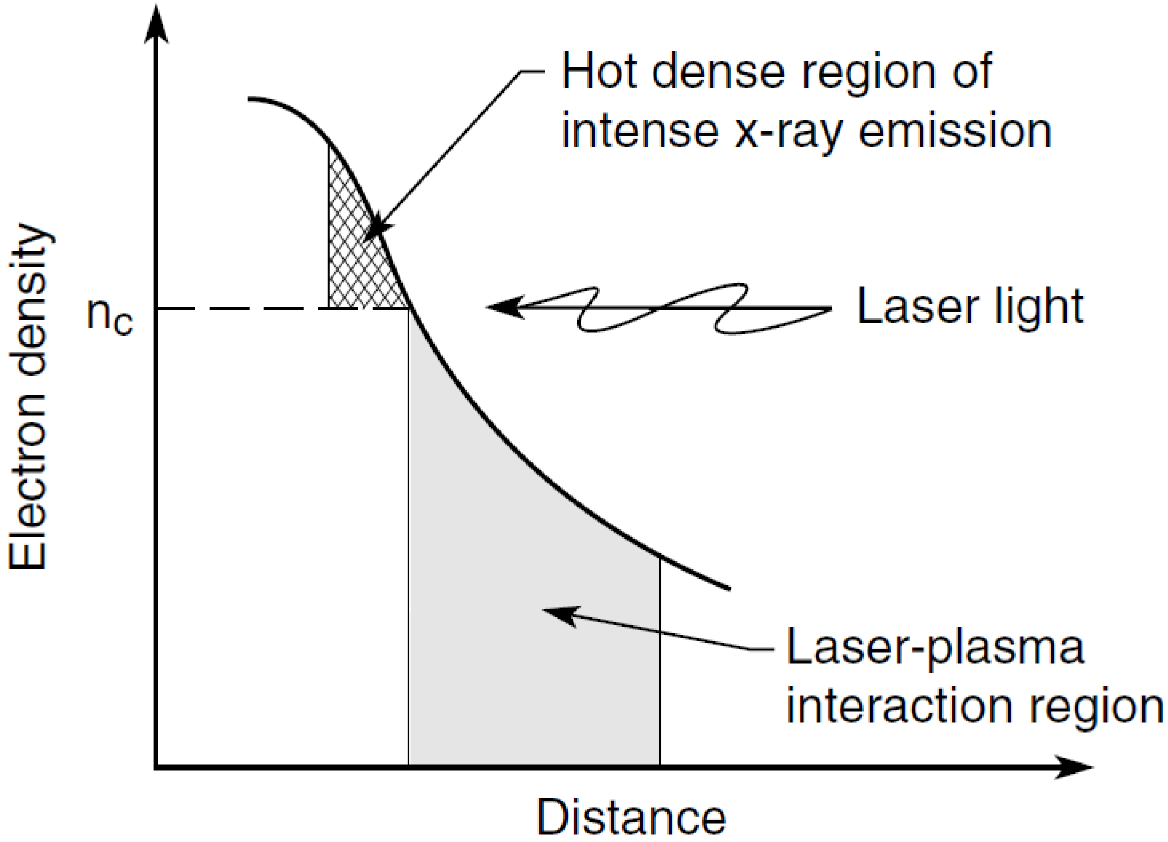
Multilayer coated normal incidence cassegrain objective

EIT composite image

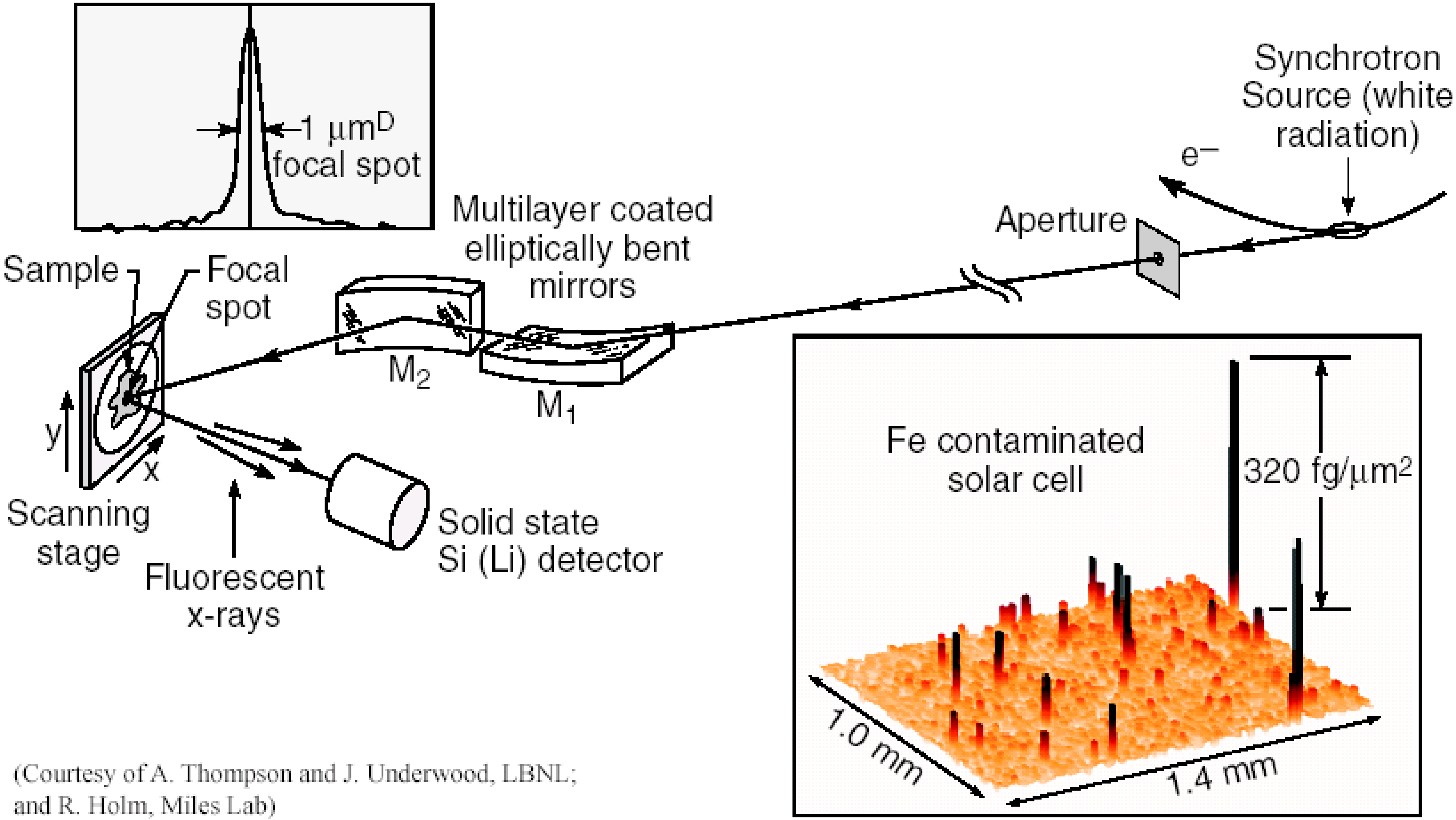


17,1 nm (blue)
19.5 nm (green)
28,4 nm (red)

Soft X-Ray/EUV Emission from a Hot-Dense Plasma



- $\kappa T_e \sim 50$ eV to 1 keV
- $n_e \sim 10^{20}$ to 10^{22} e/cm^3

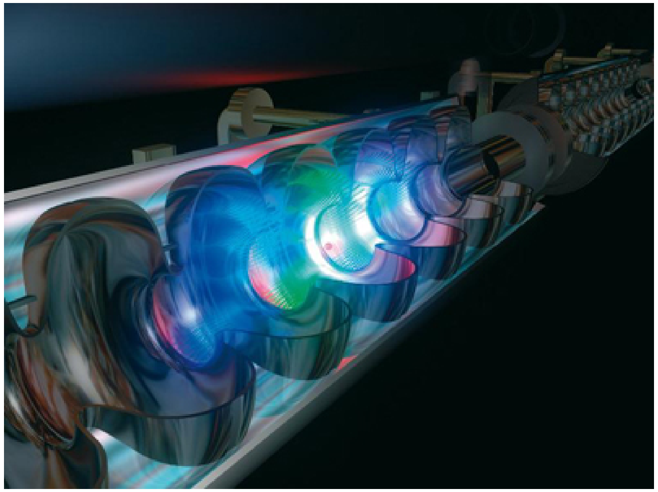


(Courtesy of A. Thompson and J. Underwood, LBNL;
and R. Holm, Miles Lab)

Motivation

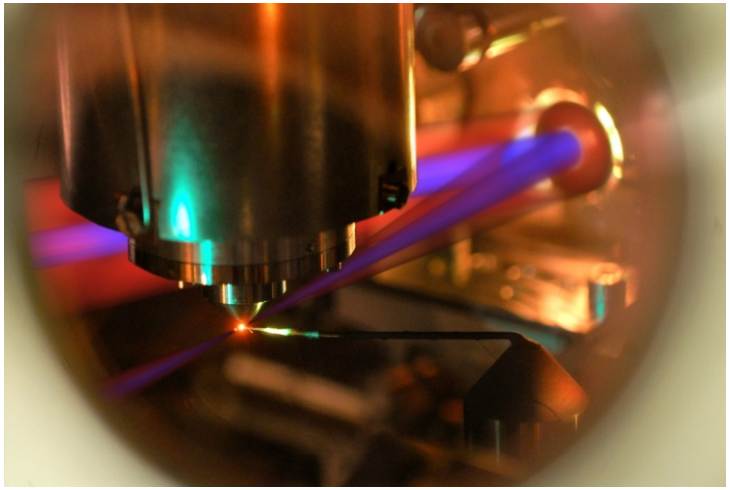
Excellent XUV optics for sources emitting ultrashort pulses:

FEL



(aspiration for sub-) fs pulses
grazing optics due to high intensities

HHG



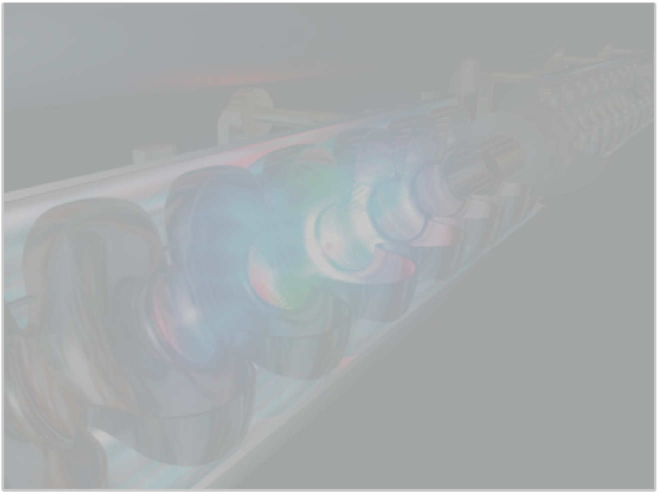
as pulses (requires large ΔE)
normal incidence optics possible

Both require optics for spectral filtering, phase shaping, …

Motivation

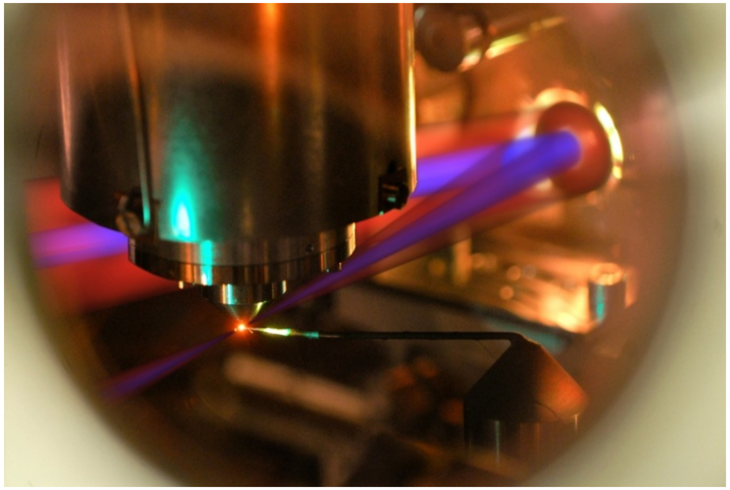
Excellent XUV optics for sources emitting ultrashort pulses:

FEL



(aspiration for sub-) fs pulses
grazing optics due to high intensities

OUR FOCUS: HHG

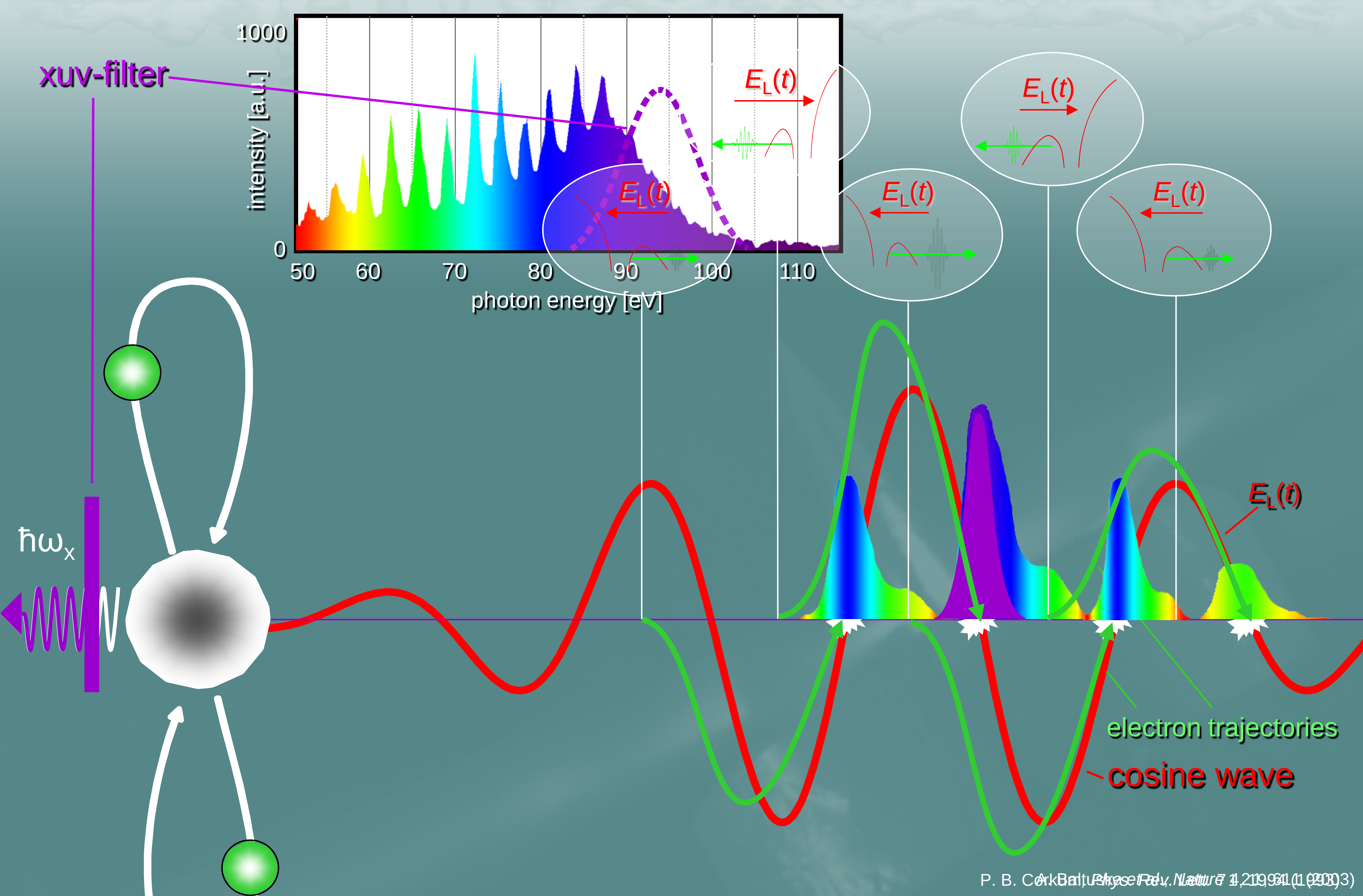


as pulses (requires large ΔE)
normal incidence optics possible

Photon flux essential!

Both require optics for spectral filtering, phase shaping, …

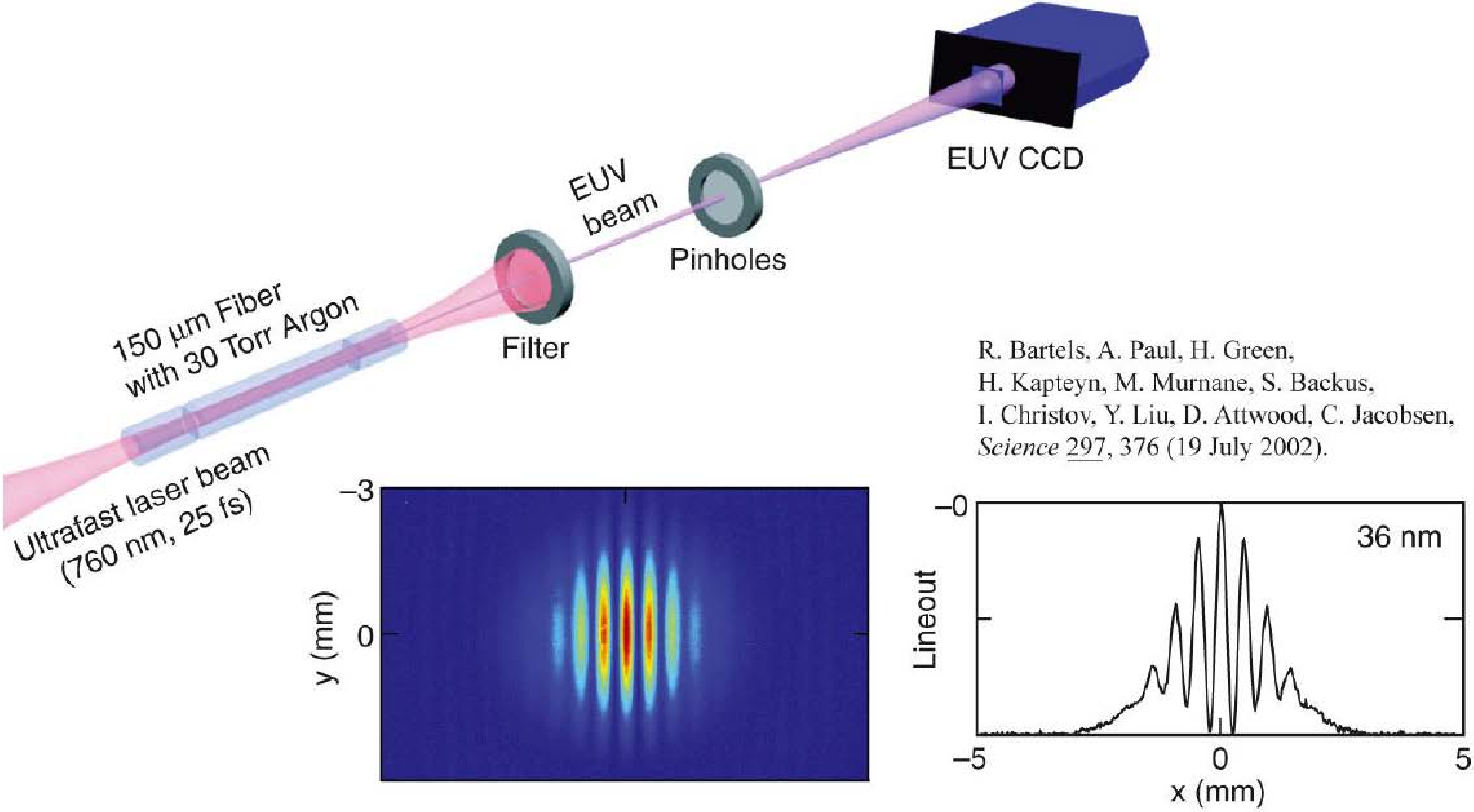
steering bound electrons with controlled light fields:
the birth of an attosecond pulse



P. B. Corkum, *Phys. Rev. Lett.* 71, 1994 (1993)

A. Baltuška et al., *Nature* 421, 611 (2003)

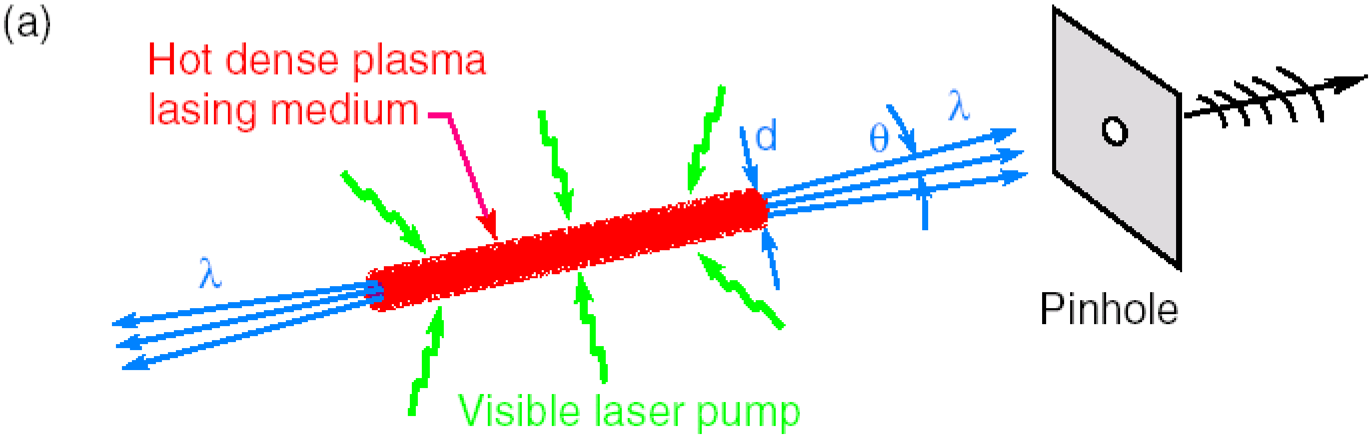
High Harmonic Generation (HHG) Provides Coherent, Femtosecond Pulses

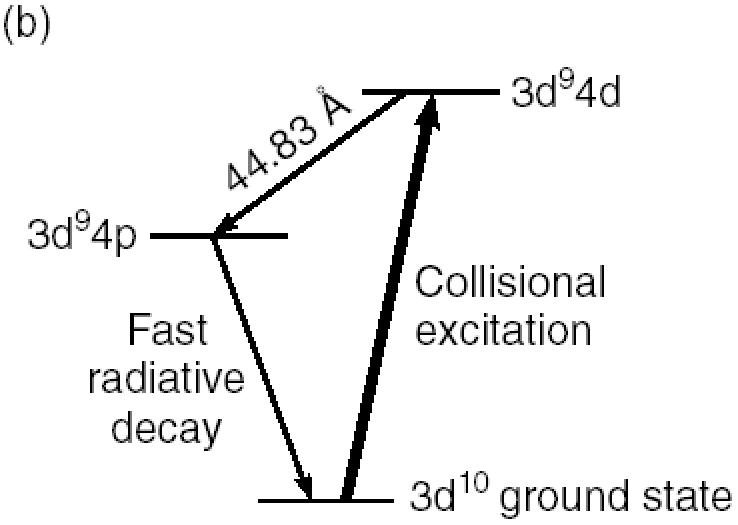


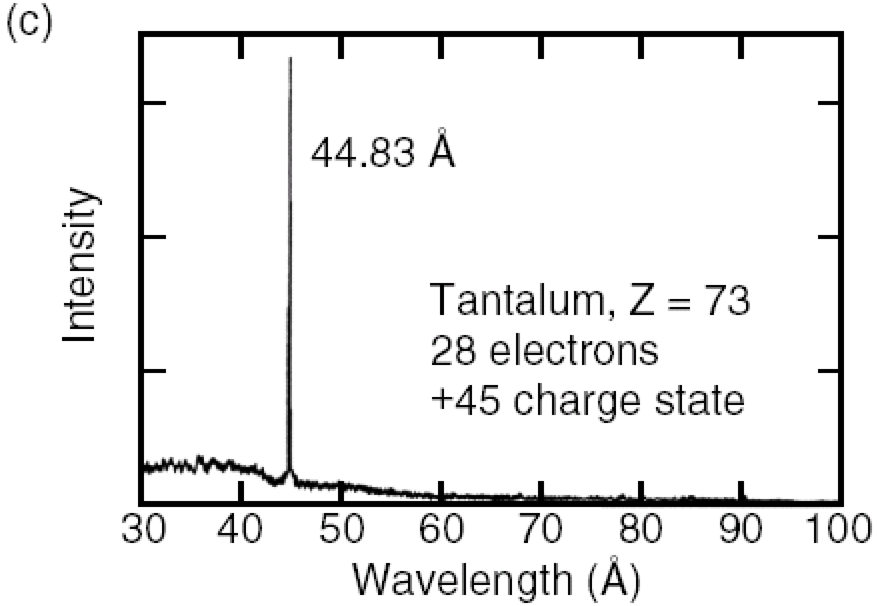
R. Bartels, A. Paul, H. Green,
H. Kapteyn, M. Murnane, S. Backus,
I. Christov, Y. Liu, D. Attwood, C. Jacobsen,
Science 297, 376 (19 July 2002).

$$P \simeq 10\ \mu W \rightarrow 2 \times 10^{12}\ \text{ph/sec @ 36 nm } (n = 21;\ 34\ \text{eV})$$

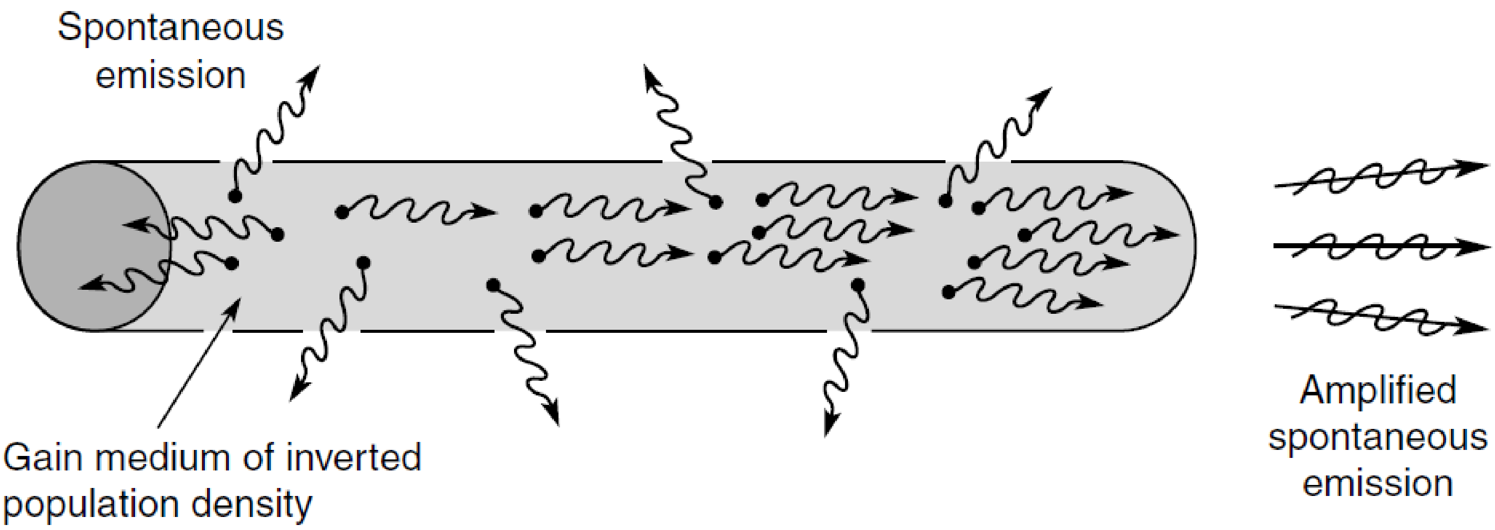
Courtesy of Professors Margaret Murnane and Henry Kapteyn, Univ. Colorado


(a)
Hot dense plasma
lasing medium
d
θ
λ
λ
Pinhole
Visible laser pump

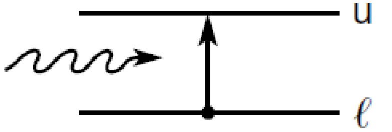

(b)
3d⁹4d
44.83 Å
3d⁹4p
Collisional
excitation
Fast
radiative
decay
3d¹⁰ ground state


(c)
44.83 Å
Intensity
Tantalum, Z = 73
28 electrons
+45 charge state
30
40
50
60
70
80
90
100
Wavelength (Å)

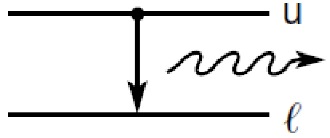
Lasing Begins with Amplified Spontaneous Emission



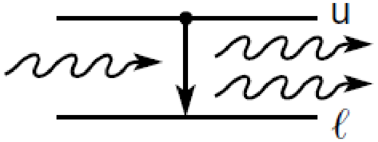
(a) Absorption



(b) Spontaneous emission



(b) Stimulated emission



$$\frac{I}{I_0} = e^{GL} \tag{7.2}$$

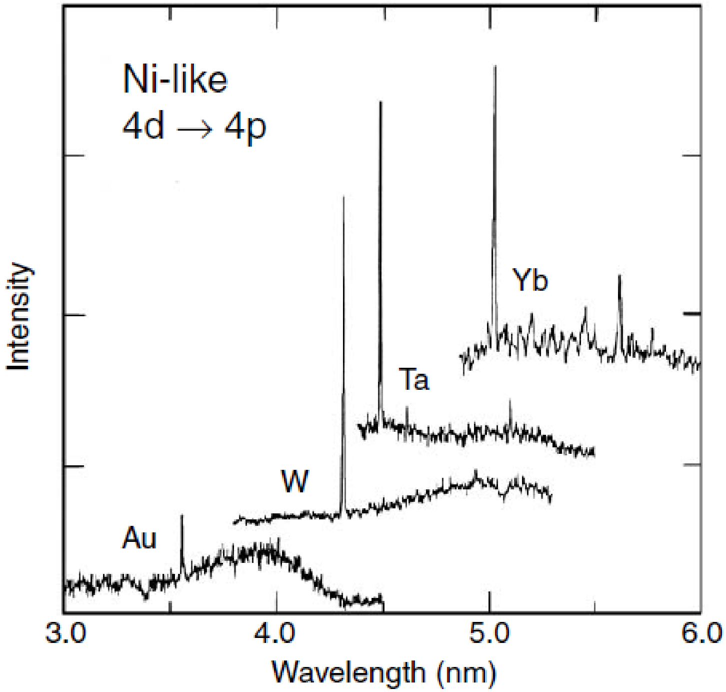
$$G = n_u \sigma_{\text{stim}} F \tag{7.4}$$

$$\sigma_{\text{stim}} = \frac{\pi \lambda r_e}{(\Delta\lambda/\lambda)} \left(\frac{g_l}{g_u} \right) f_{lu} \tag{7.18}$$

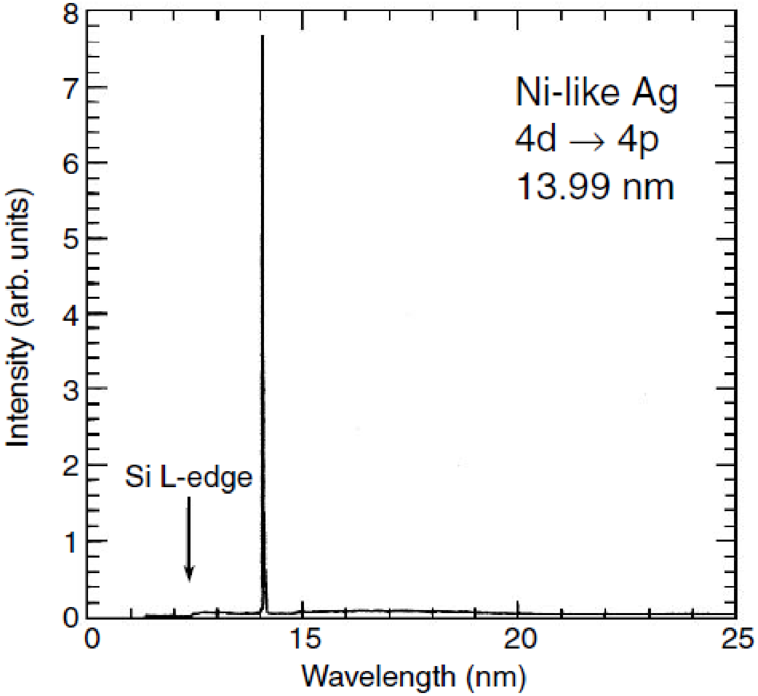
$$\frac{P}{A} = \frac{16\pi^2 c^2 \hbar (\Delta\lambda/\lambda) GL}{\lambda^4} \tag{7.22}$$

Mirror-less SXR/EUV Lasing (ASE) at Various Labs Around the World

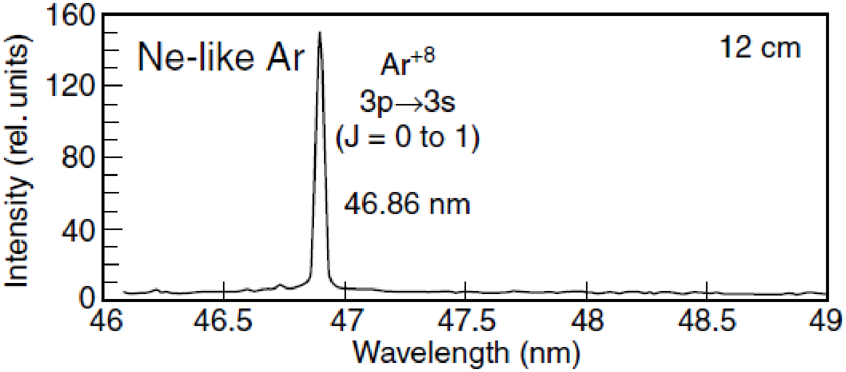
B. MacGowan, et al., Lawrence Livermore Lab



J. Zhang, et al., Rutherford-Appleton



J. Rocca, et al., Colorado State Univ.



S. Suckewer, Princeton Univ.

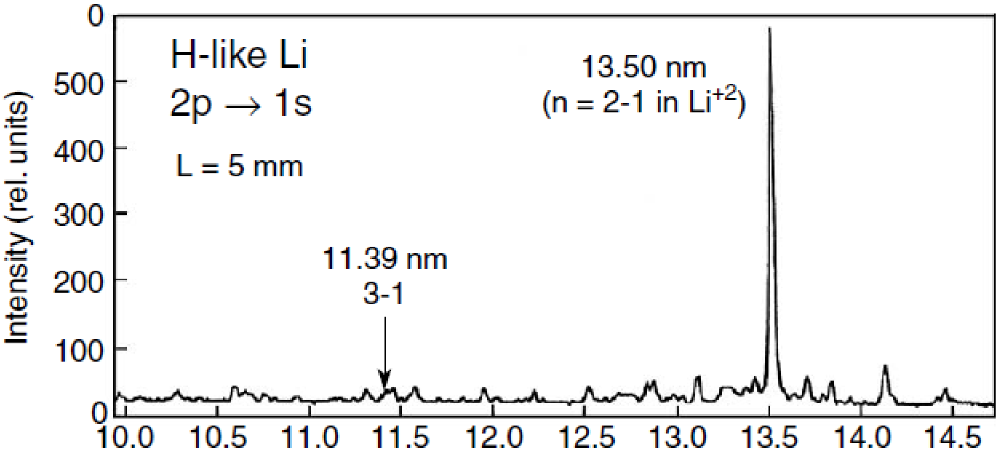
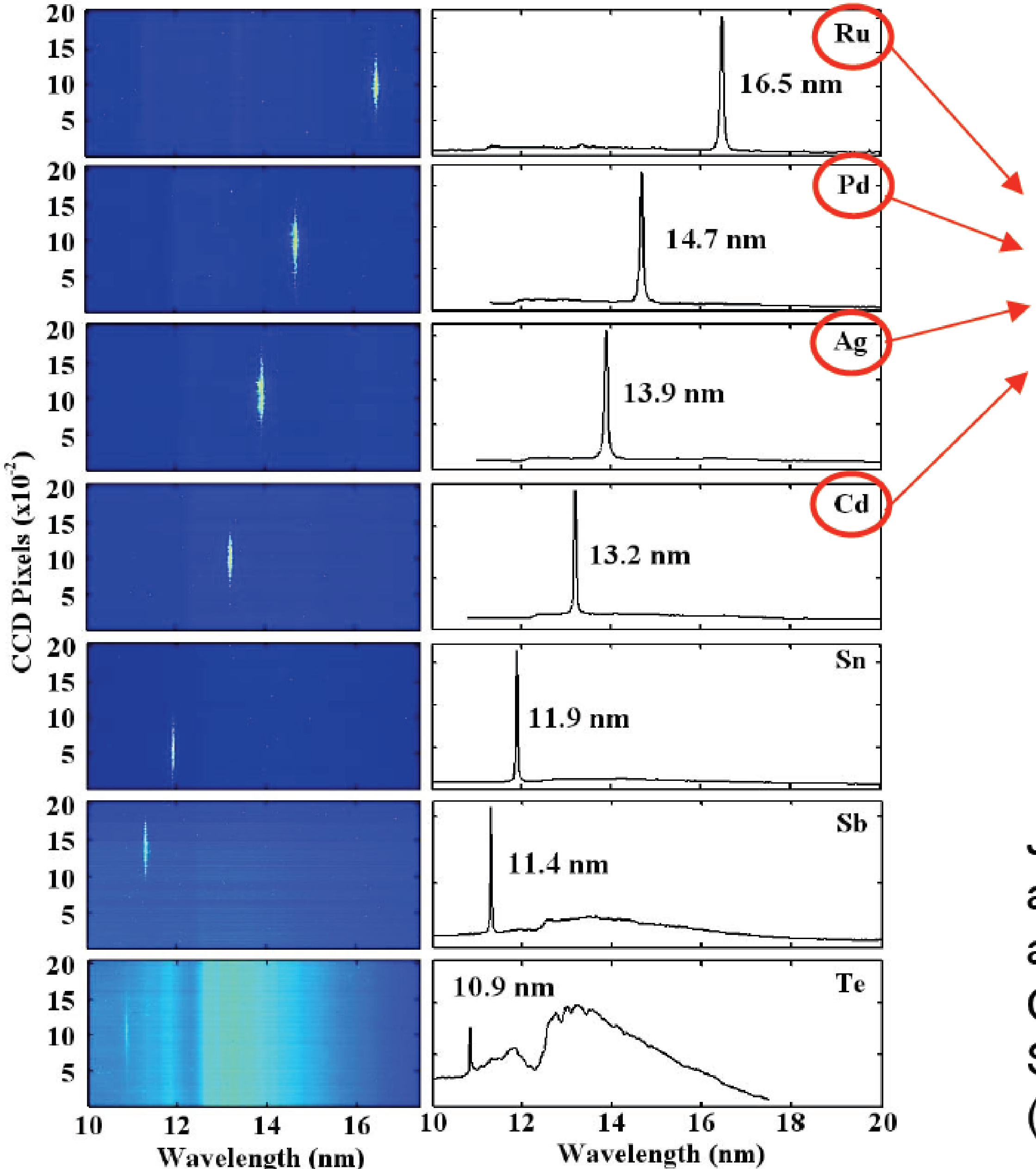


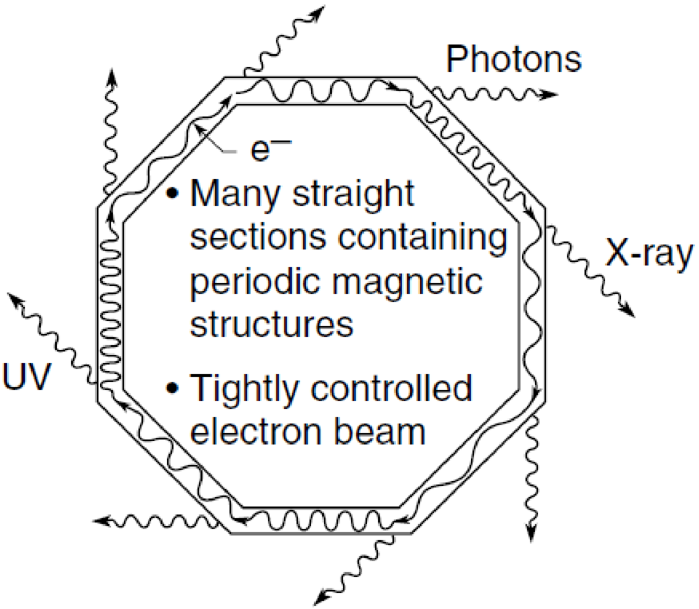
Table-top EUV Lasers



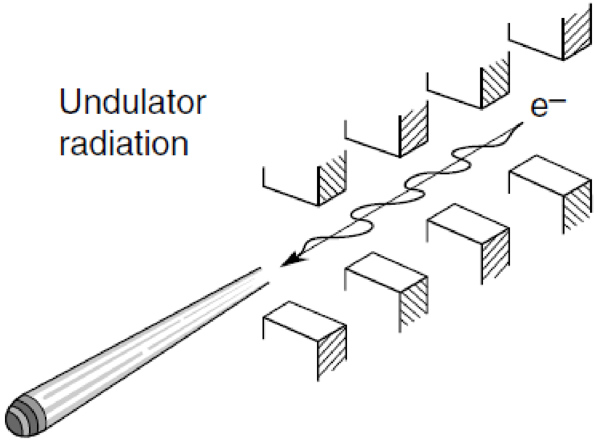
Gain saturated operation demonstrated

J.J. Rocca et al. Presented at SPIE Conf. 5919. San Diego (2005)

Synchrotron Radiation



- Many straight sections containing periodic magnetic structures
- Tightly controlled electron beam



Bending Magnet:

$$\hbar\omega_c = \frac{3e\hbar B\gamma^2}{2m} \qquad (5.7)$$

Wiggler:

$$\hbar\omega_c = \frac{3e\hbar B\gamma^2}{2m} \qquad (5.80)$$

$$n_c = \frac{3K}{4}\left(1 + \frac{K^2}{2}\right) \qquad (5.82)$$

$$P_T = \frac{\pi e K^2 \gamma^2 I N}{3\epsilon_0 \lambda_u} \qquad (5.85)$$

Undulator:

$$\lambda = \frac{\lambda_u}{2\gamma^2}\left(1 + \frac{K^2}{2} + \gamma^2\theta^2\right) \qquad (5.28)$$

$$K = \frac{eB_0\lambda_u}{2\pi mc} \qquad (5.18)$$

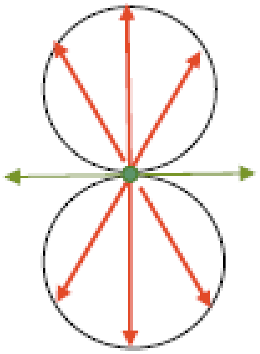
$$\theta_{\text{cen}} = \frac{1}{\gamma^* \sqrt{N}} \qquad (5.15)$$

$$\left.\frac{\Delta\lambda}{\lambda}\right|_{\text{cen}} = \frac{1}{N} \qquad (5.14)$$

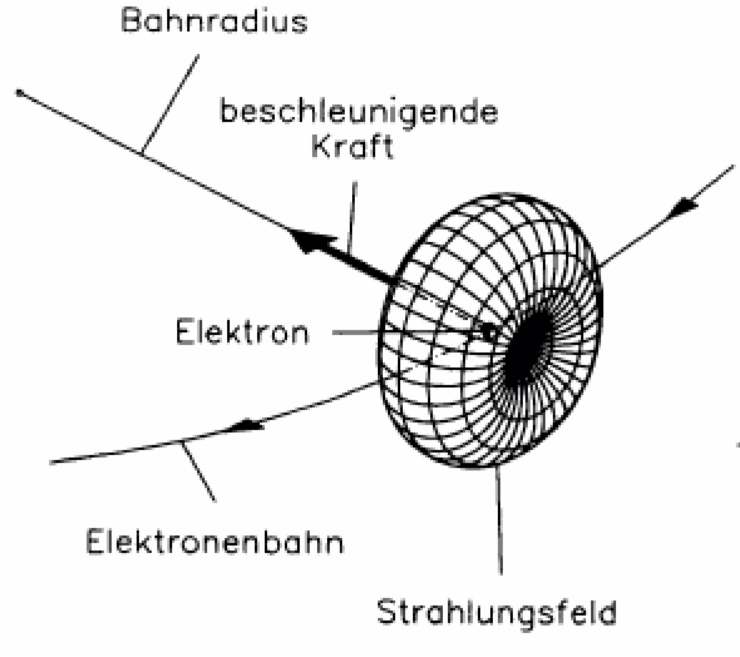
$$\bar{P}_{\text{cen}} = \frac{\pi e \gamma^2 I}{\epsilon_0 \lambda_u} \frac{K^2}{\left(1 + \frac{K^2}{2}\right)^2} f(K) \qquad (5.41)$$

IV.1.2 Synchrotronstrahlungsquellen

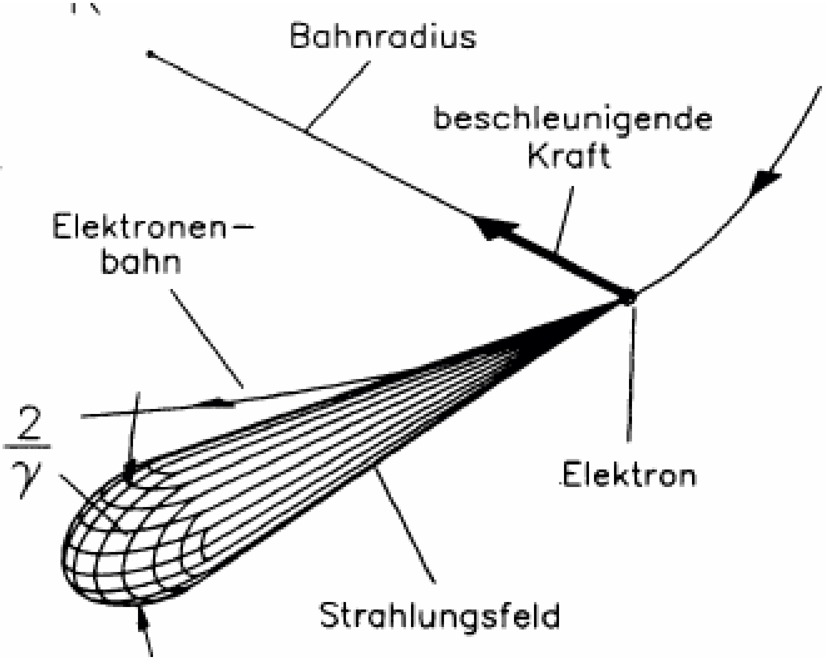
Prinzip: Abstrahlung elektromagnetischer Wellen
durch beschleunigte Ladung
(vgl. oszillierender Dipol)



hier: Querbeschleunigung der Ladungen
bei relativistischer Geschwindigkeit

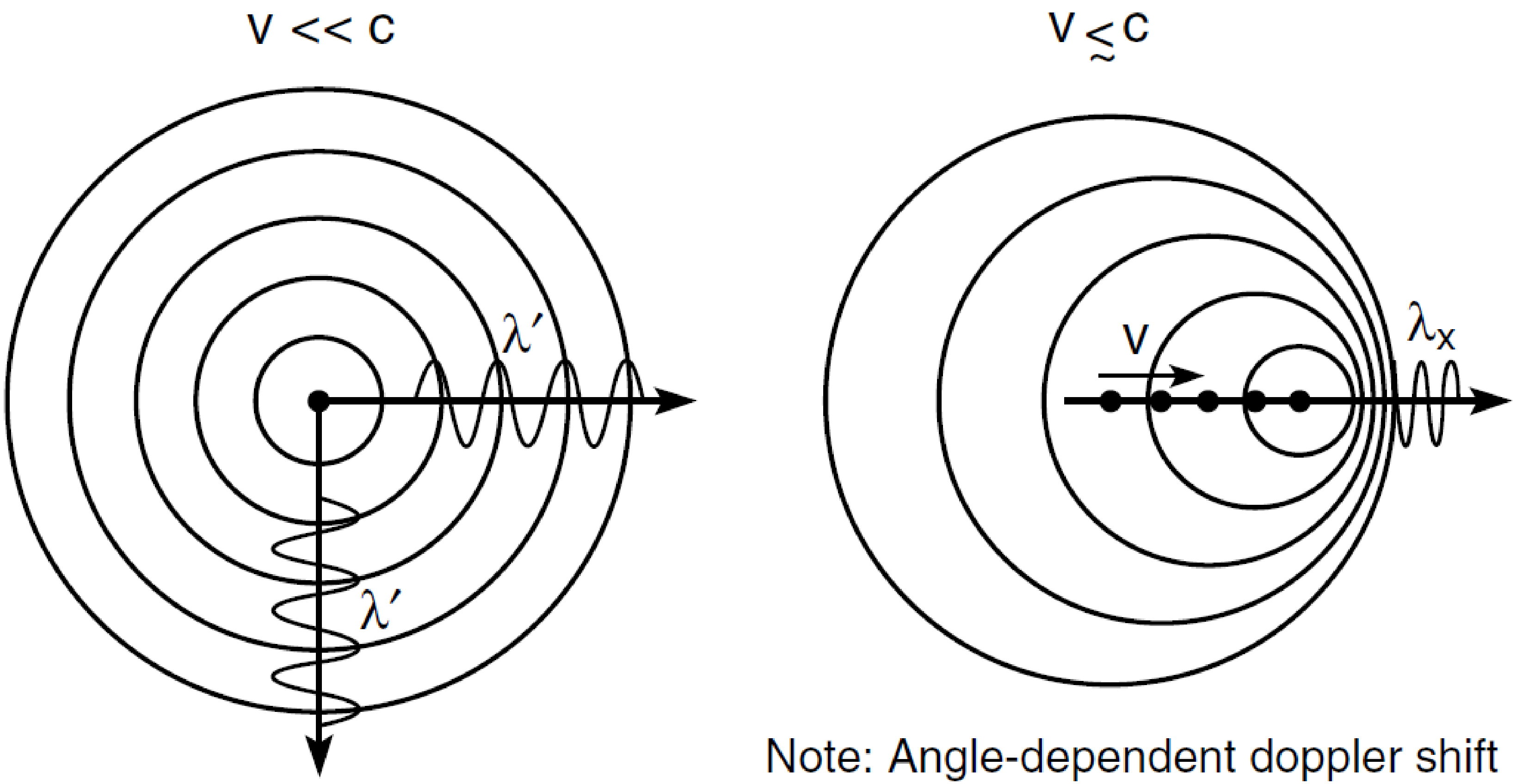


Schwerpunktsystem des Elektrons



Laborsystem

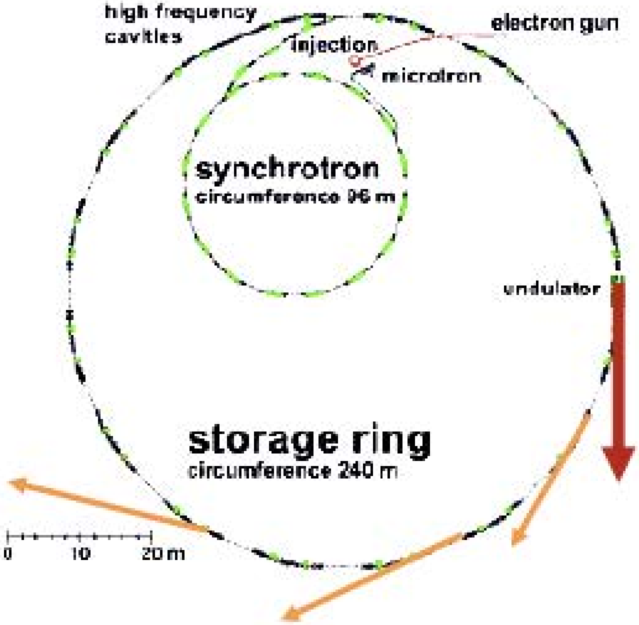
Synchrotron Radiation from Relativistic Electrons

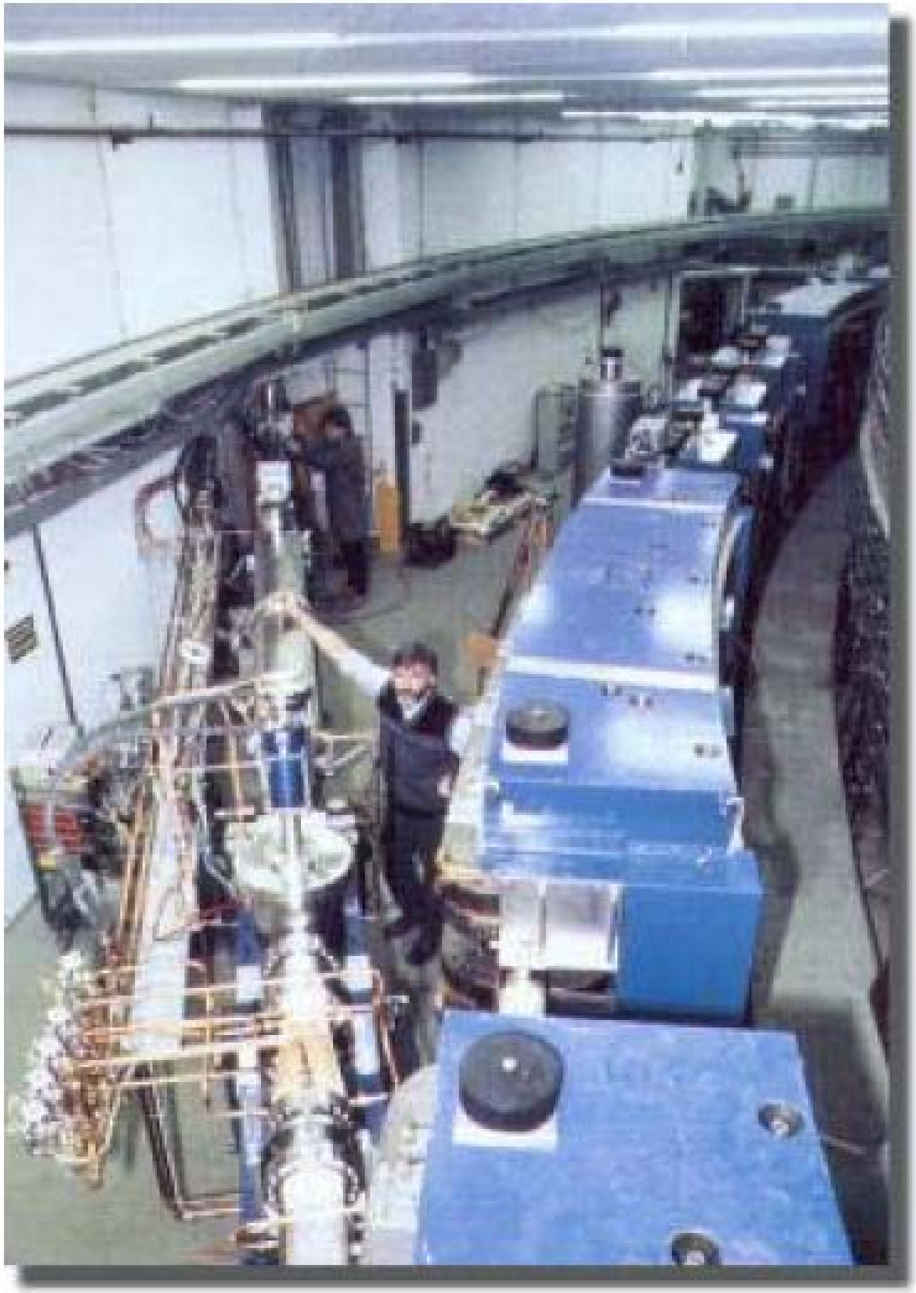


Note: Angle-dependent doppler shift

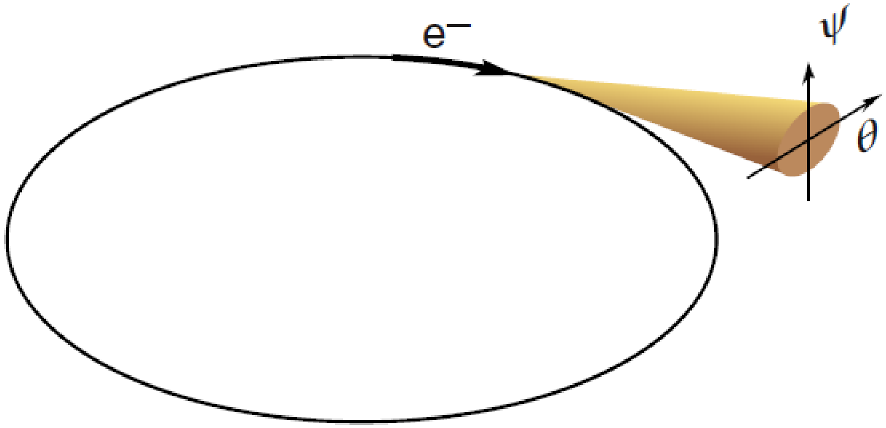
Synchrotronstrahlung

Abstrahlung im Ablenkmagnet





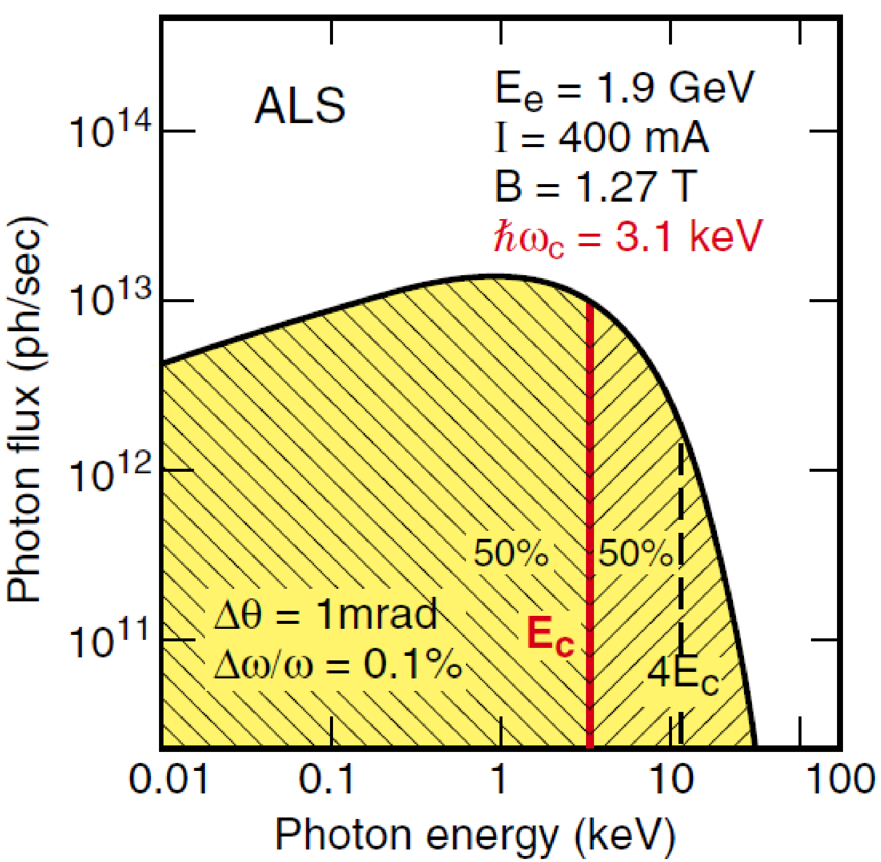
Bending Magnet Photon Flux at the ALS



$$E_c = \hbar\omega_c = \frac{3e\hbar B\gamma^2}{2m} \qquad (5.7a)$$

$$E_c(\text{keV}) = 0.6650 E_e^2(\text{GeV}) B(\text{T}) \qquad (5.7b)$$

$$\gamma = \frac{E_e}{mc^2} = 1957 E_e(\text{GeV}) \qquad (5.5)$$



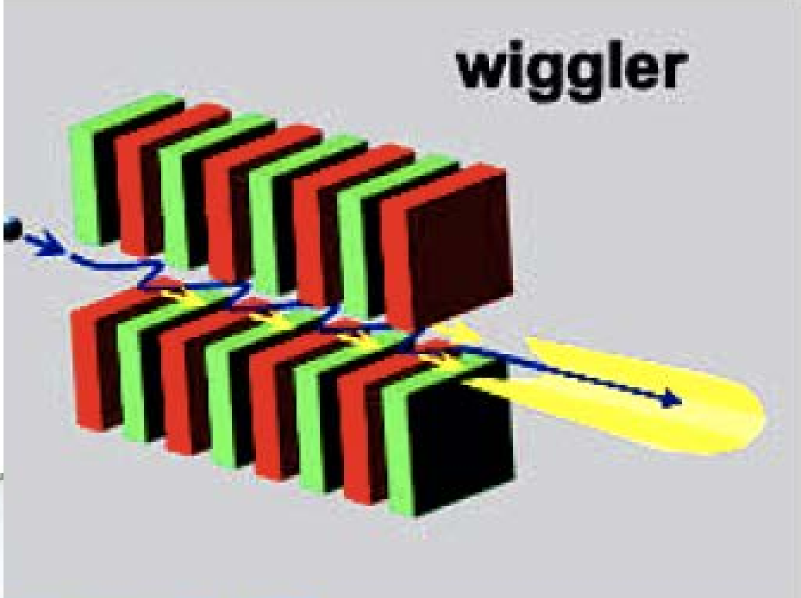
Advantages:
- covers broad spectral range
- least expensive
- most accessable

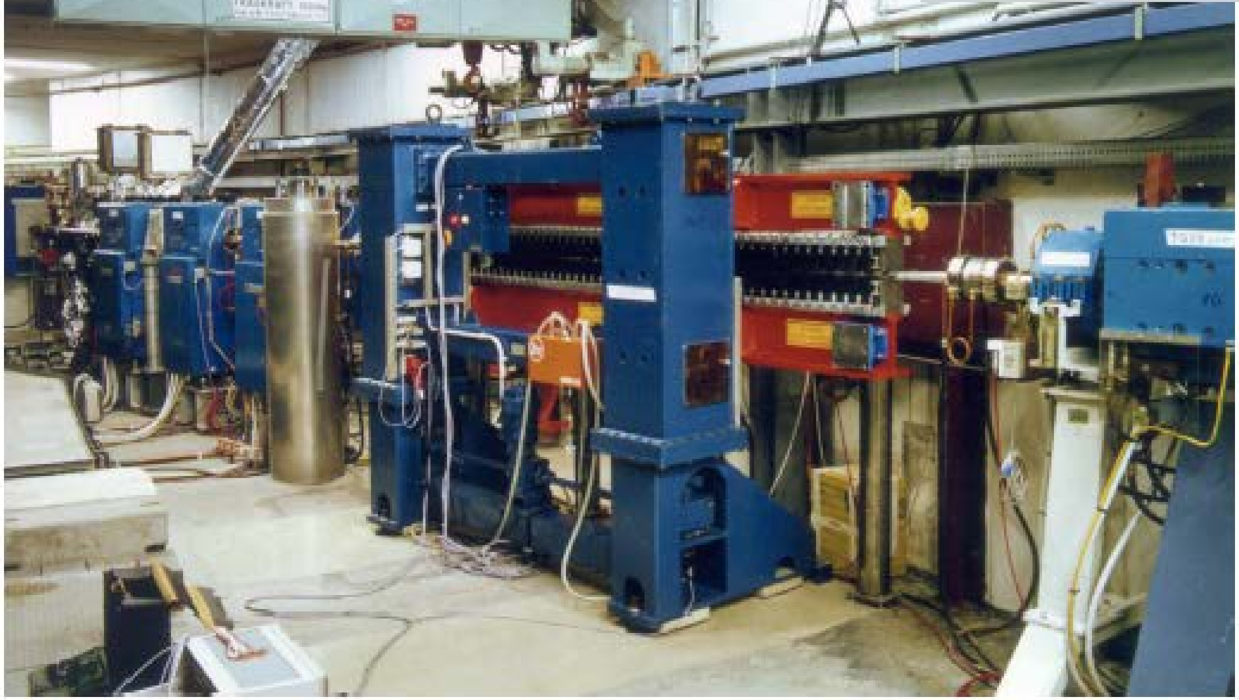
Disadvantages:
- limited coverage of hard x-rays
- not as bright as undulator

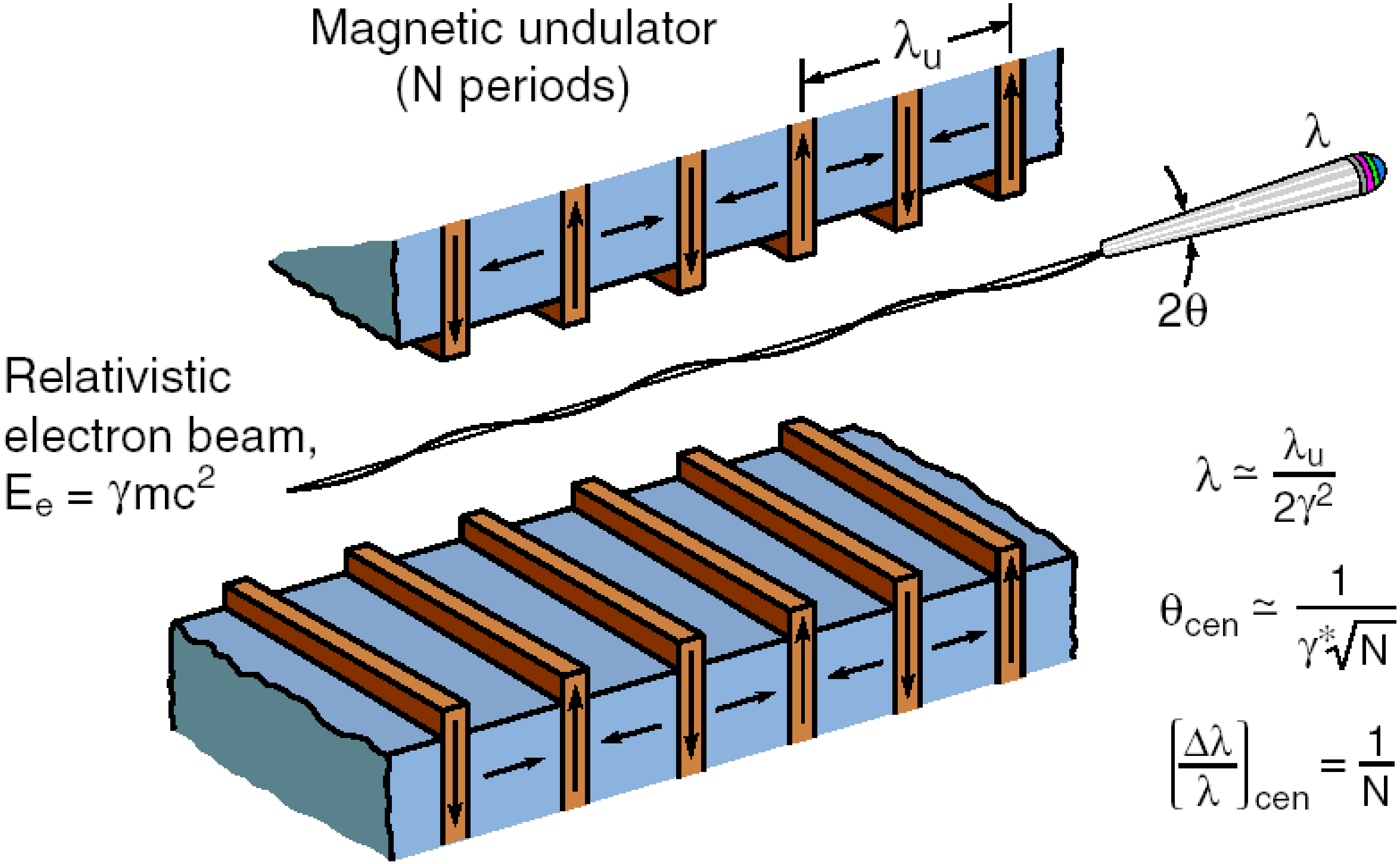
Synchrotronstrahlung

durch alternierende Magnete:

Überlagerung der Abstrahlprozesse







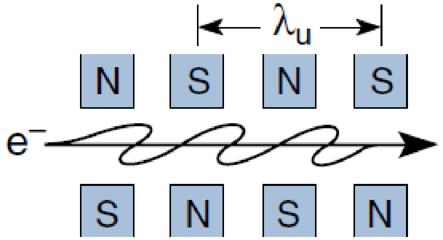
$$\lambda \simeq \frac{\lambda_u}{2\gamma^2}$$

$$\theta_{cen} \simeq \frac{1}{\gamma^* \sqrt{N}}$$

$$\left[\frac{\Delta\lambda}{\lambda}\right]_{cen} = \frac{1}{N}$$

Undulator Radiation

Laboratory Frame of Reference

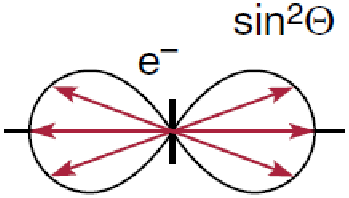


$E = \gamma mc^2$

$$\gamma = \frac{1}{\sqrt{1 - \frac{v^2}{c^2}}}$$

N = # periods

Frame of Moving e⁻



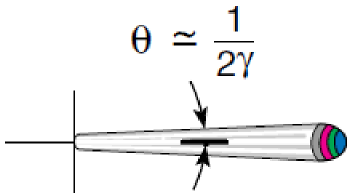
e^- radiates at the Lorentz contracted wavelength:

$$\lambda' = \frac{\lambda_u}{\gamma}$$

Bandwidth:

$$\frac{\lambda'}{\Delta\lambda'} \simeq N$$

Frame of Observer



Doppler shortened wavelength on axis:

$$\lambda = \lambda'\gamma(1 - \beta\cos\theta)$$

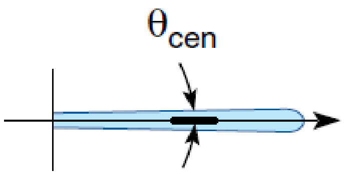
$$\lambda = \frac{\lambda_u}{2\gamma^2}(1 + \gamma^2\theta^2)$$

Accounting for transverse motion due to the periodic magnetic field:

$$\boxed{\lambda = \frac{\lambda_u}{2\gamma^2}\left(1 + \frac{K^2}{2} + \gamma^2\theta^2\right)}$$

where $K = eB_0\lambda_u/2\pi mc$

Following Monochromator



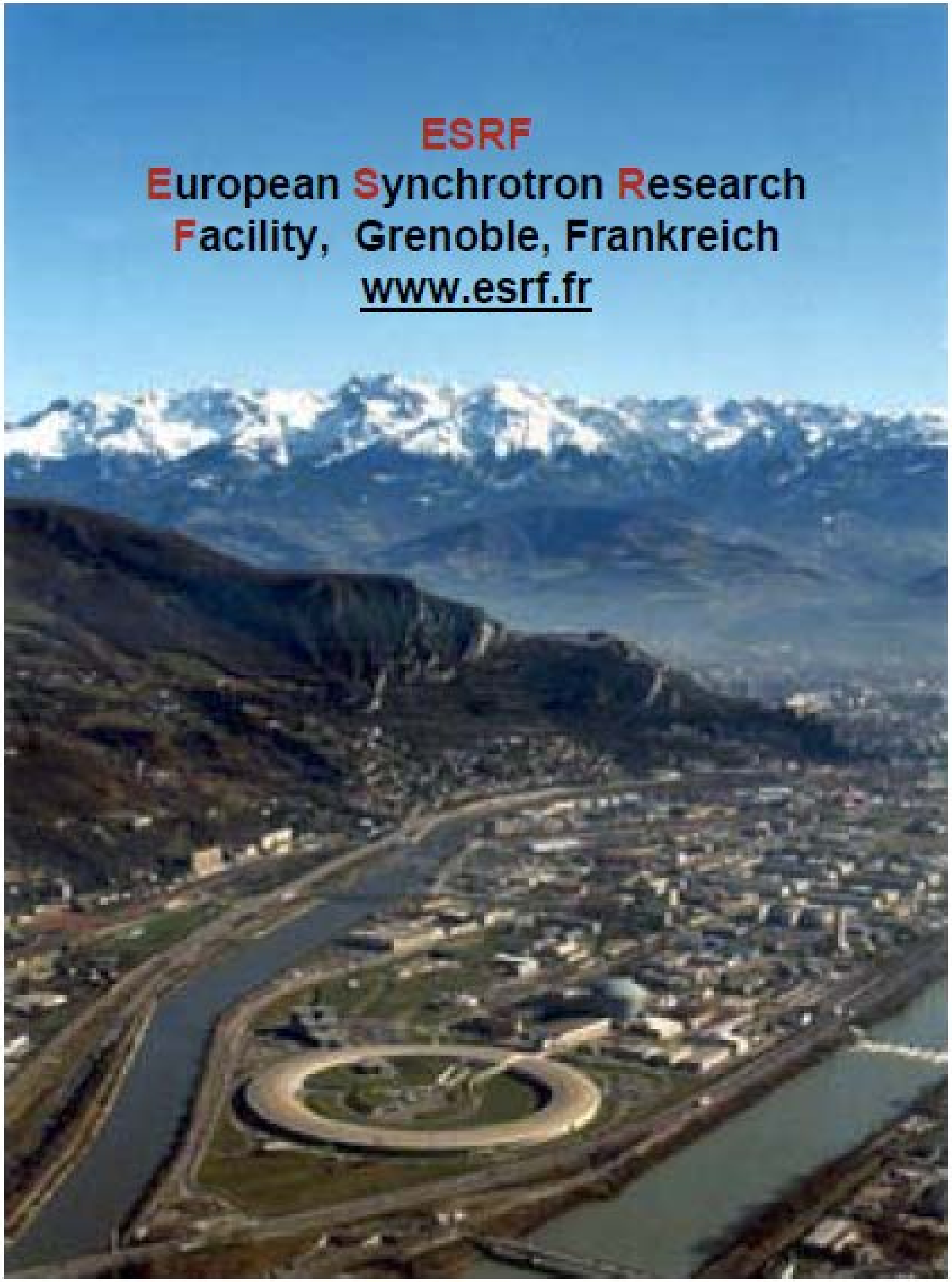
For $\frac{\Delta\lambda}{\lambda} \simeq \frac{1}{N}$

$$\theta_{cen} \simeq \frac{1}{\gamma\sqrt{N}}$$

typically

$$\theta_{cen} \simeq 40\ \mu\text{rad}$$

Info über Synchrotronstrahlung im Internet



ESRF
European Synchrotron Research Facility, Grenoble, Frankreich
www.esrf.fr

DESY
Deutsches Elektronensynchrotron
HASYLAB: Hamburger Synchrotronstrahlungslabor
www-hasylab.desy.de

BESSY
Berliner Elektronenspeicherring – Gesellschaft für Synchrotronstrahlung
www.bessy.de/guided_tour/

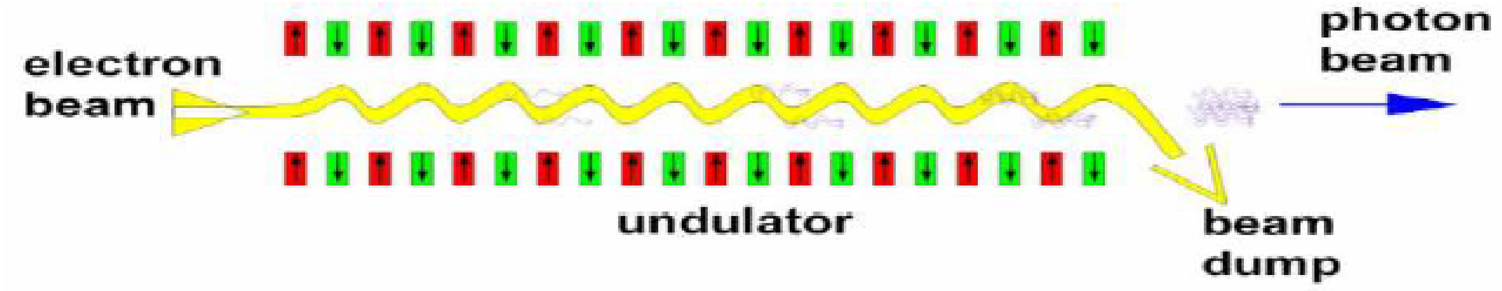
Preis ≥ € 1.000.000.000

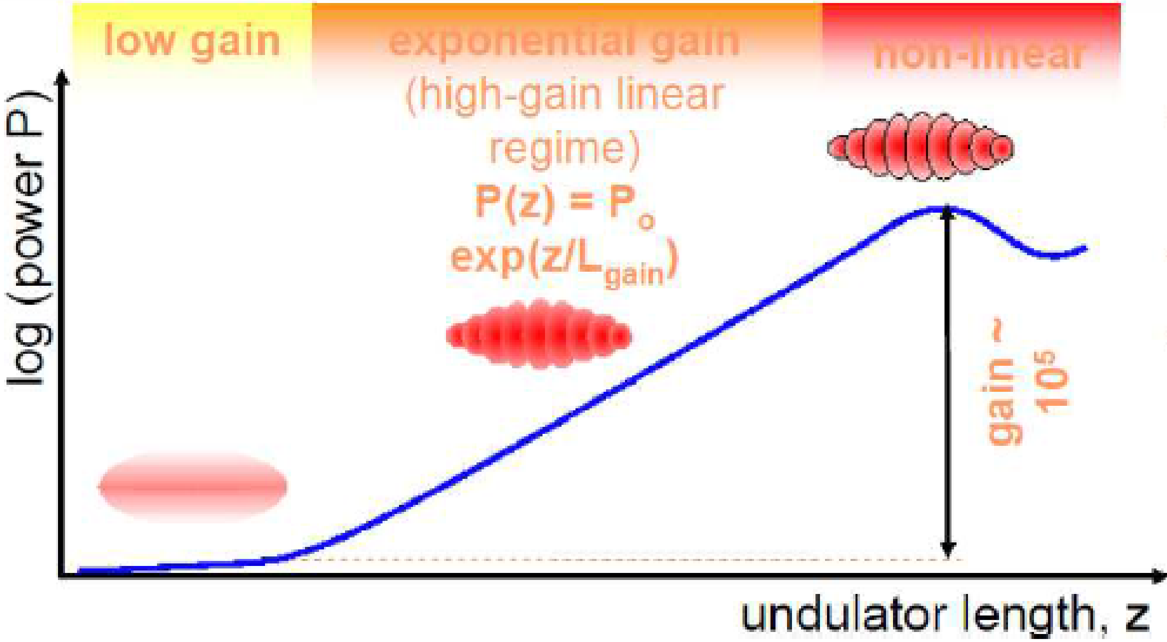
Höchstbrillante Röntgenquelle : Der Freie Elektronenlaser

SASE Prinzip

SASE = **S**elf **A**mplification of **S**pontaneous **E**mission

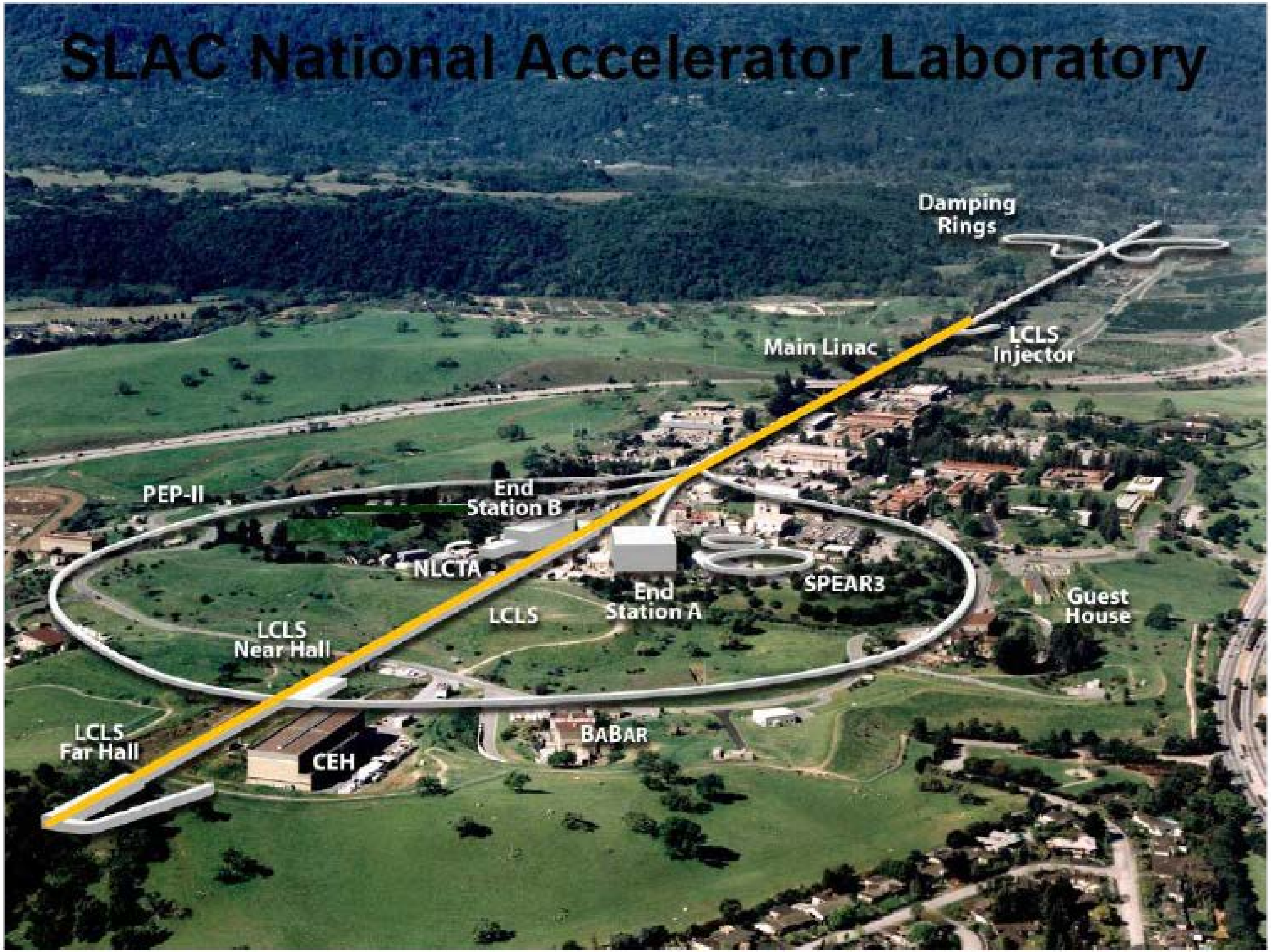
Saldin, Schneidmiller, Yurkov





- Bunch wechselwirkt mit eigenem Photonfeld
- Mikrobunche entstehen
- Elektronen strahlen kohärent ~N_e^2 mit $N_e \approx 10^6$

► Verstärkung bis zu N_e !



www6.slac.stanford.edu

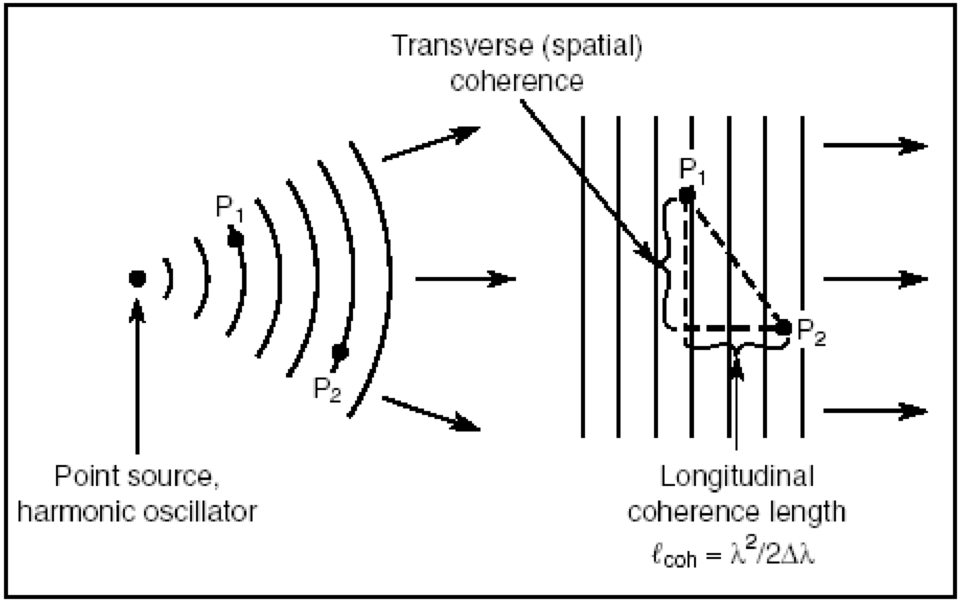
Mutual coherence factor

$$\Gamma_{12}(\tau) \equiv \langle E_1(t+\tau)E_2^*(t)\rangle \qquad (8.1)$$

Normalize degree of spatial coherence (complex coherence factor)

$$\mu_{12} = \frac{\langle E_1(t)E_2^*(t)\rangle}{\sqrt{\langle |E_1|^2\rangle}\sqrt{\langle |E_2|^2\rangle}} \qquad (8.12)$$

A high degree of coherence ($\mu \rightarrow 1$) implies an ability to form a high contrast interference (fringe) pattern. A low degree of coherence ($\mu \rightarrow 0$) implies an absence of interference, except with great care. In general radiation is partially coherent.

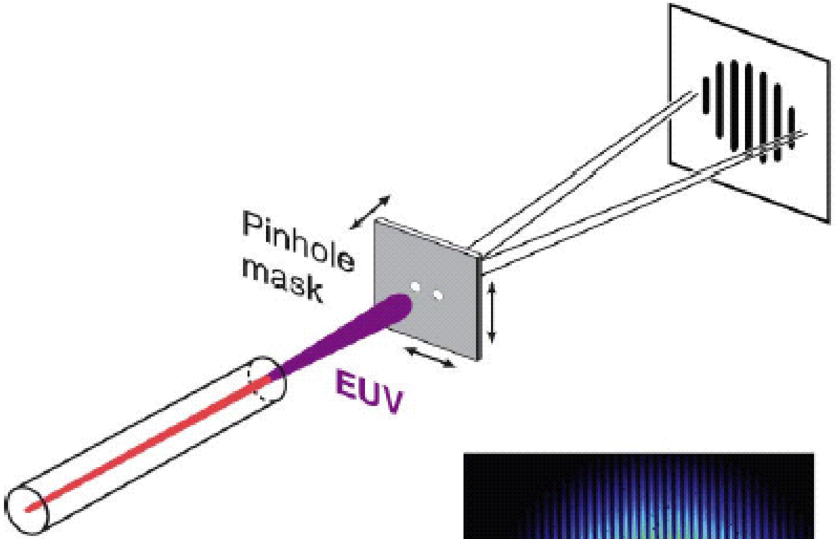


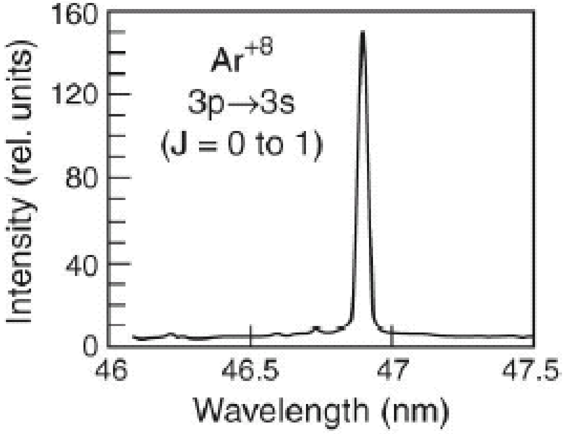
Longitudinal (temporal) coherence length

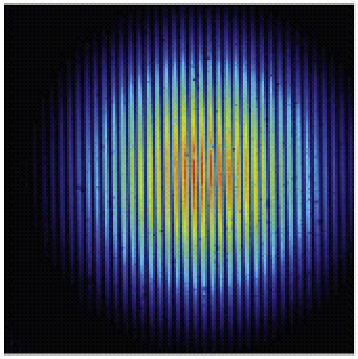
$$\boxed{\ell_{coh} = \frac{\lambda^2}{2\,\Delta\lambda}} \qquad (8.3)$$

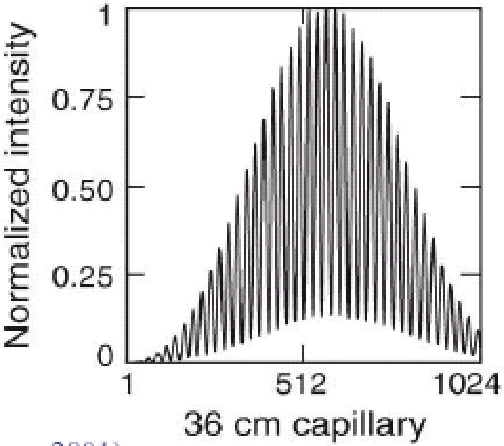
Full spatial (transverse) coherence

$$\boxed{d \cdot \theta = \lambda/2\pi} \qquad (8.5)$$







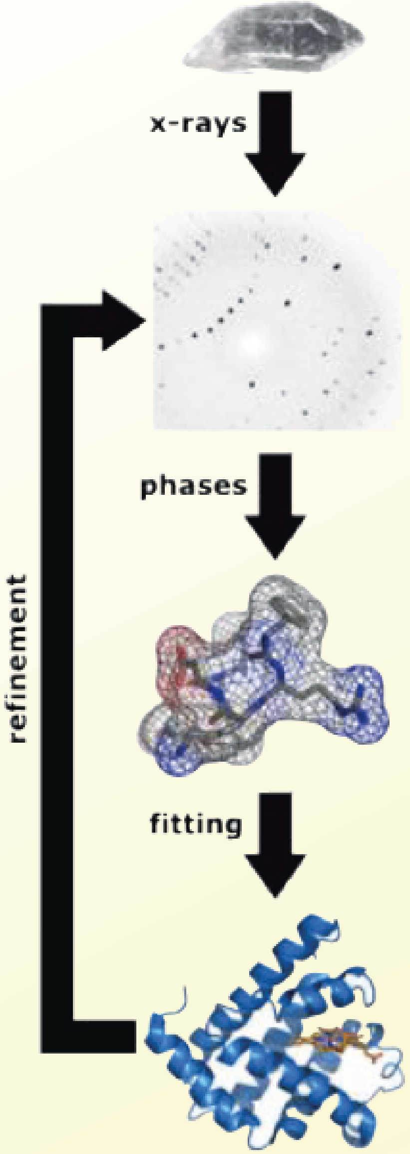


Y.Liu, et al., *Phys. Rev. A* (5 February 2001)

$$P_{coh} = 3\ \mathrm{mW} \rightarrow 7 \times 10^{14}\ \mathrm{ph/sec}\ @\ 46.9\ \mathrm{nm}$$

Courtesy of Prof. Jorge Rocca, Colorado State Univ.

Crystallography overcomes radiation damage and optics limitations, but requires crystals

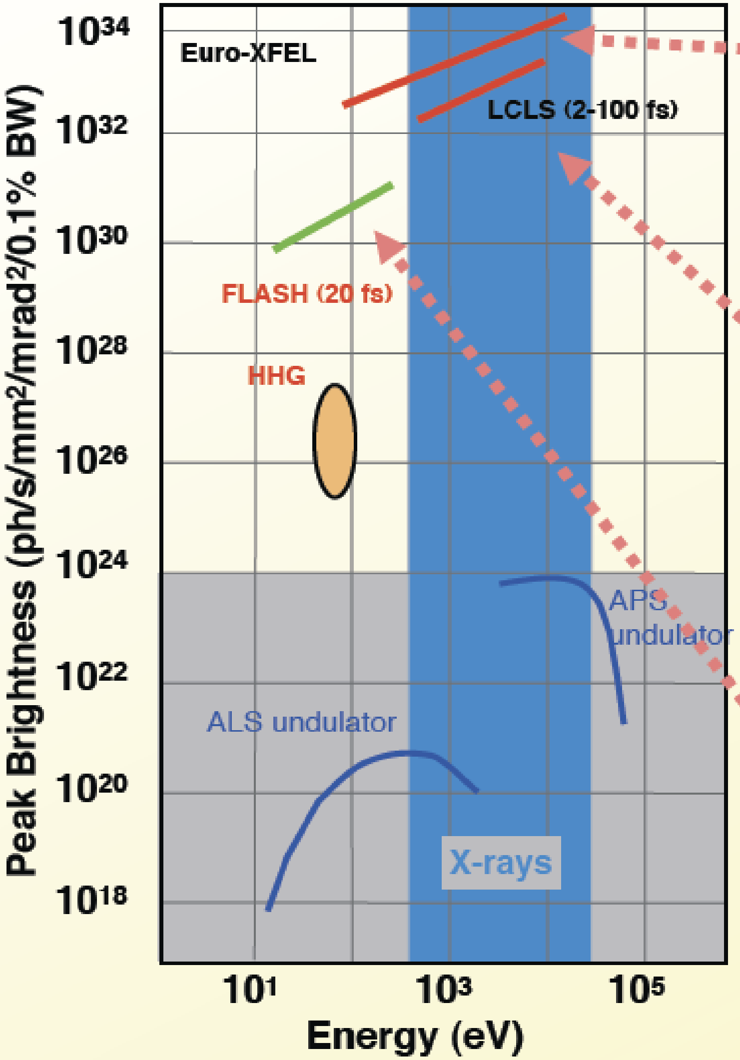


- ★ Radiation damage is spread out over 10^{10} identical unit cells
- ★ Diffraction from unit cells adds up coherently to form strong Bragg peaks
- ★ ~ 60,000 structures solved (in protein data bank), but ~15,000 distinct structures

- The bottleneck is in growing crystals

http://en.wikipedia.org/wiki/Image:X_ray_diffraction.png

X-ray free-electron lasers provide pulses that are *intense, short duration, short wavelength,* and *coherent*

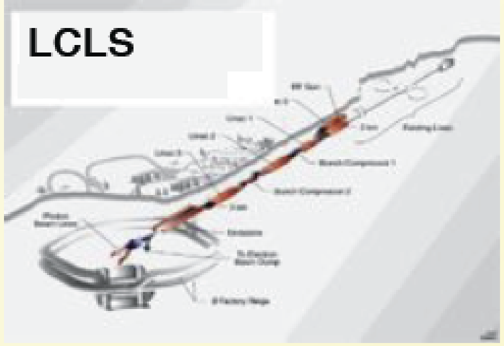


APS=Advanced Photon Source (ANL)
ALS=Advanced Light Source (LBNL)

operational 2013

12 keV, 50 fs, 10^{13} photons

European X-ray FEL,
DESY, Hamburg



operational now

800 eV to 2 keV in 2009
8 keV, 100 fs, 10^{12} photons

Linac Coherent Light Source,
SLAC, Stanford

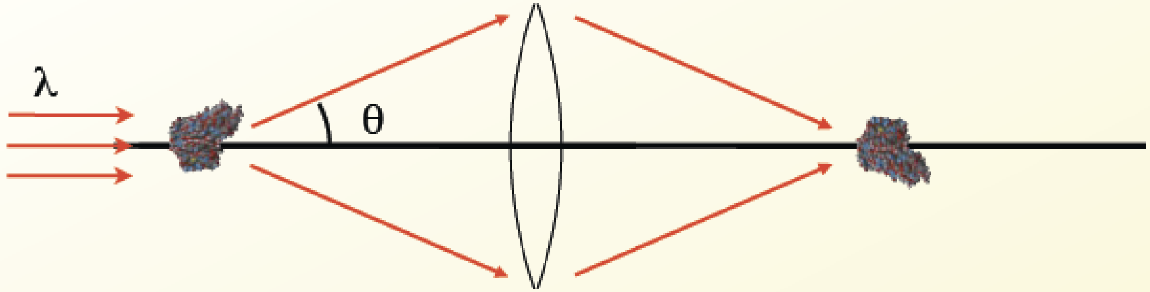
operational now

200 eV, 25 fs, 10^{12} photons
upgrade to 300 eV, 400 fs

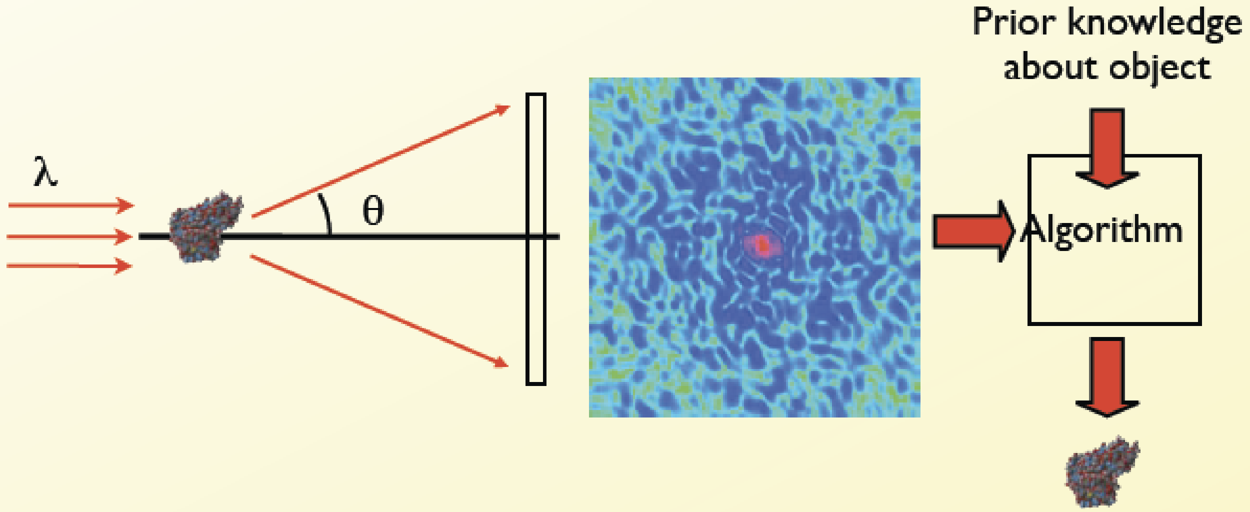
FLASH
DESY, Hamburg

Coherent diffractive imaging is lensless

Use a computer to phase the scattered light, rather than a lens



A lens recombines the scattered rays with correct phases to give the image



Prior knowledge about object

Algorithm

An algorithm finds the phases that are consistent with measurements and prior knowledge

Resolution: $\delta = \lambda / \sin\theta$

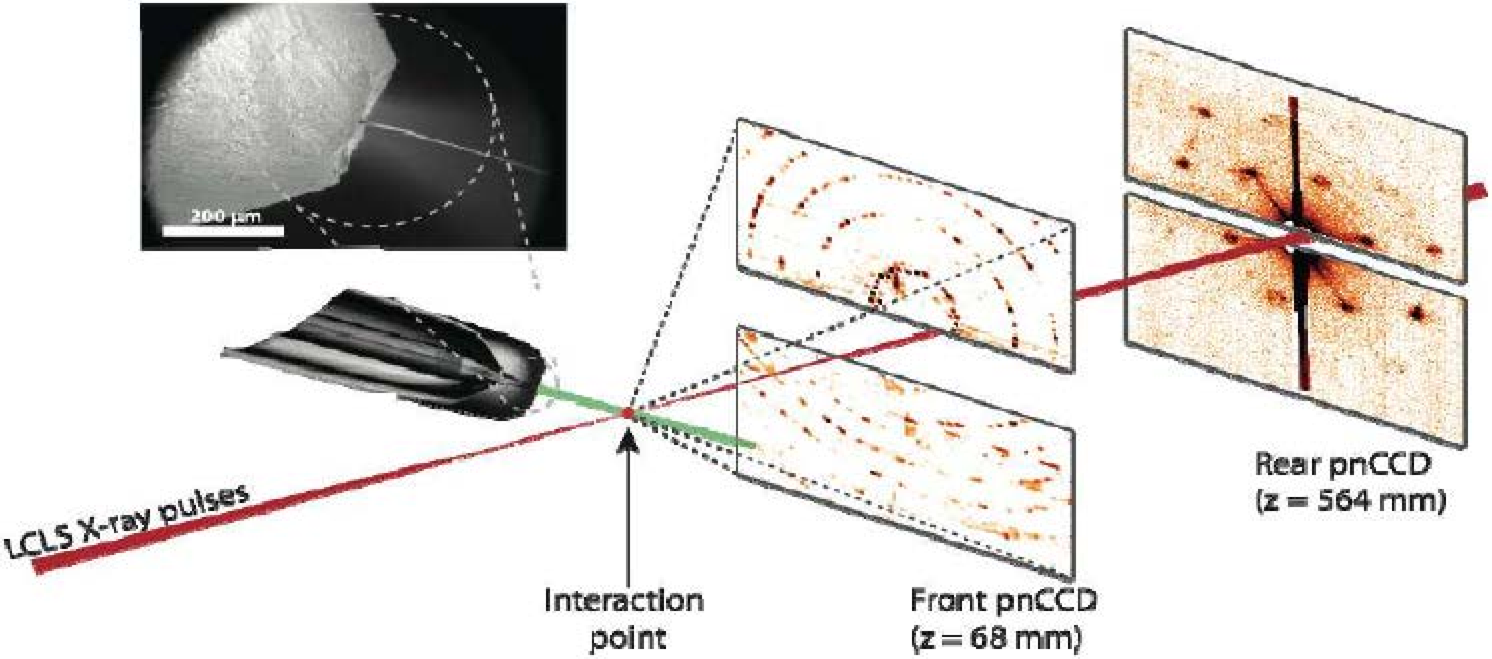
J. Fienup, Appl. Opt. **21** 2758 (1987)

J. Miao et al, Nature **400** 342 (1999)

Nanocrystallography carried out in a flowing water microjet

- Single pulse diffraction from Photosystem 1 nanocrystals at LCLS
- *E* = 1.8 keV
- <10, 60, 200 fs pulse

- 2 mJ pulse energy
- patterns collected at 30 Hz
- hit rate >50%
- 5 Tb data in one night!



Chapter One :

- **Basic Absorption and Emission Processes**
- **Atomic Energy Levels and Allowed Transistions**
- **Scattering, Diffraction and Refraction**

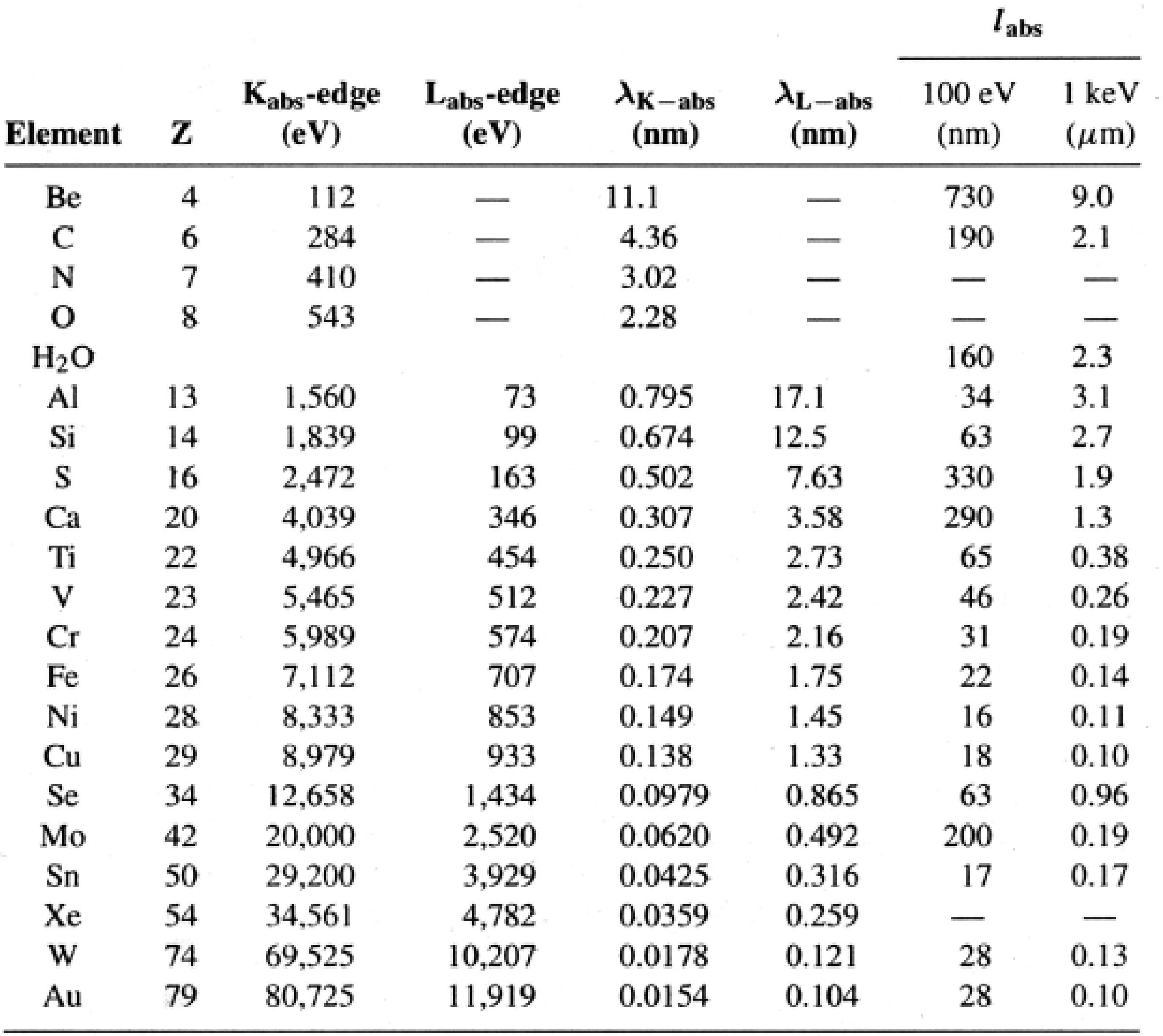
Photon Energy, Wavelength, Power

$$\boxed{\hbar\omega \cdot \lambda = hc = 1239.842 \text{ eV nm}} \tag{1.1}$$

$$\boxed{1 \text{ joule} \Rightarrow 5.034 \times 10^{15} \lambda[\text{nm}] \text{ photons}} \tag{1.2a}$$

$$\boxed{1 \text{ watt} \Rightarrow 5.034 \times 10^{15} \lambda[\text{nm}] \, \frac{\text{photons}}{\text{s}}} \tag{1.2b}$$

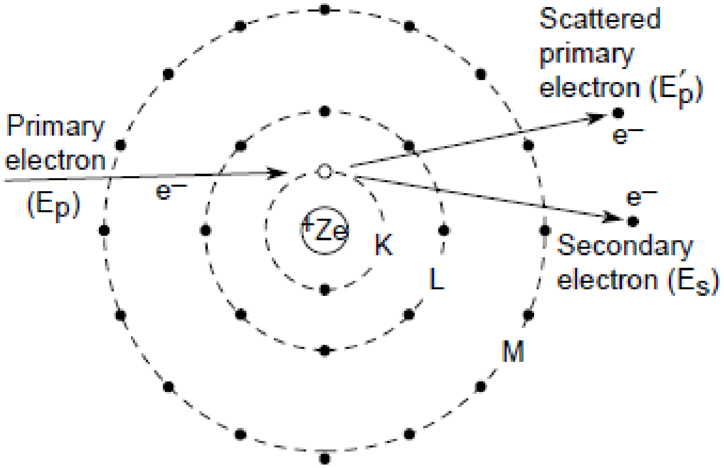
K and L_3-Absorption Edges for Selected Elements



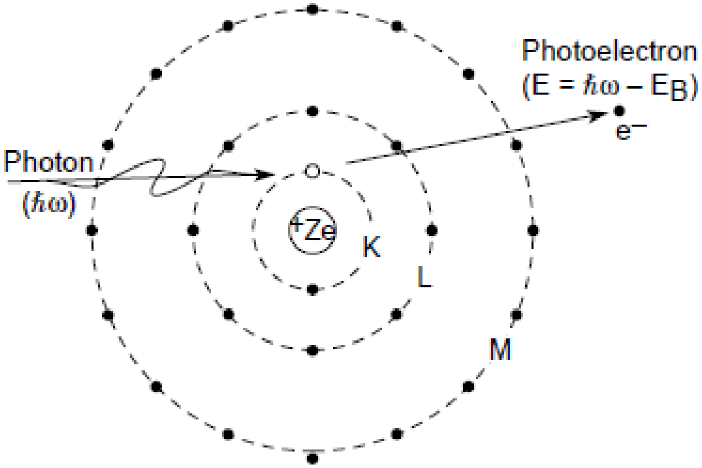
						l_{abs}	
Element	**Z**	**K_{abs}-edge (eV)**	**L_{abs}-edge (eV)**	**λ_{K-abs} (nm)**	**λ_{L-abs} (nm)**	100 eV (nm)	1 keV (μm)
Be	4	112	—	11.1	—	730	9.0
C	6	284	—	4.36	—	190	2.1
N	7	410	—	3.02	—	—	—
O	8	543	—	2.28	—	—	—
H_2O						160	2.3
Al	13	1,560	73	0.795	17.1	34	3.1
Si	14	1,839	99	0.674	12.5	63	2.7
S	16	2,472	163	0.502	7.63	330	1.9
Ca	20	4,039	346	0.307	3.58	290	1.3
Ti	22	4,966	454	0.250	2.73	65	0.38
V	23	5,465	512	0.227	2.42	46	0.26
Cr	24	5,989	574	0.207	2.16	31	0.19
Fe	26	7,112	707	0.174	1.75	22	0.14
Ni	28	8,333	853	0.149	1.45	16	0.11
Cu	29	8,979	933	0.138	1.33	18	0.10
Se	34	12,658	1,434	0.0979	0.865	63	0.96
Mo	42	20,000	2,520	0.0620	0.492	200	0.19
Sn	50	29,200	3,929	0.0425	0.316	17	0.17
Xe	54	34,561	4,782	0.0359	0.259	—	—
W	74	69,525	10,207	0.0178	0.121	28	0.13
Au	79	80,725	11,919	0.0154	0.104	28	0.10

Basic Ionization and Emission Processes in Isolated Atoms

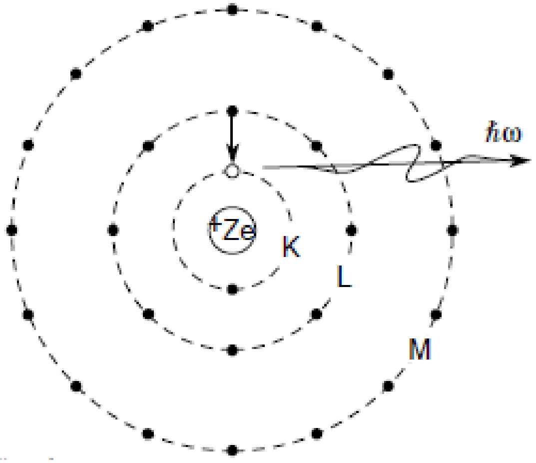
(a) Electron collision induced ionization



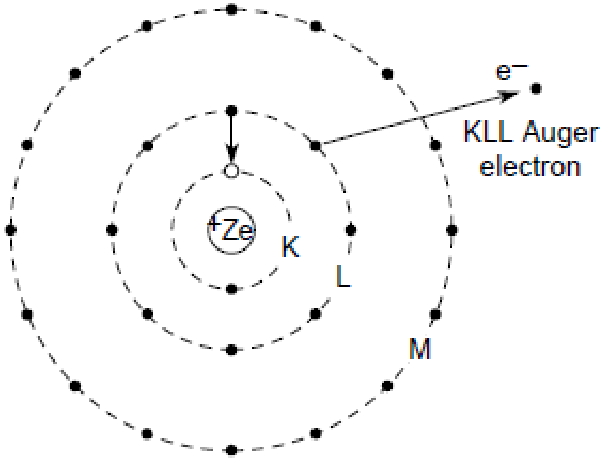
(b) Photoionization



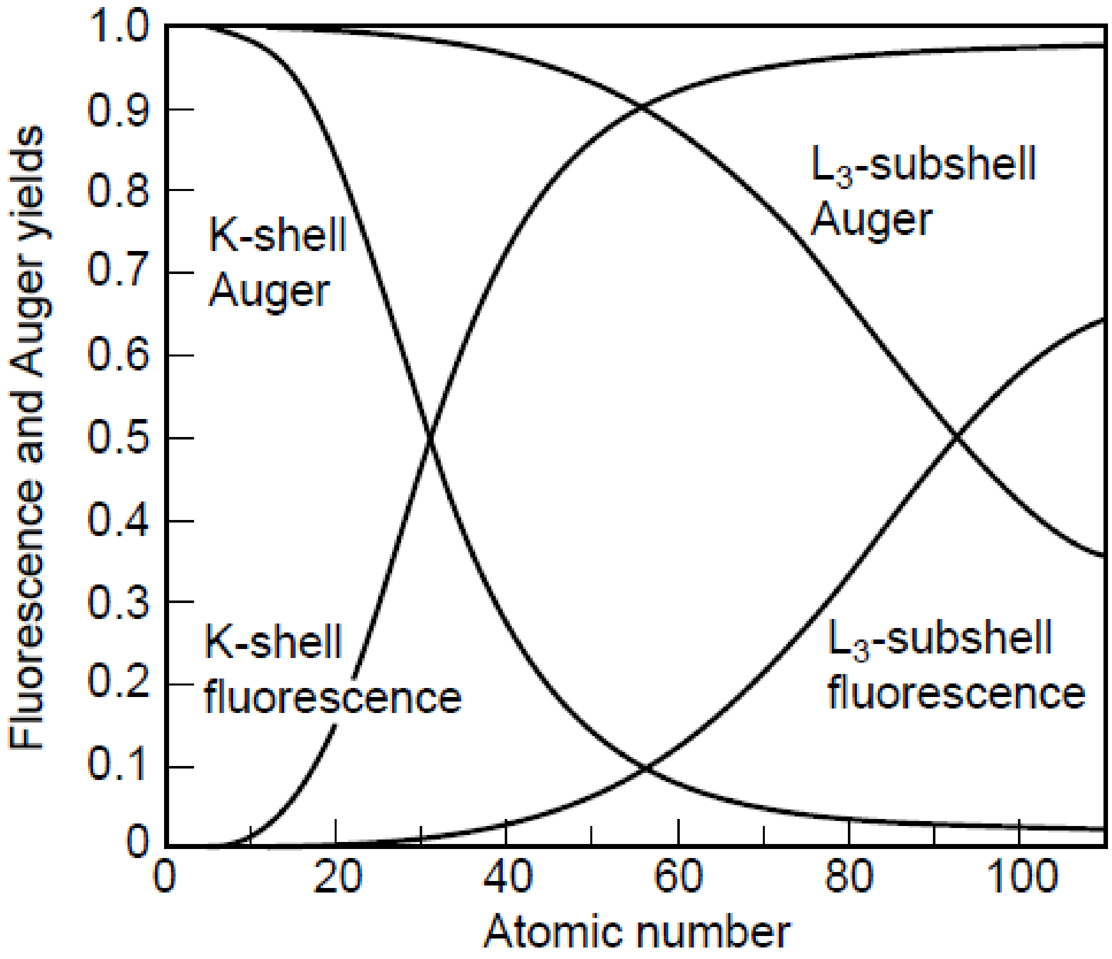
(c) Fluorescent emission of characteristic radiation



(d) Non-radiative Auger process

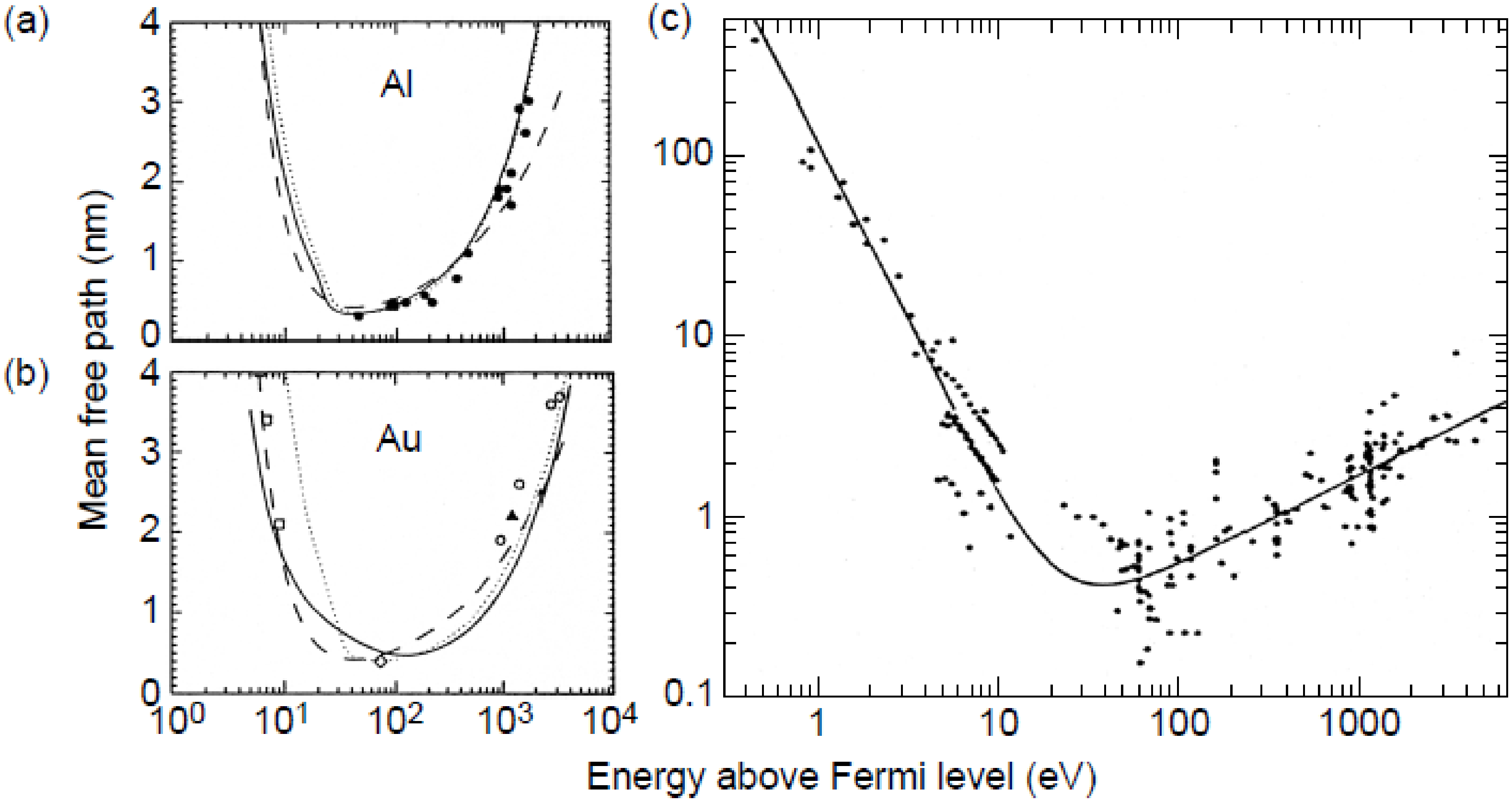


Fluorescence and Auger Emission Yields



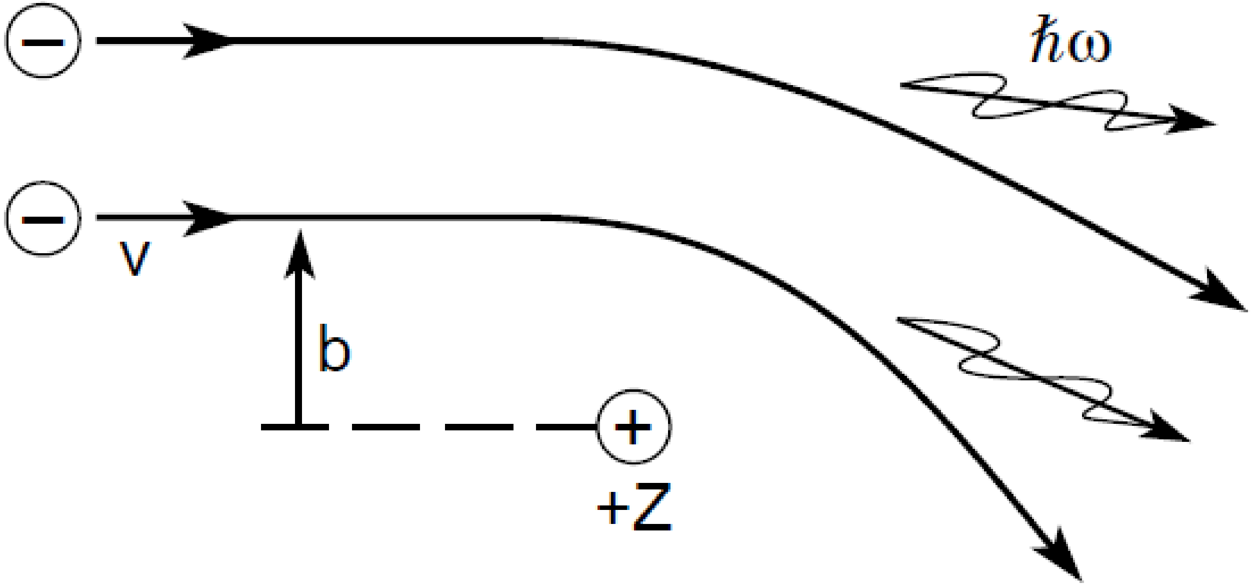
(Courtesy of M. Krause, Oak Ridge)

Electron Mean Free Paths As a Function of Energy

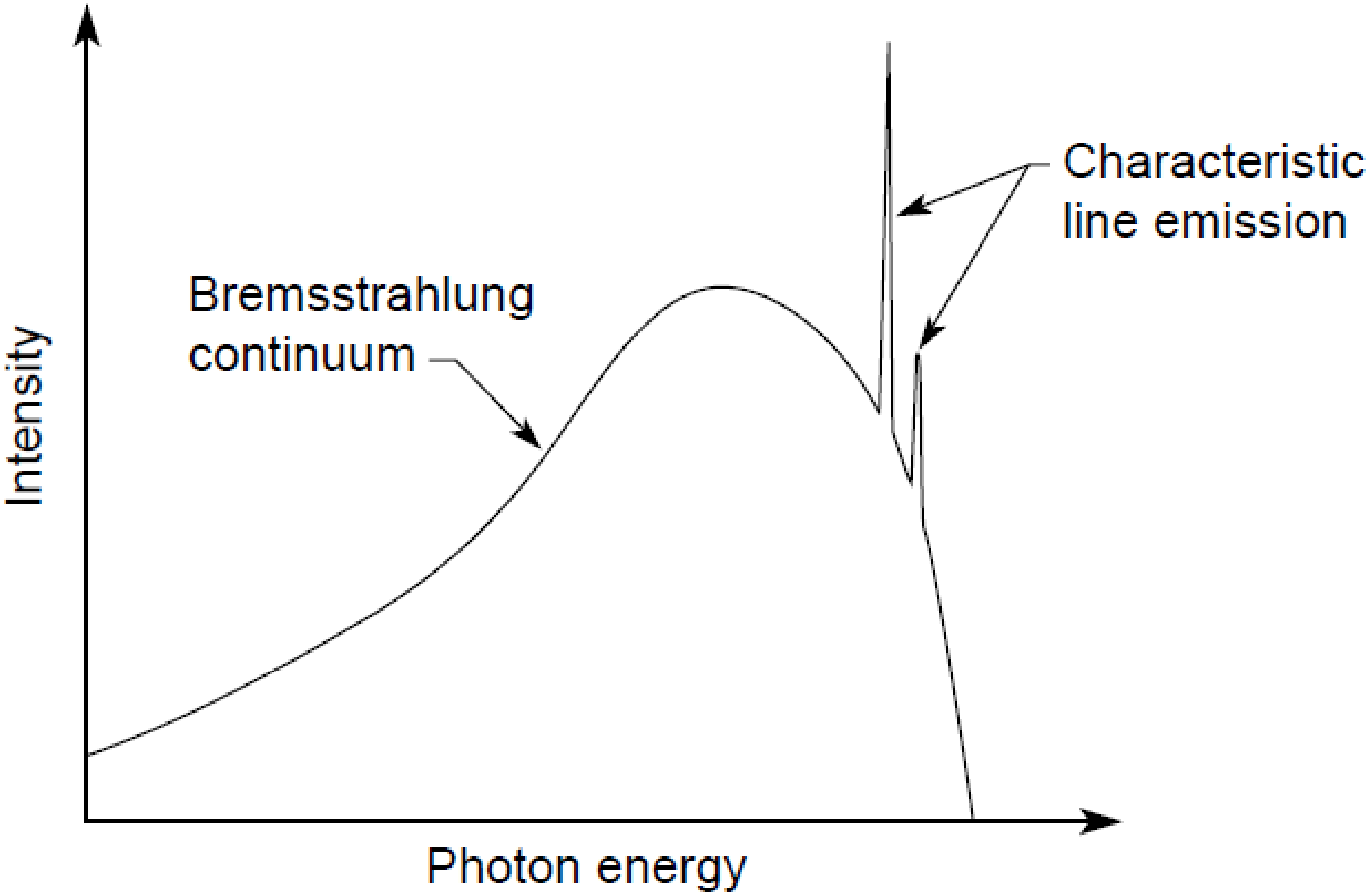


Courtesy of: Penn (a & b), Seah and Dench (c)

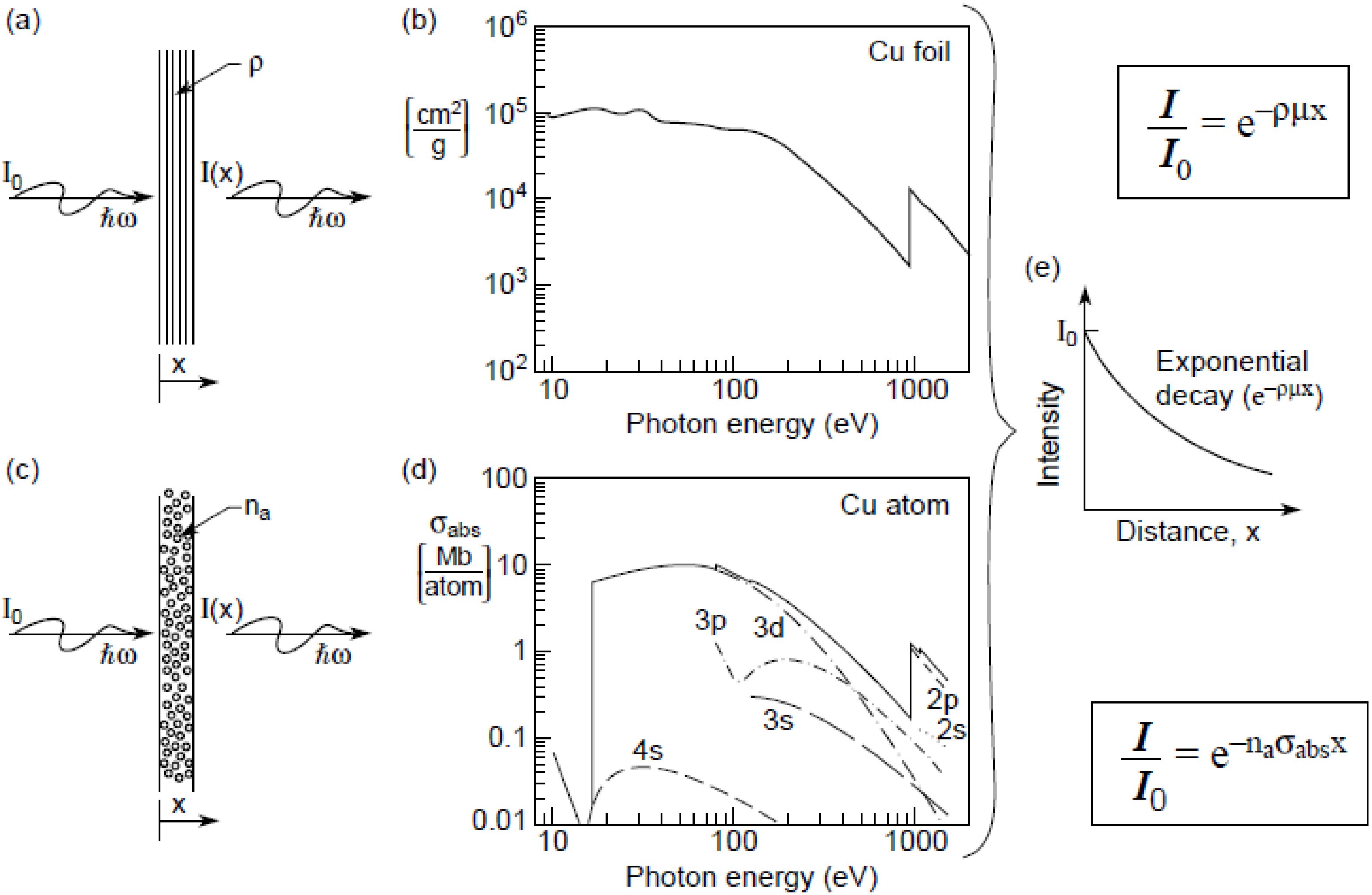
Bremsstrahlung Radiation: Braking Radiation from an Accelerated Charge



Continuum Bremsstrahlung Radiation and Narrow Characteristic Line Emission from a Solid Target with Electron Bombardment



Photoabsorption by Thin Foils and Isolated Atoms



$$\frac{I}{I_0} = e^{-\rho\mu x}$$

$$\frac{I}{I_0} = e^{-n_a\sigma_{abs}x}$$

Atomic Energy Levels and Allowed Transitions in the Bohr Atom

Equate Coulomb Force $Ze^2/4\pi\epsilon_0 r^2$ to the centripetal force mv^2/r:

$$E_n = \frac{mZ^2e^4}{32\pi^2\epsilon_0^2\hbar^2}\,\frac{1}{n^2} \tag{1.4}$$

$$r_n = \frac{4\pi\epsilon_0\hbar^2}{me^2Z}\cdot n^2 \tag{1.5}$$

$$\hbar\omega = E_i - E_f = \underbrace{\frac{me^4}{32\pi^2\epsilon_0\hbar^2}}_{13.6\ \text{eV}}\left[\frac{1}{n_{\text{f}}^2} - \frac{1}{n_{\text{i}}^2}\right]Z^2 \tag{1.6}$$

$$r_n = \frac{a_0 n^2}{Z} \quad ; \quad a_0 = 0.529\ \text{Å} \tag{1.9}$$

Quantum Mechanics Based on a Probabilistic Wave Function, $\Psi(\mathbf{r}, t)$

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(\mathbf{r}, t) + V(\mathbf{r}, t)\Psi(\mathbf{r}, t) = i\hbar\frac{\partial\Psi(\mathbf{r}, t)}{\partial t} \qquad (1.10)$$

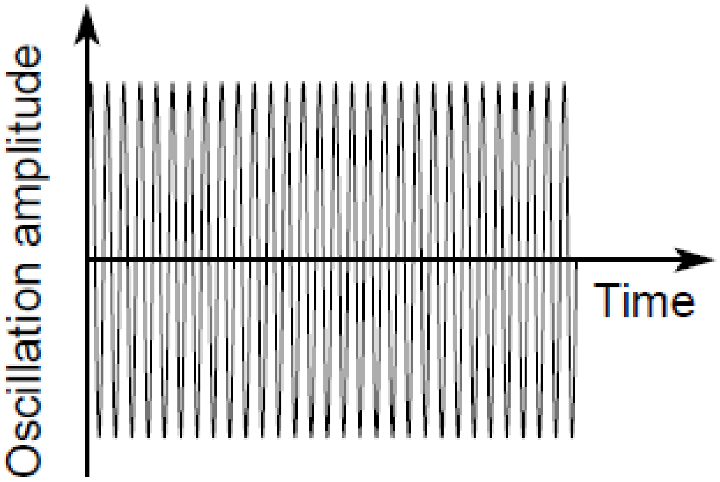
$$P(\mathbf{r}, t)d\mathbf{r} = \Psi^*(\mathbf{r}, t)\,\Psi(\mathbf{r}, t)d\mathbf{r} \qquad (1.13)$$

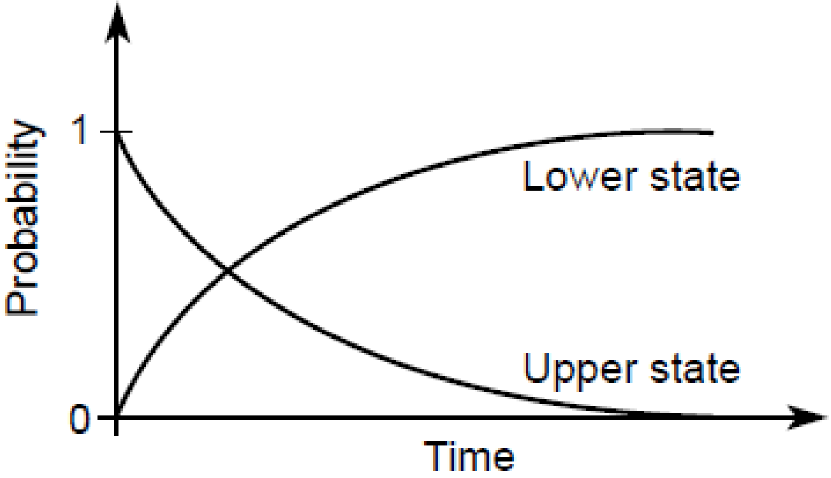
$$\bar{\mathbf{r}} = \int\!\!\int\!\!\int \mathbf{r}P(\mathbf{r}, t)d\mathbf{r} = \int\!\!\int\!\!\int \Psi^*(\mathbf{r}, t)\mathbf{r}\Psi(\mathbf{r}, t)d\mathbf{r} \qquad (1.15)$$

quantum numbers: n, ℓ, m_ℓ, m_s

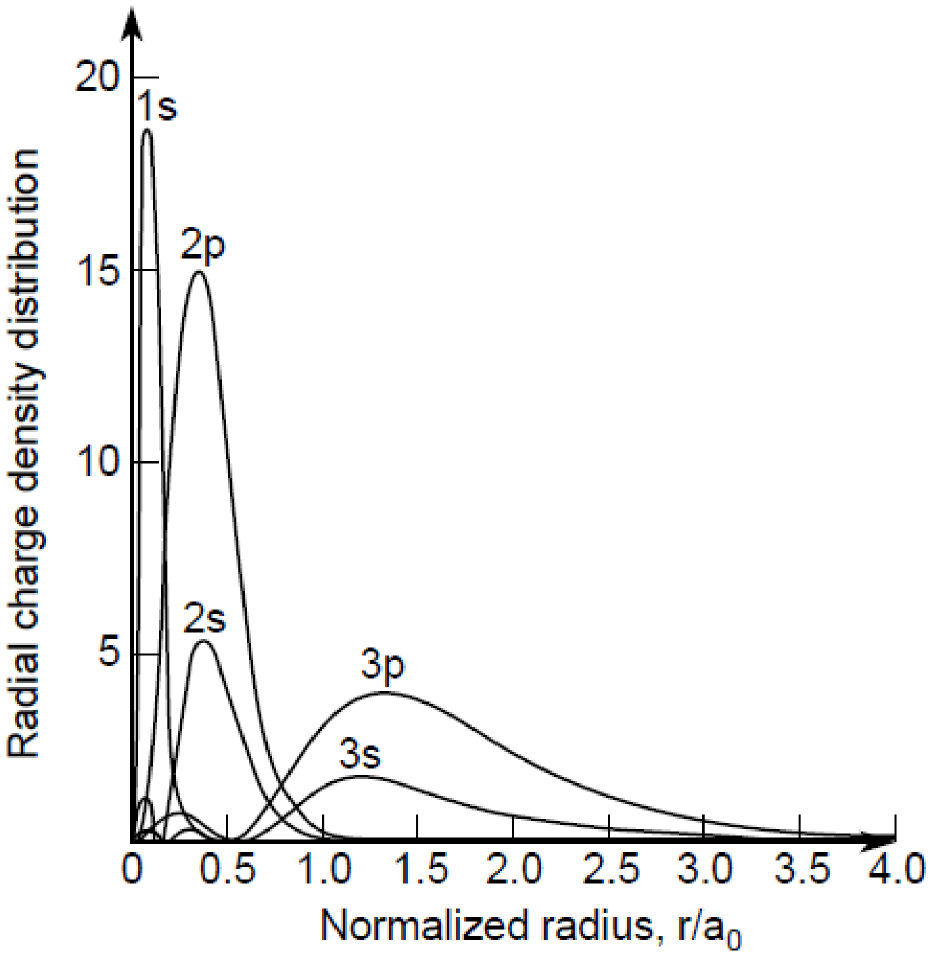
selection rules for allowed transitions: $\Delta\ell = \pm 1$
$\Delta j = 0, \pm 1$

Radiative Decay Involves An Atom Oscillating Between Two Stationary States at the Frequency $\omega_{if} = (E_i - E_f) / \hbar$



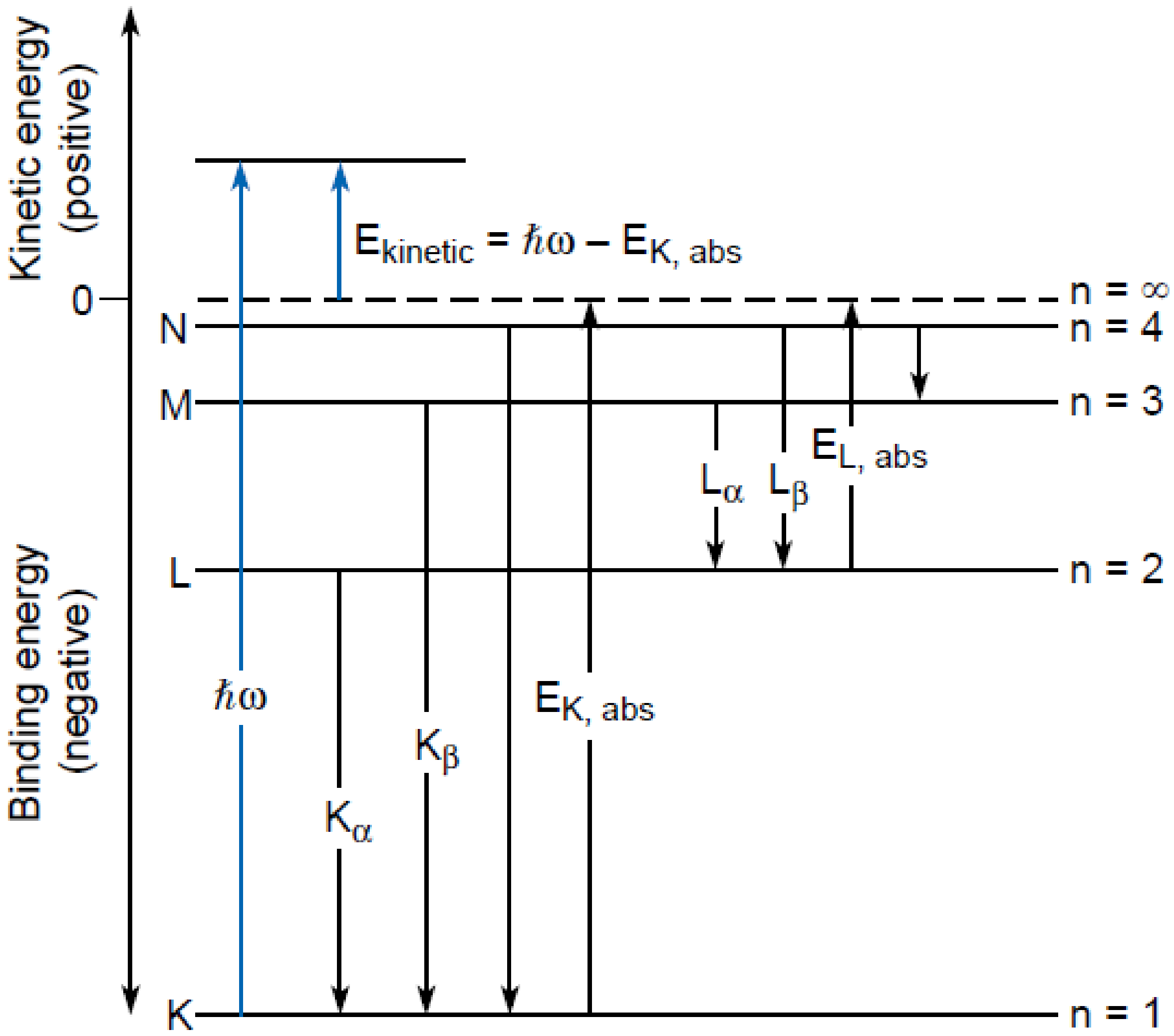


Probabilistic Radial Charge Distribution (e/Å) in the Argon Atom

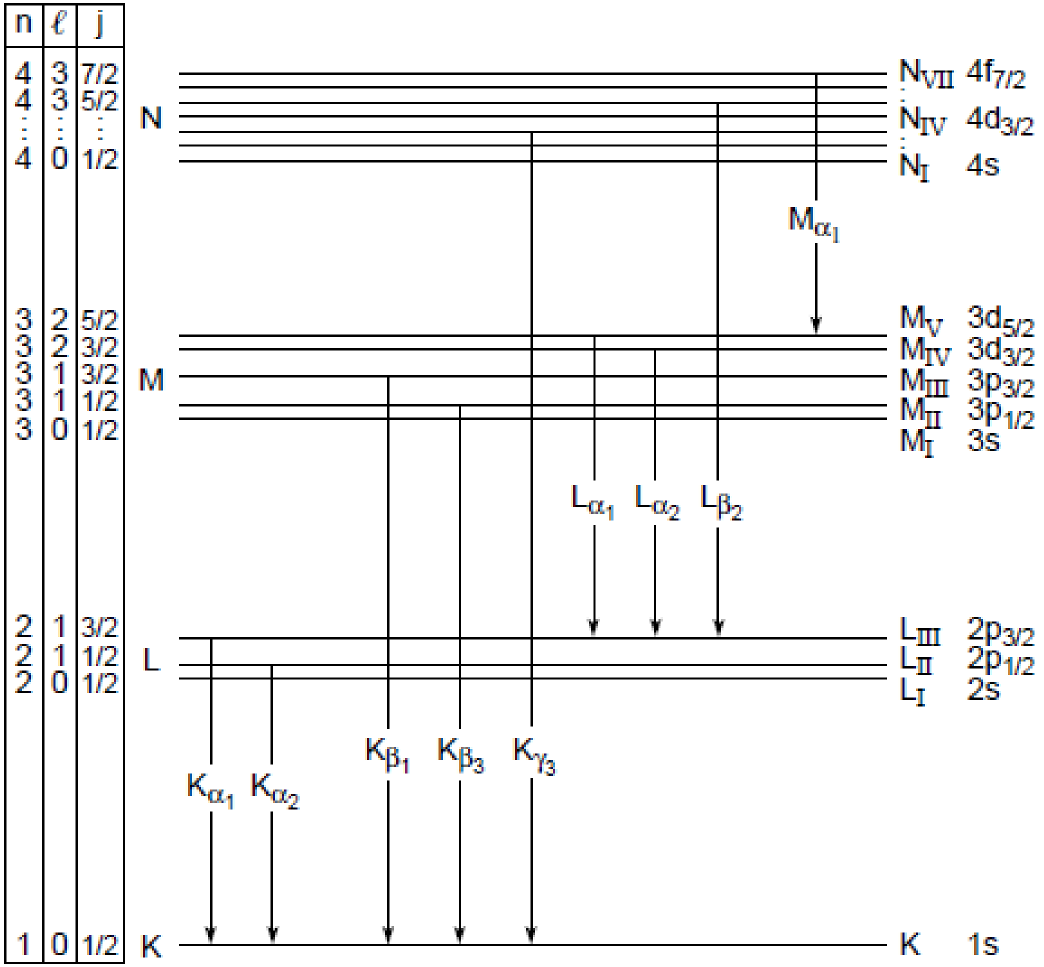


Courtesy of Eisberg and Resnick, *Quantum Physics of Atoms, Molecules, Solids, Nuclei, and Particles*.

Energy Levels, Absorption Edges, and Characteristic Line Emissions for a Multi-Electron Atom



Energy Levels, Quantum Numbers, and Allowed Transitions for the Copper Atom



Absorption edges for copper (Z = 29):

$E_{N_1,\,abs}$ = 7.7 eV

$E_{M_3,\,abs}$ = 75 eV

$E_{M_1,\,abs}$ = 123 eV

$E_{L_3,\,abs}$ = 933 eV
$E_{L_2,\,abs}$ = 952 eV
$E_{L_1,\,abs}$ = 1,097 eV

$E_{K,\,abs}$ = 8,979 eV
(1.381Å)

Cu K_{α_1} = 8,048 eV (1.541Å)	Cu L_{α_1} = 930 eV
Cu K_{α_2} = 8,028 eV (1.544Å)	Cu L_{α_2} = 930 eV
Cu K_{β_1} = 8,905 eV	Cu L_{β_1} = 950 eV

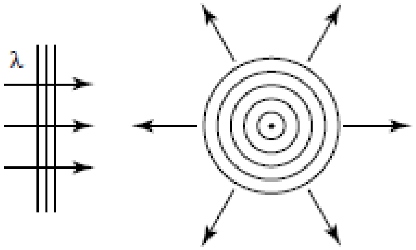
TABLE B.1. Electron binding energies in electron volts for the elements in their natural forms.[a]

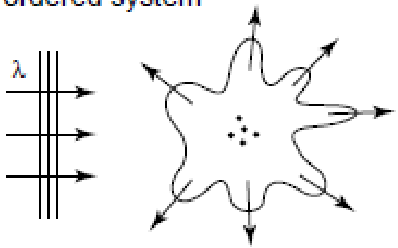
Element	K 1s	$L_1$2s	L_2 $2p_{1/2}$	L_3 $2p_{3/2}$	$M_1$3s	M_2 $3p_{1/2}$	M_3 $3p_{3/2}$	M_4 $3d_{3/2}$	M_5 $3d_{5/2}$	$N_1$4s	N_2 $4p_{1/2}$	N_3 $4p_{3/2}$
1 H	13.6											
2 He	24.6[b]											
3 Li	54.7[b]											
4 Be	111.5[b]											
5 B	188[b]											
6 C	284.2[b]											
7 N	409.9[b]	37.3[b]										
8 O	543.1[b]	41.6[b]										
9 F	696.7[b]											
10 Ne	870.2[b]	48.5[b]	21.7[b]	21.6[b]								
11 Na	1070.8[c]	63.5[c]	30.4[c]	30.5[b]								
12 Mg	1303.0[c]	88.6[b]	49.6[c]	49.2[c]								
13 Al	1559.6	117.8[b]	72.9[b]	72.5[b]								
14 Si	1838.9	149.7[b]	99.8[b]	99.2[b]								
15 P	2145.5	189[b]	136[b]	135[b]								
16 S	2472	230.9[b]	163.6[b]	162.5[b]								
17 Cl	2822.4	270.2[b]	202[b]	200[b]								
18 Ar	3205.9[b]	326.3[b]	250.6[b]	248.4[b]	29.3[b]	15.9[b]	15.7[b]					
19 K	3608.4[b]	378.6[b]	297.3[b]	294.6[b]	34.8[b]	18.3[b]	18.3[b]					
20 Ca	4038.5[b]	438.4[c]	349.7[c]	346.2[c]	44.3[c]	25.4[c]	25.4[c]					
21 Sc	4492.8	498.0[b]	403.6[b]	398.7[b]	51.1[b]	28.3[b]	28.3[b]					
22 Ti	4966.4	560.9[c]	461.2[c]	453.8[c]	58.7[c]	32.6[c]	32.6[c]					
23 V	5465.1	626.7[c]	519.8[c]	512.1[c]	66.3[c]	37.2[c]	37.2[c]					
24 Cr	5989.2	695.7[c]	583.8[c]	574.1[c]	74.1[c]	42.2[c]	42.2[c]					
25 Mn	6539.0	769.1[c]	649.9[c]	638.7[c]	82.3[c]	47.2[c]	47.2[c]					
26 Fe	7112.0	844.6[c]	719.9[c]	706.8[c]	91.3[c]	52.7[c]	52.7[c]					
27 Co	7708.9	925.1[c]	793.3[c]	778.1[c]	101.0[c]	58.9[c]	58.9[c]					
28 Ni	8332.8	1008.6[c]	870.0[c]	852.7[c]	110.8[c]	68.0[c]	66.2[c]					
29 Cu	8978.9	1096.7[c]	952.3[c]	932.5[c]	122.5[c]	77.3[c]	75.1[c]					
30 Zn	9658.6	1196.2[b]	1044.9[b]	1021.8[b]	139.8[b]	91.4[b]	88.6[b]	10.2[b]	10.1[b]			

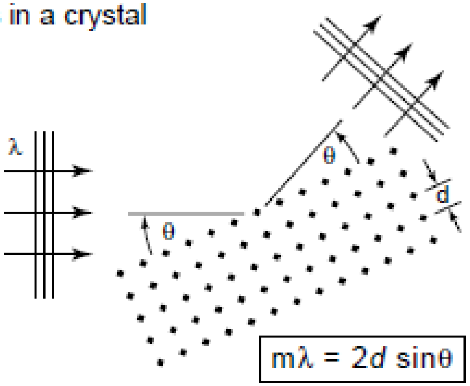
TABLE B.2. Photon energies, in electron volts, of principal K and L shell emission lines.[a]

Element	$K\alpha_1$	$K\alpha_2$	$K\beta_1$	$L\alpha_1$	$L\alpha_2$	$L\beta_1$	$L\beta_2$	$L\gamma_1$
3 Li	54.3							
4 Be	108.5							
5 B	183.3							
6 C	277							
7 N	392.4							
8 O	524.9							
9 F	676.8							
10 Ne	848.6	848.6						
11 Na	1,040.98	1,040.98	1,071.1					
12 Mg	1,253.60	1,253.60	1,302.2					
13 Al	1,486.70	1,486.27	1,557.45					
14 Si	1,739.98	1,739.38	1,835.94					
15 P	2,013.7	2,012.7	2,139.1					
16 S	2,307.84	2,306.64	2,464.04					
17 Cl	2,622.39	2,620.78	2,815.6					
18 Ar	2,957.70	2,955.63	3,190.5					
19 K	3,313.8	3,311.1	3,589.6					
20 Ca	3,691.68	3,688.09	4,012.7	341.3	341.3	344.9		
21 Sc	4,090.6	4,086.1	4,460.5	395.4	395.4	399.6		
22 Ti	4,510.84	4,504.86	4,931.81	452.2	452.2	458.4		
23 V	4,952.20	4,944.64	5,427.29	511.3	511.3	519.2		
24 Cr	5,414.72	5,405.509	5,946.71	572.8	572.8	582.8		
25 Mn	5,898.75	5,887.65	6,490.45	637.4	637.4	648.8		
26 Fe	6,403.84	6,390.84	7,057.98	705.0	705.0	718.5		
27 Co	6,930.32	6,915.30	7,649.43	776.2	776.2	791.4		
28 Ni	7,478.15	7,460.89	8,264.66	851.5	851.5	868.8		
29 Cu	8,047.78	8,027.83	8,905.29	929.7	929.7	949.8		
30 Zn	8,638.86	8,615.78	9,572.0	1,011.7	1,011.7	1,034.7		

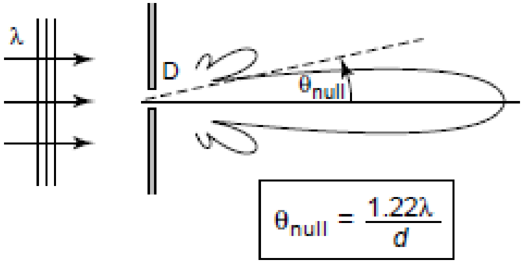
Scattering, Diffraction, and Refraction


(a) Isotropic scattering from a point object

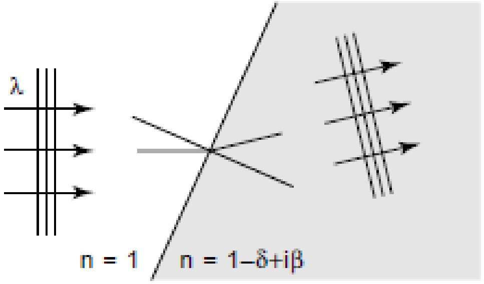

(b) Non-isotropic scattering from a partially ordered system

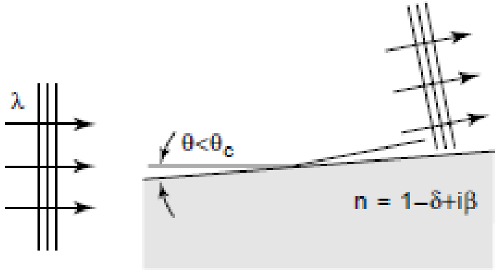

(c) Diffraction by an ordered array of atoms, as in a crystal

$$m\lambda = 2d \sin\theta$$

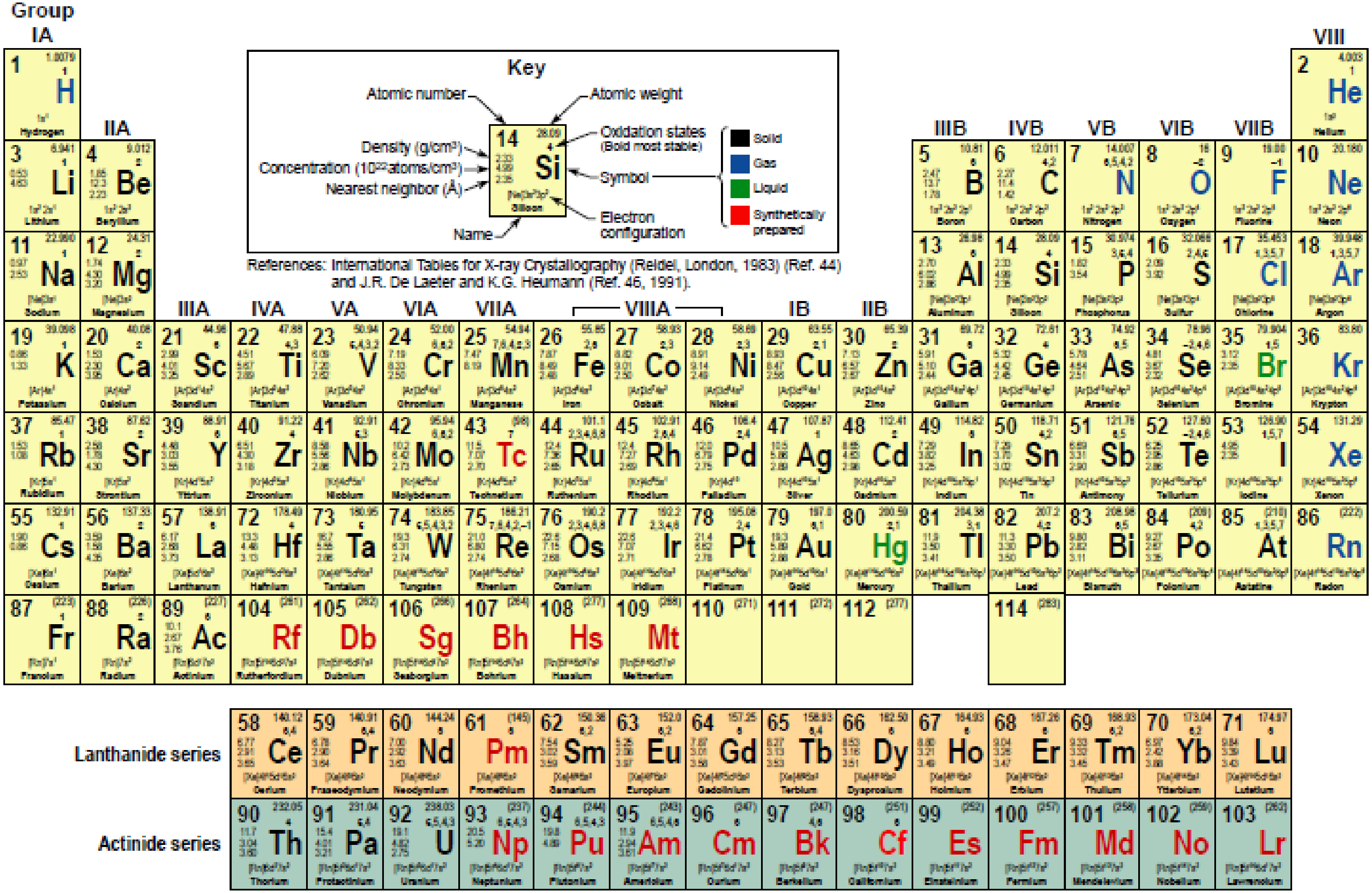

(d) Diffraction from a well-defined geometric structure, such as a pinhole

$$\theta_{null} = \frac{1.22\lambda}{d}$$


(e) Refraction at an interface


(f) Total external reflection

Periodic Table of the Elements



Key

14 28.09 4 Si 2.33 4.99 2.35 [Ne]3s²3p² Silicon

■ Solid
🟦 Gas
🟩 Liquid
🟥 Synthetically prepared

References: International Tables for X-ray Crystallography (Reidel, London, 1983) (Ref. 44) and J.R. De Laeter and K.G. Heumann (Ref. 46, 1991).

IA	IIA	IIIA	IVA	VA	VIA	VIIA	VIIIA	VIIIA	VIIIA	IB	IIB	IIIB	IVB	VB	VIB	VIIB	VIII
1 H																	2 He
3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
55 Cs	56 Ba	57 La	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
87 Fr	88 Ra	89 Ac	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110	111	112		114				

Lanthanide series	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
Actinide series	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr