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X-Ray Interaction with Matter: Absorption, Scattering, Refraction

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X-Ray Interaction with Matter: Absorption, Scattering, Refraction

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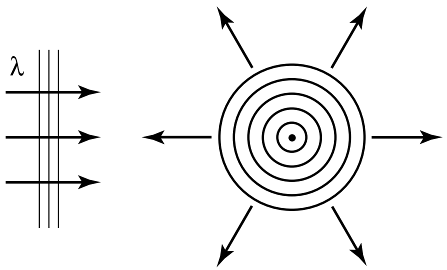
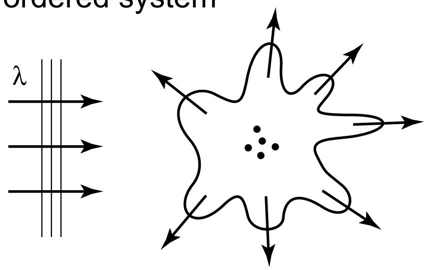
Scattering, Diffraction, and Refraction

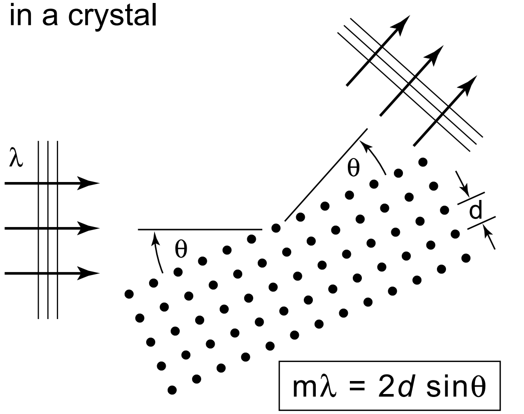
(a) Isotropic scattering from a point object



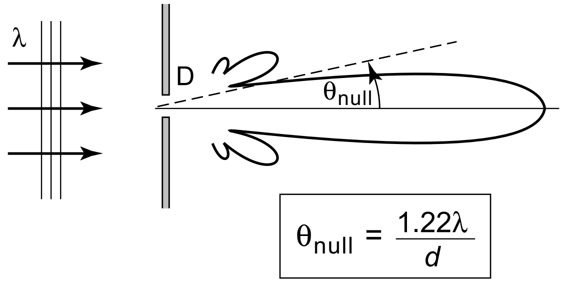
(b) Non-isotropic scattering from a partially ordered system



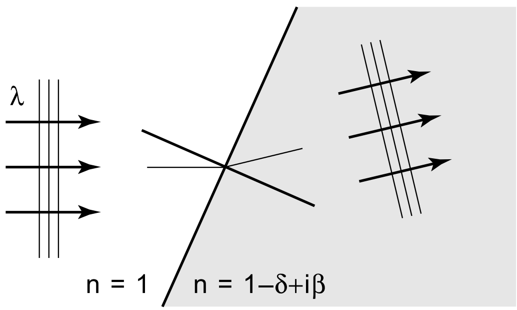
(c) Diffraction by an ordered array of atoms, as in a crystal



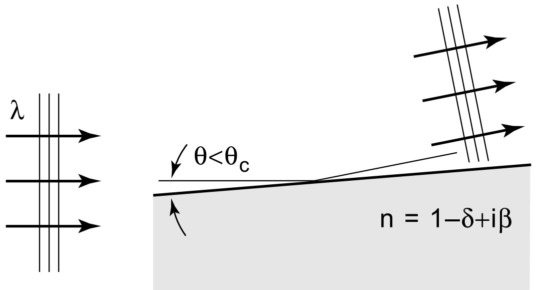
(d) Diffraction from a well-defined geometric structure, such as a pinhole



(e) Refraction at an interface



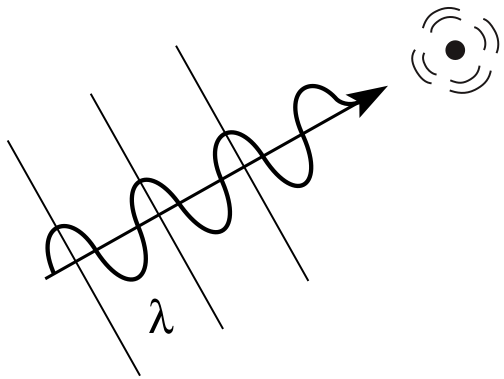
(f) Total external reflection

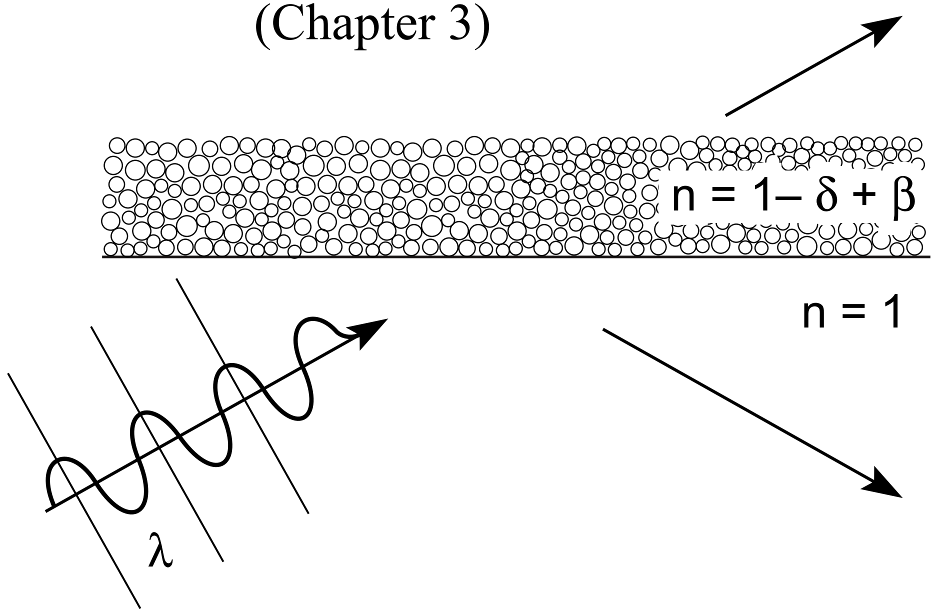


Scattering, Refraction, and Reflection

Single scatterer, electron or atom, in vacuum. (Chapter 2)

Many atoms, each with many electrons, constituting a “material”. (Chapter 3)





- How are scattering, refraction, and reflection related?
- How do these differ for amorphous and ordered (crystalline) materials?
- What is the role of forward scattering?

Maxwell's Equations

↓

Wave Equation

(in vacuum) (Chapter 2) ↙ ↘ (in a material) (Chapter 3)

Radiation by a single electron ("dipole radiation")

Scattering cross-sections

Scattering by a free electron ("Thomson scattering")

Scattering by a single bound electron ("Rayleigh scattering")

Scattering by a multi-electron atom

Atomic "scattering factors", f_0' and f_0''

Refractive index with many atoms present

Role of forward scattering

Contributions to refractive index by bound electrons

Refractive index for soft x-rays and EUV

$$n = 1 - \delta + i\beta \quad (\delta, \beta << 1)$$

$\delta \rightarrow f_0'$, $\beta \rightarrow f_0''$

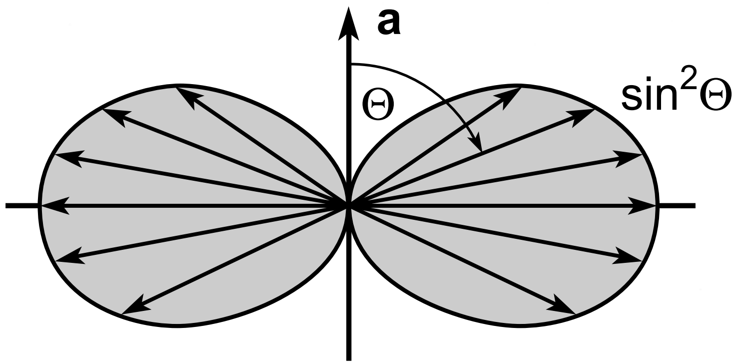
Determining f_0' and f_0''; measurements and Kramers-Kronig

Total external reflection

Reflectivity vs. angle

Brewster's angle

Radiation by an Accelerated Charge: Scattering by Free and Bound Electrons



$$\frac{dP}{d\Omega} = \frac{e^2|\mathbf{a}|^2 \sin^2\Theta}{16\pi^2\epsilon_0 c^3} \qquad (2.34)$$

$$r_e = \frac{e^2}{4\pi\epsilon_0 mc^2} \qquad (2.44)$$

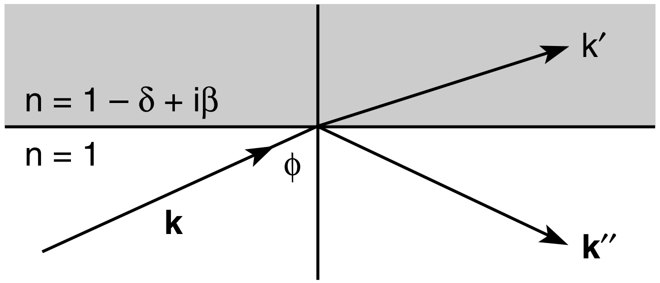
$$\sigma_e = \frac{8\pi}{3} r_e^2 \qquad (2.45)$$

$$\sigma = \frac{8\pi}{3} r_e^2 \frac{\omega^4}{(\omega^2 - \omega_s^2)^2 + (\gamma\omega)^2} \qquad (2.51)$$

$$f(\Delta\mathbf{k}, \omega) = \sum_{s=1}^{Z} \frac{\omega^2 e^{-i\Delta\mathbf{k}\cdot\Delta\mathbf{r}_s}}{\omega^2 - \omega_s^2 + i\gamma\omega} \qquad (2.66)$$

$$f^0(\omega) = \sum_{s=1}^{Z} \frac{\omega^2}{\omega^2 - \omega_s^2 + i\gamma\omega} \qquad (2.72)$$

WAVE PROPAGATION AND REFRACTIVE INDEX AT EUV AND SOFT X-RAY WAVELENGTHS



$$n(\omega) = 1 - \frac{n_a r_e \lambda^2}{2\pi}\left(f_1^0 - i f_2^0\right) \quad (3.9)$$

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

$$l_{\text{abs}} = \frac{\lambda}{4\pi\beta} \quad (3.22)$$

$$\sigma_{\text{abs.}} = 2 r_e \lambda f_2^0(\omega) \quad (3.28)$$

$$\Delta\phi = \left(\frac{2\pi\delta}{\lambda}\right)\Delta r \quad (3.29)$$

$$\theta_c = \sqrt{2\delta} \quad (3.41)$$

$$R_{s,\perp} \simeq \frac{\delta^2 + \beta^2}{4} \quad (3.50)$$

$$\phi_B \simeq \frac{\pi}{4} - \frac{\delta}{2} \quad (3.60)$$

Maxwell's Equations and the Wave Equation

Maxwell's equations:

$$\nabla \times \mathbf{H} = \frac{\partial \mathbf{D}}{\partial t} + \mathbf{J} \qquad \text{(Ampere's law)} \qquad (2.1) \quad , \quad \mathbf{J} = -en\mathbf{v} \qquad (2.10)$$

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \qquad \text{(Faraday's law)} \qquad (2.2)$$

$$\nabla \cdot \mathbf{B} = 0 \qquad (2.3)$$

$$\nabla \cdot \mathbf{D} = \rho \qquad \text{(Coulomb's law)} \qquad (2.4)$$

$$\mathbf{D} = \epsilon_0 \mathbf{E} \qquad (2.5)$$

$$\mathbf{B} = \mu_0 \mathbf{H} \qquad (2.6)$$

The transverse wave equation:

$$\left(\frac{\partial^2}{\partial t^2} - c^2 \nabla^2\right) \mathbf{E}_T(\mathbf{r}, t) = -\frac{1}{\epsilon_0} \frac{\partial \mathbf{J}_T(\mathbf{r}, t)}{\partial t} \qquad (3.1)$$

The Wave Equation

From Maxwell's Equations, take the curl of equation 2.2

$$\nabla \times \boxed{\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}} \qquad (2.2)$$

and use the vector identity from Appendix D.1, pg. 440,

$$\nabla \times (\nabla \times \mathbf{A}) = \nabla(\nabla \cdot \mathbf{A}) - \nabla^2 \mathbf{A} \qquad (D.7)$$

to form the Wave Equation

$$\left(\frac{\partial^2}{\partial t^2} - c^2\nabla^2\right)\mathbf{E}(\mathbf{r}, t) = -\frac{1}{\epsilon_0}\left[\frac{\partial \mathbf{J}(\mathbf{r}, t)}{\partial t} + c^2\nabla\rho(\mathbf{r}, t)\right] \qquad (2.7)$$

where

$$c \equiv \frac{1}{\sqrt{\epsilon_0 \mu_0}} \qquad (2.8)$$

where $\mathbf{J}(\mathbf{r},t)$ is the current density in vacuum and ρ is the charge density:

$$\mathbf{J}(\mathbf{r},t) = qn(\mathbf{r},t)\mathbf{v}(\mathbf{r},t) \qquad (2.10)$$

For transverse waves the Wave Equation reduces to

$$\boxed{\left(\frac{\partial^2}{\partial t^2} - c^2\nabla^2\right)\mathbf{E}_T(\mathbf{r}, t) = -\frac{1}{\epsilon_0}\frac{\partial \mathbf{J}_T(\mathbf{r}, t)}{\partial t}} \qquad (3.1)$$

Relationships Among E, H and S for a Plane Wave in Vacuum

Among **E** and **H**, take $\nabla \times \mathbf{E}(\mathbf{r}, t) = -\frac{\partial \mathbf{B}(\mathbf{r}, t)}{\partial t}$, with $\mathbf{B} = \mu_0 \mathbf{H}$ in vacuum to obtain

$$\nabla \times \mathbf{E} = -\mu_0 \frac{\partial \mathbf{H}}{\partial t}$$

Write **E** and **H**, in terms of Fourier representations

$$\mathbf{E}(\mathbf{r}, t) = \iint_{\mathbf{k}\omega} \mathbf{E}_{\mathbf{k}\omega}\, e^{-i(\omega t - \mathbf{k} \cdot \mathbf{r})} \frac{d\omega d\mathbf{k}}{(2\pi)^4} \quad \text{and} \quad \mathbf{H}(\mathbf{r}, t) = \iint_{\mathbf{k}\omega} \mathbf{H}_{\mathbf{k}\omega}\, e^{-i(\omega t - \mathbf{k} \cdot \mathbf{r})} \frac{d\omega d\mathbf{k}}{(2\pi)^4}$$

The ∇ and $\partial/\partial t$ operates on the fields become algebraic multipliers on the Fourier-Laplace coefficients $\mathbf{E}_{\mathbf{k}\omega}$ and $\mathbf{H}_{\mathbf{k}\omega}$

$$\mathbf{H}_{k\omega} = \sqrt{\frac{\epsilon_0}{\mu_0}}\, \mathbf{k}_0 \times \mathbf{E}_{k\omega}$$

using the inverse transforms

$$\boxed{\mathbf{H}(\mathbf{r}, t) = \sqrt{\frac{\epsilon_0}{\mu_0}}\, \mathbf{k}_0 \times \mathbf{E}(\mathbf{r}, t)} \qquad (2.29)$$

and

$$\boxed{\mathbf{S}(\mathbf{r}, t) = \sqrt{\frac{\epsilon_0}{\mu_0}}\, |\mathbf{E}|^2 \mathbf{k}_0} \qquad (2.31)$$

Electric Field Radiated by an Accelerated Charge

Inverting eq. (3.1) in **k**, ω - space

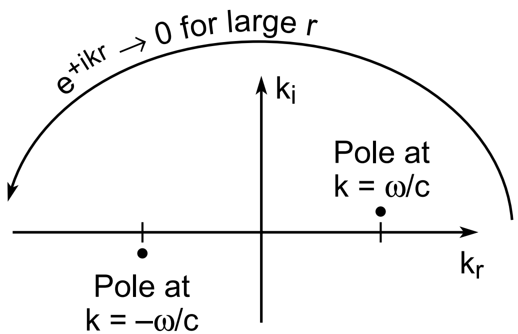
$$\mathbf{E}(\mathbf{r}, t) = \int_{\mathbf{k}} \int_{\omega} \left(-\frac{i\omega}{\epsilon_0}\right) \frac{\mathbf{J}_{T_{k\omega}} e^{-i(\omega t - \mathbf{k}\cdot\mathbf{r})}}{(\omega^2 - k^2c^2)} \frac{d\omega\, d\mathbf{k}}{(2\pi)^4} \tag{2.19}$$

Where now for an accelerated electron

$$\mathbf{J}_{T_{k\omega}} = -e\mathbf{v}_T(\omega) \tag{2.21}$$

Then

$$\mathbf{E}(\mathbf{r}, t) = \frac{ie}{\epsilon_0} \int_{\mathbf{k}} \int_{\omega} \frac{\omega \mathbf{v}_T(\omega) e^{-i(\omega t - \mathbf{k}\cdot\mathbf{r})}}{\omega^2 - k^2c^2} \frac{d\omega\, d\mathbf{k}}{(2\pi)^4} \tag{2.22}$$



$$\mathbf{E}(\mathbf{r}, t) = \frac{e}{4\pi\epsilon_0 c^2 r} \int_{-\infty}^{\infty} (-i\omega)\mathbf{v}_T(\omega) e^{-i\omega(t - r/c)} \frac{d\omega}{2\pi} \tag{2.24}$$

$$\mathbf{E}(\mathbf{r}, t) = \frac{e}{4\pi\epsilon_0 c^2 r} \frac{d\mathbf{v}_T(t - r/c)}{dt}$$

or

$$\boxed{\mathbf{E}(\mathbf{r}, t) = \frac{e\mathbf{a}_T(t - r/c)}{4\pi\epsilon_0 c^2 r}} \tag{2.25}$$

Power Radiated by an Accelerated Point Charge

Combining $\mathbf{E}(\mathbf{r},t) = \dfrac{e\mathbf{a}_T(t-r/c)}{4\pi\epsilon_0 c^2 r}$ (2.25) and $\mathbf{S}(\mathbf{r},t) = \sqrt{\dfrac{\epsilon_0}{\mu_0}}|\mathbf{E}|^2\mathbf{k}_0$ (2.31)

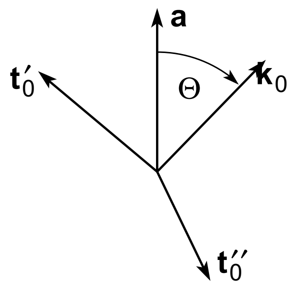
one obtains the *instantaneous power per unit area* radiated by an accelerated electron

$$\mathbf{S}(\mathbf{r},t) = \frac{e^2|\mathbf{a}_T|^2}{16\pi^2\epsilon_0 c^3 r^2}\mathbf{k}_0 \qquad (2.32)$$

$\mathbf{k}_0$, propagation direction

$|\mathbf{a}_T| = |\mathbf{a}|\sin\Theta$

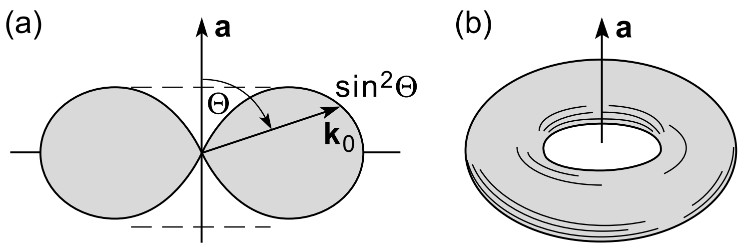
For an angle Θ between the direction of acceleration, **a**, and the observation direction, $\mathbf{k}_0$, the instantaneous power per unit area is



$$\mathbf{S}(\mathbf{r},t) = \frac{e^2|\mathbf{a}|^2\sin^2\Theta}{16\pi^2\epsilon_0 c^3 r^2}\mathbf{k}_0 \qquad (2.33)$$

Noting that $\mathbf{S} = (dP/dA)\mathbf{k}_0$ and $dA = r^2\, d\Omega$, one obtains the power per unit solid angle

$$\boxed{\frac{dP}{d\Omega} = \frac{e^2|\mathbf{a}|^2\sin^2\Theta}{16\pi^2\epsilon_0 c^3}} \qquad (2.34)$$



the well known "donut-shaped" radiation pattern characteristic of a radiator whose size is much smaller than the wavelength ("dipole radiation").

Total Power Radiated by an Accelerated Point Charge

The total power radiated, P, is determined by integrating $\mathbf{S}$ over the area of a distant sphere:

$$P = \iint_{\text{area}} \mathbf{S} \cdot d\mathbf{A} = \iint_{\substack{\text{solid}\\ \text{angle}}} \mathbf{S} \cdot (r^2\, d\Omega\, \mathbf{k}_0) \qquad (2.35)$$

where for $0 \le \Theta \le \pi$ and $0 \le \phi \le 2\pi$ we have $d\Omega = \sin\Theta\, d\Theta\, d\phi$, thus

$$P = \iint \left[\frac{e^2|\mathbf{a}|^2 \sin^2\Theta}{16\pi^2\epsilon_0 c^3 r^2}\, \mathbf{k}_0 \right] \cdot r^2 \sin\Theta\, d\Theta\, d\phi\, \mathbf{k}_0$$

Thus the *instantaneous power radiated* to all angles by an oscillating electron of acceleration a is

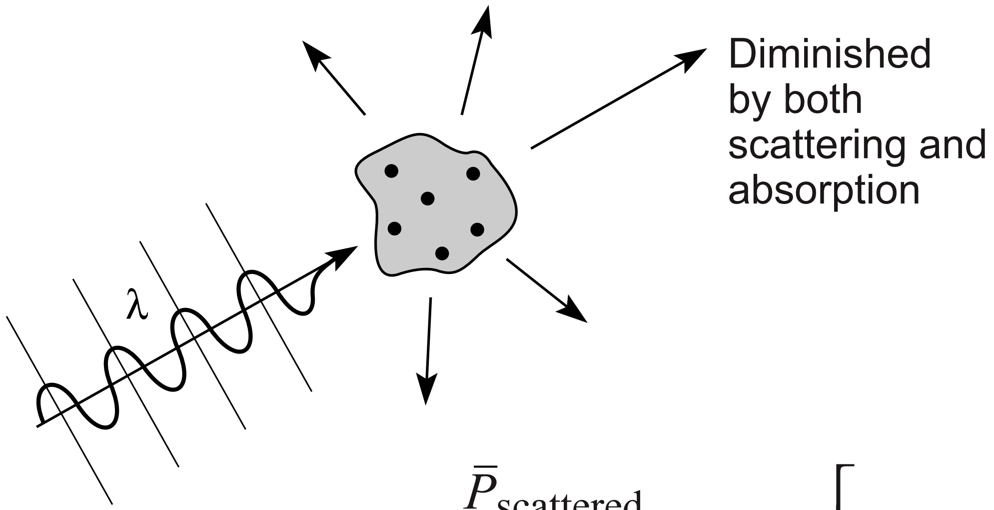
$$\boxed{P = \frac{8\pi}{3}\left(\frac{e^2|\mathbf{a}|^2}{16\pi^2\epsilon_0 c^3}\right)} \qquad (2.36)$$

For sinusoidal motion, averaging over a full cycle, $\sin^2\omega t$ or $\cos^2\omega t$, introduces a factor of 1/2

$$\bar{P} = \frac{1}{2} \cdot \frac{8\pi}{3}\left(\frac{e^2|\mathbf{a}|^2}{16\pi^2\epsilon_0 c^3}\right)$$

Scattering Cross-Sections

Measures the ability of an object to remove particles or photons from a directed beam and send them into new directions



$$\sigma \equiv \frac{\bar{P}_{\text{scattered}}}{|\bar{S}|} \qquad \left[\text{area} = \frac{(\text{power})}{(\text{power/area})} \right]$$

- Isotropic or anisotropic?
- Energy or wavelength dependent?

Scattering by a Free Electron

Define the cross-section as the average power radiated to all angles, divided by the average incident power per unit area

$$\sigma \equiv \frac{\bar{P}_{\text{scatt.}}}{|\bar{\mathbf{S}}_i|} \tag{2.38}$$

For an incident electromagnetic wave of electric field $\mathbf{E}_i(\mathbf{r},t)$

$$\bar{\mathbf{S}} = \frac{1}{2}\sqrt{\frac{\epsilon_0}{\mu_0}}\,|\mathbf{E}_i|^2\,\mathbf{k}_0 \tag{2.39}$$

For a free electron the incident field causes an oscillatory motion described by Newton's second equation of motion, $\mathbf{F} = m\mathbf{a}$, where $\mathbf{F}$ is the Lorentz force on the electron

$$m\mathbf{a} = -e[\mathbf{E}_i + \underbrace{\mathbf{v}\times\mathbf{B}_i}_{\text{small}}] \tag{2.40}$$

Thus the instantaneous acceleration is

$$\mathbf{a}(\mathbf{r},t) = -\frac{e}{m}\mathbf{E}_i(\mathbf{r},t) \tag{2.42}$$

Scattering by a Free Electron (continued)

The average power scattered by an oscillating electron is

$$\bar{P}_{\text{scatt.}} = \frac{1}{2}\,\frac{8\pi}{3}\,\frac{e^2\left(\frac{e^2}{m^2}|\mathbf{E}_i|^2\right)}{16\pi^2\epsilon_0 c^3}$$

The scattering cross-section is

$$\sigma = \frac{\bar{P}_{\text{scatt.}}}{|\bar{\mathbf{S}}|} = \frac{\frac{4\pi}{3}\left(\frac{e^4|\mathbf{E}_i|^2}{16\pi^2\epsilon_0 m^2 c^3}\right)}{\frac{1}{2}\sqrt{\frac{\epsilon_0}{\mu_0}}|\mathbf{E}_i|^2}$$

Introducing the "classical electron radius"

$$r_e = \frac{e^2}{4\pi\epsilon_0 mc^2} \qquad (2.44)$$

One obtains the scttering cross-section for a single free electron

$$\boxed{\sigma_e = \frac{8\pi}{3} r_e^2} \qquad (2.45)$$

which we observe is independent of wavelength. This is referred to as the Thomson cross-section (for a free electron), after J.J. Thomson. Numerically $r_e = 2.82 \times 10^{-13}$ cm and $\sigma_e = 6.65 \times 10^{-25}$ cm^2. The differential Thomson scattering cross-section is

Scattering by a Bound Electron

For an electromagnetic wave incident upon a bound electron of resonant frequency ω_s, the force equation can be written semi-classically as

$$m\frac{d^2\mathbf{x}}{dt^2} + m\gamma\frac{d\mathbf{x}}{dt} + m\omega_s^2\mathbf{x} = -e(\mathbf{E}_i + \underbrace{\mathbf{v}\times\mathbf{B}_i}_{\simeq 0}) \qquad (2.48)$$

with an acceleration term (m**a**), a damping term, a restoring force term, and the Lorentz force exerted by the fields. For an incident electric field

$$\mathbf{E} = \mathbf{E}_i e^{-i\omega t}$$

the harmonic motion will be driven at the same frequency, ω, so that

$$\mathbf{x} = \frac{1}{\omega^2 - \omega_s^2 + i\gamma\omega}\frac{e\mathbf{E}_i}{m} \qquad (2.49)$$

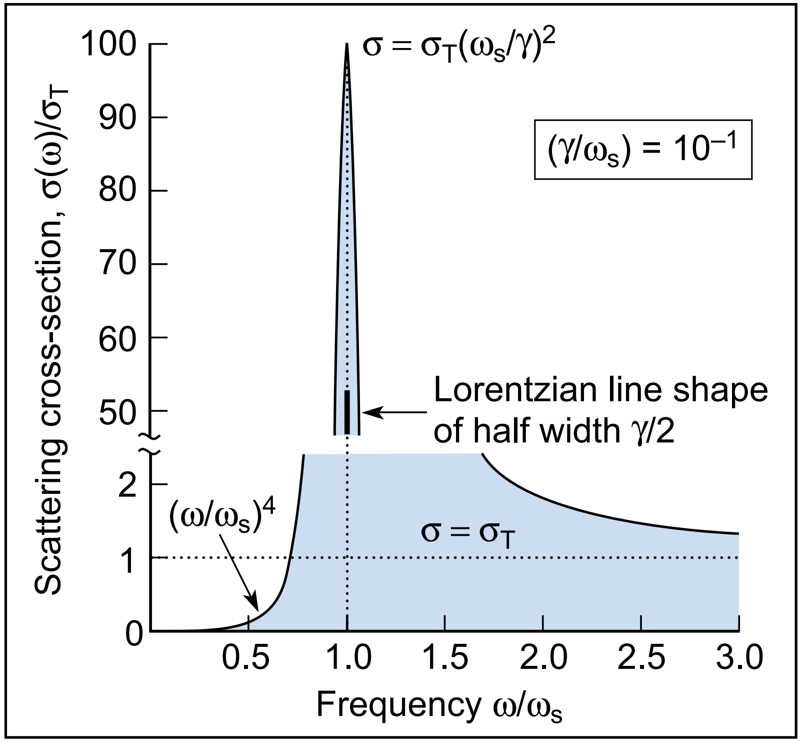
$$\mathbf{a} = \frac{-\omega^2}{\omega^2 - \omega_s^2 + i\gamma\omega}\frac{e\mathbf{E}_i}{m} \qquad (2.50)$$

Following the same procedures used earlier, one obtains the scattering cross-section for a bound electron of resonant frequency, ω_s

$$\boxed{\sigma = \frac{8\pi}{3}r_e^2\frac{\omega^4}{\left(\omega^2 - \omega_s^2\right)^2 + (\gamma\omega)^2}} \qquad (2.51)$$

Semi-Classical Scattering Cross-Section for a Bound Electron

$$\sigma = \frac{8\pi}{3} r_e^2 \frac{\omega^4}{(\omega^2 - \omega_s^2)^2 + (\gamma\omega)^2} \qquad (2.51)$$

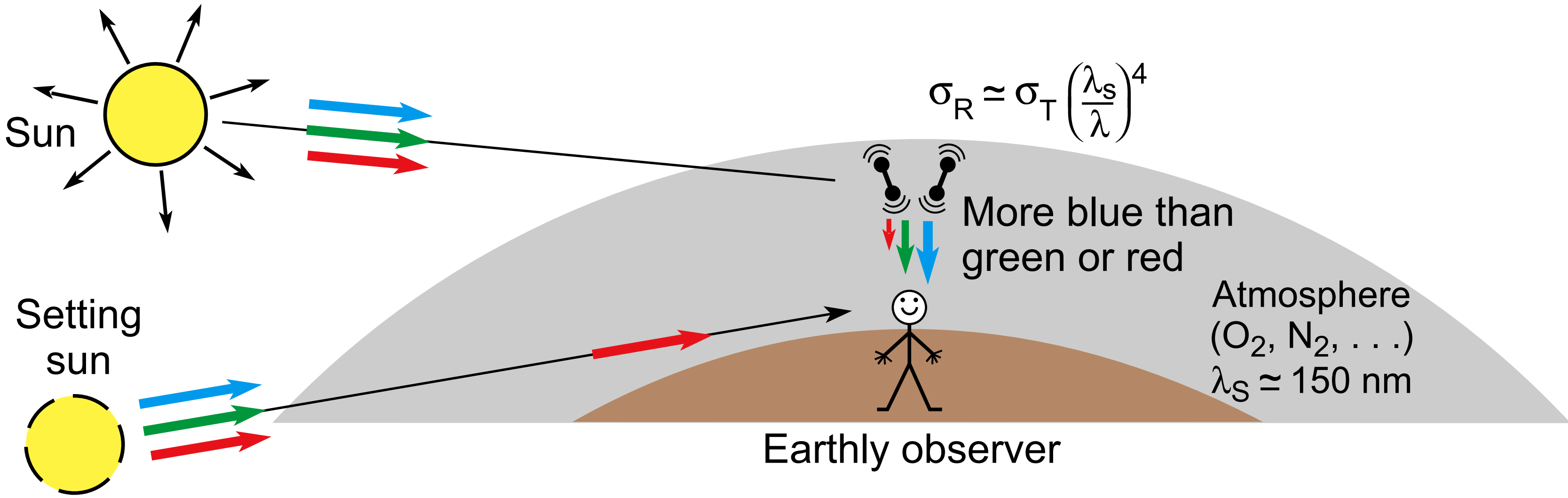


Note that below the resonance, for $\omega^2 << \omega_s^2$

$$\sigma_R = \frac{8\pi}{3} r_e^2 \left(\frac{\omega}{\omega_s}\right)^4 = \frac{8\pi}{3} r_e^2 \left(\frac{\lambda_s}{\lambda}\right)^4 \qquad (2.52)$$

This is the Rayleigh scattering cross-section (1899) for a bound electron, with $\omega/\omega_s << 1$, which displays a very strong λ^{-4} wavelength dependence.

The sky appears blue because of the strong wave length dependence of scattering by bound electrons.

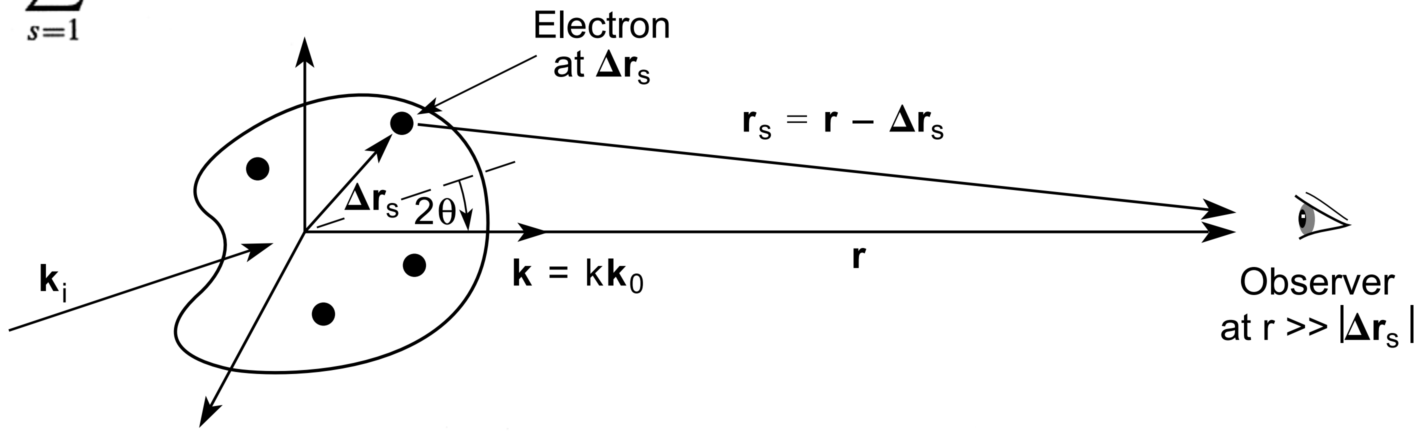


- UV resonances in O_2 and N_2, at 8.6 and 8.2 eV
- Red (1.8 eV, 700 nm), green (2.3 eV, 530 nm), and blue light (3.3 eV, 380 nm)
- Density fluctuations essential
- Long path at sunset, color of clouds
- Photon energy and wavelength effects. Volcanic eruptions

Scattering by a Multi-Electron Atom

Semi-classical model of an atom with Z electrons and nucleus of charge +Ze at $\mathbf{r} = 0$.

$$n(\mathbf{r}, t) = \sum_{s=1}^{Z} \delta[\mathbf{r} - \Delta\mathbf{r}_s(t)] \quad (2.53)$$



For each electron
$$m\frac{d^2\mathbf{x}_s}{dt^2} + m\gamma\frac{d\mathbf{x}_s}{dt} + m\omega_s^2\mathbf{x}_s = -e(\mathbf{E}_i + \underbrace{\mathbf{v}_s \times \mathbf{B}}_{\simeq 0}) \quad (2.58)$$

The acceleration has an additional phase term due to the position, $\Delta\mathbf{r}_s$, within the atom:

$$\mathbf{a}_s(t) = \frac{-\omega^2}{\omega^2 - \omega_s^2 + i\gamma\omega}\frac{e}{m}\mathbf{E}_i\, e^{-i(\omega t - \mathbf{k}_i \cdot \Delta\mathbf{r}_s)} \quad (2.61)$$

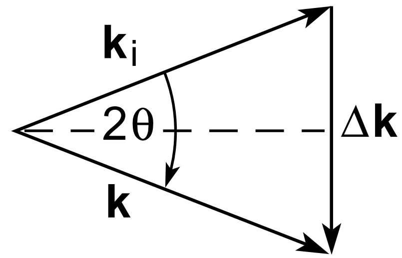
The scattered electric field at a distance **r** summed for all Z electrons, is

$$E(\mathbf{r}, t) = \frac{-e^2}{4\pi\epsilon_0 mc^2}\sum_{s=1}^{Z}\frac{\omega^2 E_i \sin\Theta}{\omega^2 - \omega_s^2 + i\gamma\omega}\frac{1}{r_s}e^{-i[\omega(t - r_s/c) - \mathbf{k}_i \cdot \Delta\mathbf{r}_s]}$$

where $\mathbf{r}_s \equiv \mathbf{r} - \Delta\mathbf{r}_s$ and $r_s = |\mathbf{r}_s|$. For $r >> \Delta\mathbf{r}_s$, $r_s \simeq r - \mathbf{k}_0 \cdot \Delta\mathbf{r}_s$ (2.62)

Scattering by a Multi-Electron Atom (continued)

$$E(\mathbf{r}, t) = -\frac{r_e}{r}\underbrace{\left[\sum_{s=1}^{Z}\frac{\omega^2 e^{-i\Delta\mathbf{k}\cdot\Delta\mathbf{r}_s}}{\omega^2-\omega_s^2+i\gamma\omega}\right]}_{f(\Delta\mathbf{k},\,\omega)} E_i \sin\Theta\, e^{-i\omega(t-r/c)} \qquad (2.65)$$



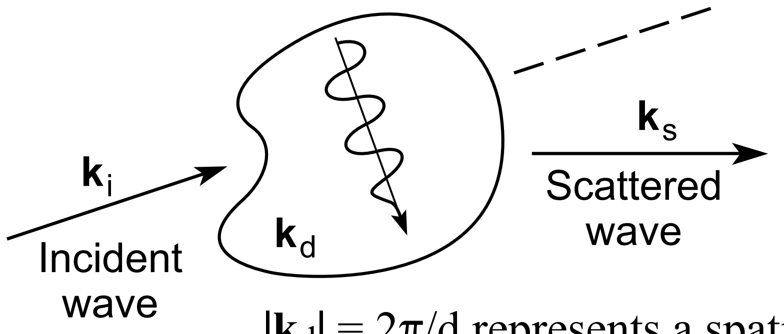
$$\Delta\mathbf{k} = \mathbf{k} - \mathbf{k}_i$$

$$|\Delta\mathbf{k}| = 2k_i \sin\theta$$

where the quantity $f(\Delta\mathbf{k}, \omega)$ is the complex atomic scattering factor, which tells us the scattered electric field due to a multi-electron atom, relative to that of a single free electron (eq. 2.43). Note the dependence on frequency ω (photon energy $\hbar\omega$), the various resonant frequencies ω_s (resonant energies $\hbar\omega_s$), and the phase terms due to the various positions of electrons within the atom, $\Delta\mathbf{k}\cdot\Delta\mathbf{r}_s$.

A General Scattering Diagram

$$\mathbf{J}(r,t) = -e\, n(r,t)\mathbf{v}(r,t) \qquad (2.10)$$



$$J_{scatt} e^{-i(\omega_s t - \mathbf{k}_s \cdot \mathbf{r})} = -e f^0(\omega_i) n_d e^{-i(\omega_d t - \mathbf{k}_d \cdot \mathbf{r})} \frac{-e\mathbf{E}_i}{-i\omega_i m} e^{-i(\omega_i t - \mathbf{k}_i \cdot \mathbf{r})}$$

matching exponents

$$\omega_s = \omega_i + \omega_d$$

$$\mathbf{k}_s = \mathbf{k}_i + \mathbf{k}_d$$

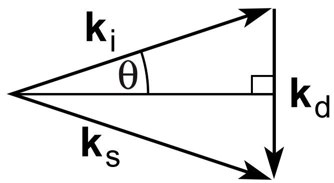
$|\mathbf{k}_d| = 2\pi/d$ represents a spatial non-uniformity in the medium, such as atoms of periodicity d, a grating, or a density distribution due to a wave motion.

If the density distribution is stationary

$$|\mathbf{k}_i| = \frac{\omega}{c} = \frac{2\pi}{\lambda}$$

$$|\mathbf{k}_s| = \frac{\omega}{c} = \frac{2\pi}{\lambda}$$

∴ the scattering diagram is isosceles



$$\mathbf{k}_i + \mathbf{k}_d = \mathbf{k}_s$$

$$\sin\theta = \frac{k_d/2}{k_i}$$

$$\sin\theta = \frac{\lambda}{2d}$$

$$\lambda = 2d \sin\theta \qquad (2.62)$$

(Bragg's Law, 1913)

(Reference: See chapter 4, eqs. 4.1 to 4.6)

The Atomic Scattering Factor

$$f(\Delta\mathbf{k}, \omega) = \sum_{s=1}^{Z} \frac{\omega^2 e^{-i\Delta\mathbf{k}\cdot\Delta\mathbf{r}_s}}{\omega^2 - \omega_s^2 + i\gamma\omega} \qquad (2.66)$$

In general the $\Delta\mathbf{k} \cdot \Delta\mathbf{r}_s$ phase terms do not simplify, but in two cases they do. Noting that $|\Delta\mathbf{k}| = 2k_i \sin\theta = 4\pi/\lambda \sin\theta$, and that the radius of the atom is of order the Bohr radius, a_0, the phase factor is then bounded by

$$|\Delta\mathbf{k} \cdot \Delta\mathbf{r}_s| \leq \frac{4\pi a_0}{\lambda} \sin\theta \qquad (2.70)$$

The atomic scattering factor $f(\Delta\mathbf{k},\omega)$ simplifies significantly when

$$|\Delta\mathbf{k} \cdot \Delta\mathbf{r}_s| \to 0 \quad \text{for } a_0/\lambda \ll 1 \qquad \text{(long wavelength limit)} \qquad (2.71a)$$

$$|\Delta\mathbf{k} \cdot \Delta\mathbf{r}_s| \to 0 \quad \text{for } \theta \ll 1 \qquad \text{(forward scattering)} \qquad (2.71b)$$

In each of these two cases the atomic scattering factor $f(\Delta\mathbf{k},\omega)$ reduces to

$$f^0(\omega) = \sum_{s=1}^{Z} \frac{\omega^2}{\omega^2 - \omega_s^2 + i\gamma\omega} \qquad (2.72)$$

where we denote these special cases by the superscript zero.

Complex Atomic Scattering Factors

$$f^0(\omega) = \sum_{s=1}^{Z} \frac{\omega^2}{\omega^2 - \omega_s^2 + i\gamma\omega} = f_1^0(\omega) - i f_2^0(\omega) \qquad (2.72)\ (2.79)$$

which some write as

$$f(\omega) = Z - f_1(\omega) - i f_2(\omega)$$

Atomic Scattering Cross-Sections

Comparing the scattered electric field for a multi-electron atom (2.65) with that for the free electron (2.43), the atomic scattering cross-sections are readily determined by the earlier proceedures to be

$$\frac{d\sigma(\omega)}{d\Omega} = r_e^2 |f^0(\omega)|^2 \sin^2\Theta \tag{2.75}$$

$$\sigma(\omega) = \frac{8\pi}{3} r_e^2 |f^0(\omega)|^2 \tag{2.76}$$

where

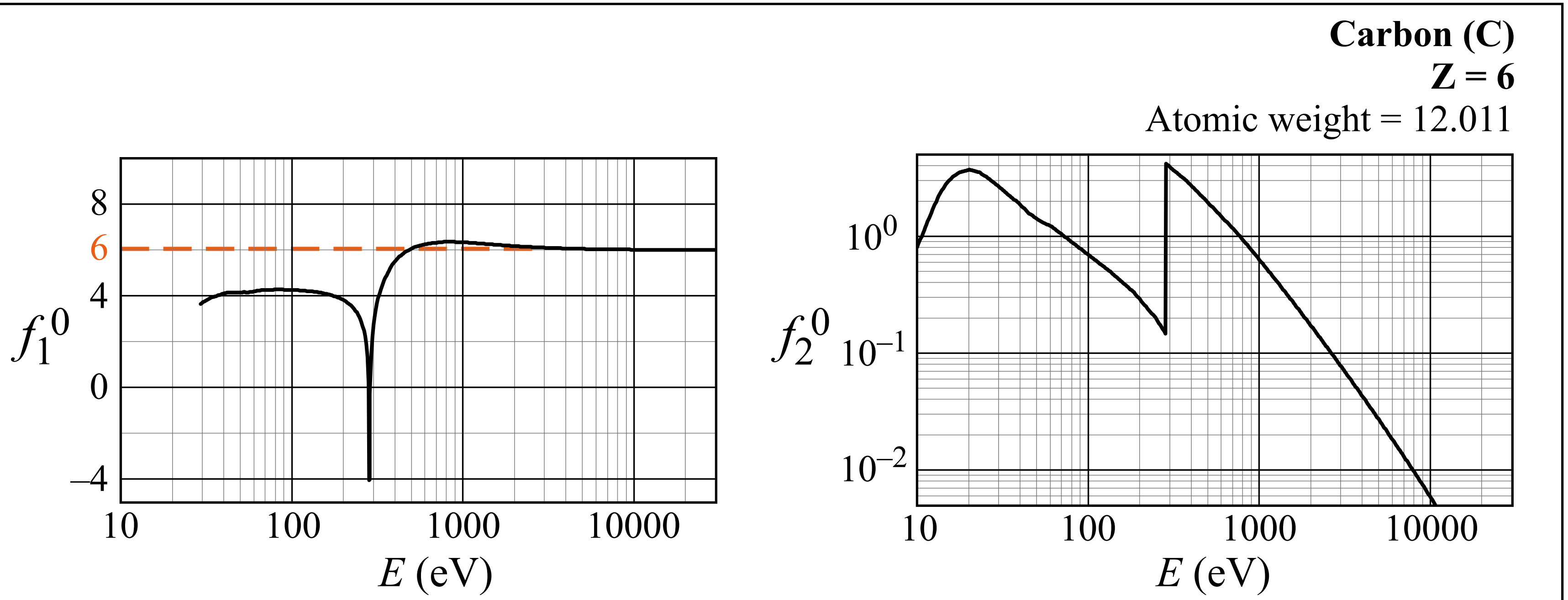
$$f^0(\omega) = \sum_s \frac{g_s \omega^2}{\omega^2 - \omega_s^2 + i\gamma\omega} \tag{2.77}$$

and where the super-script zero refers to the special circumstances of long wavelength ($\lambda >> a_0$) or forward scattering ($\theta << 1$). With the Bohr radius $a_0 = 0.529$ Å, the long wavelength condition is easily satisfied for soft x-rays and EUV. Note too that we have introduced the concept of oscillator strengths, g_s, associated with each resonance, normalized by the condition

$$\sum_s g_s = Z \tag{2.73}$$

Example:
Complex Atomic Scattering Factor for Carbon

$$f^0(\omega) = f_1^0(\omega) - i f_2^0(\omega) \qquad (2.79)$$



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

Note that for $\hbar\omega >> \hbar\omega_s$, $f_1^0 \rightarrow Z$. This works here for carbon $f_1^0 \rightarrow 6$, but note that in general this conflicts with the condition $\lambda >> a_0$. For the case of carbon at 4 Å wavelength ($\lambda >> a_0$), and thus $\hbar\omega = 3$ keV ($>> \hbar\omega_s \sim 274$ eV), the atomic scattering cross-section (2.76) becomes

$$\sigma(\omega) \simeq \frac{8\pi}{3} r_e^2 Z^2 = Z^2 \sigma_e \qquad (2.78c)$$

that is, all Z electrons are scattering cooperatively (in-phase) - the so-called N^2 effect.

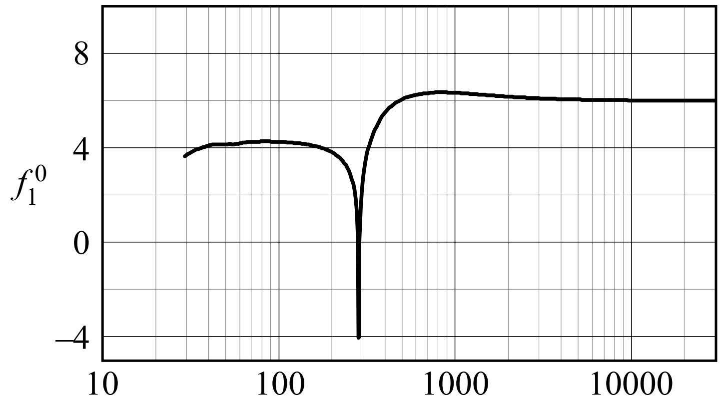
Atomic Scattering Factors for Carbon (Z = 6)

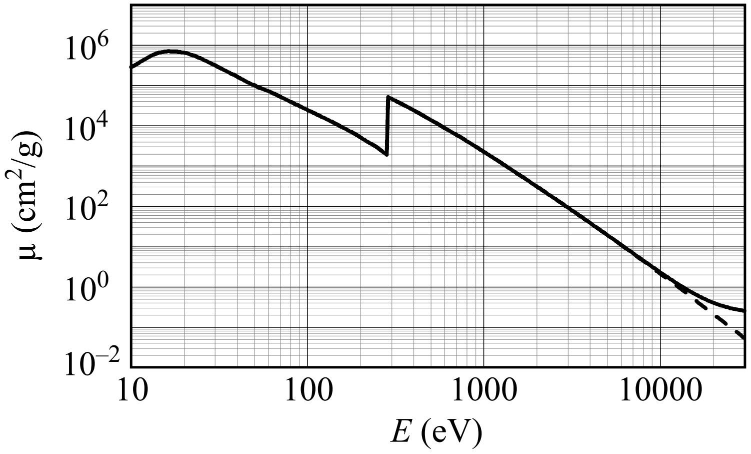
σ_a(barns/atom) = μ(cm^2/g) × 19.95

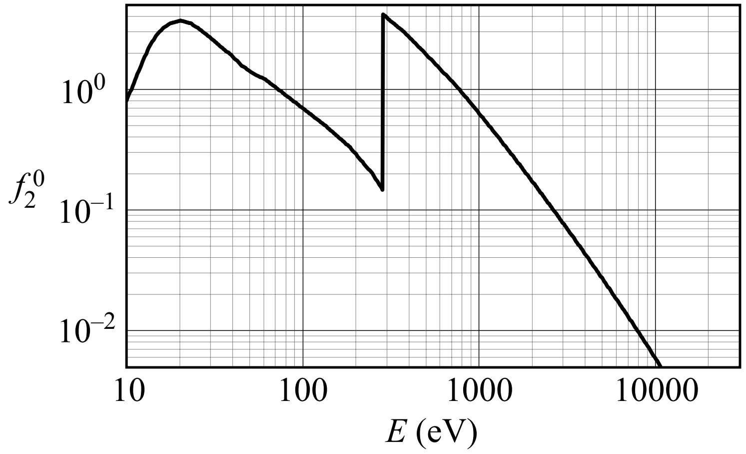
E(keV)μ(cm^2/g) = f_2^0 × 3503.31

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

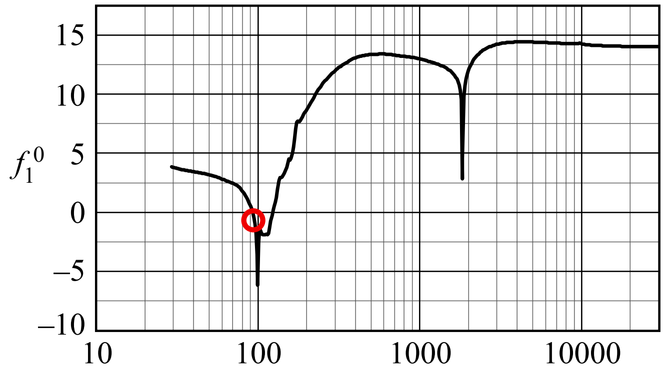
(Henke and Gullikson; www-cxro.LBL.gov)

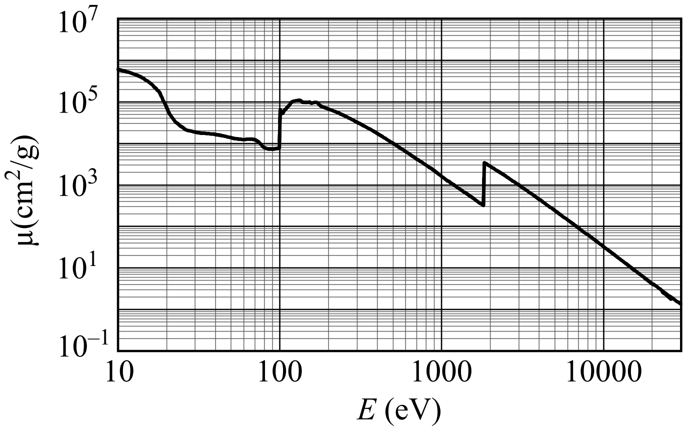
Atomic Scattering Factors for Silicon (Z = 14)

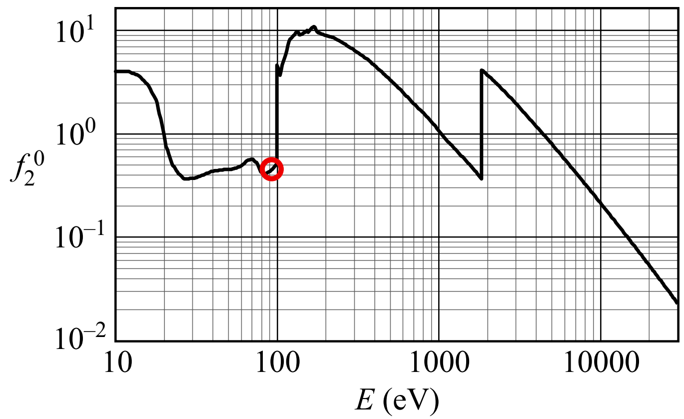
σ_a(barns/atom) = μ(cm^2/g) × 46.64
E(keV)μ(cm^2/g) = f_2^0 × 1498.22

Silicon (Si)
Z = 14
Atomic weight = 28.086

Energy (eV)	f_1^0	f_2^0	μ(cm^2/g)
30	3.799	3.734E–01	1.865E+04
70	2.448	5.701E–01	1.220E+04
100	–5.657	4.580E+00	6.862E+04
300	12.00	6.439E+00	3.216E+04
700	13.31	1.951E+00	4.175E+03
1000	13.00	1.070E+00	1.602E+03
3000	14.23	1.961E+00	9.792E+02
7000	14.33	4.240E–01	9.075E+01
10000	14.28	2.135E–01	3.199E+01
30000	14.02	2.285E–02	1.141E+00







Edge Energies: K 1838.9 eV
L_1 149.7 eV
L_2 99.8 eV
L_3 99.2 eV

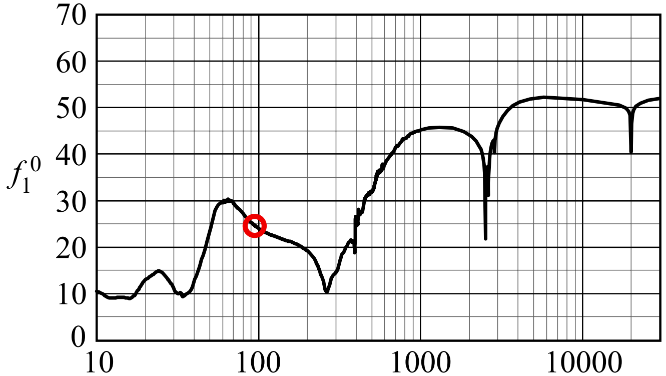
(Henke and Gullikson; www-cxro.LBL.gov)

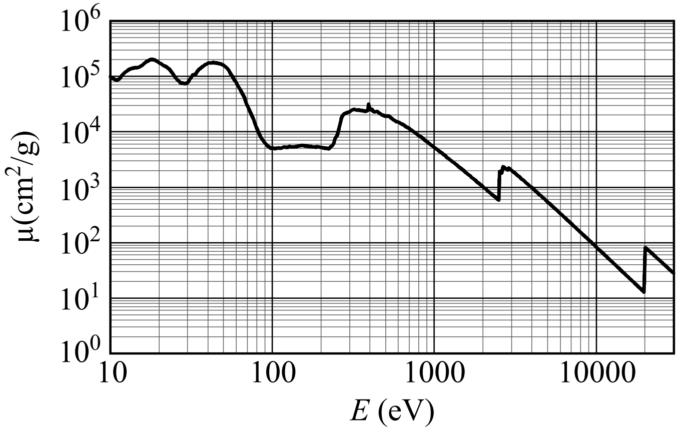
Atomic Scattering Factors for Molybdenum (Z = 42)

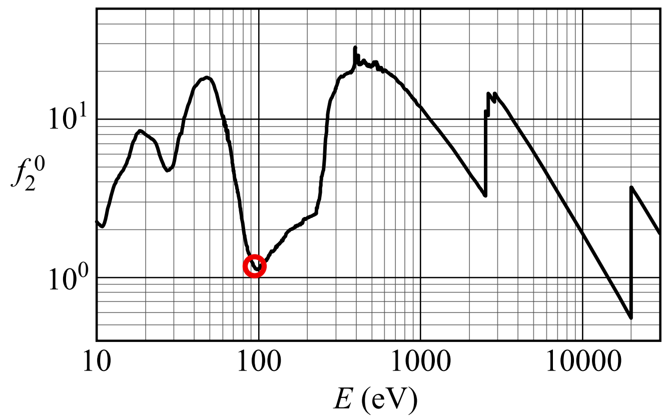
σ_a(barns/atom) = μ(cm^2/g) × 159.31
E(keV)μ(cm^2/g) = f_2^0 × 438.59

Molybdenum (Mo)
Z = 42
Atomic weight = 95.940

Energy (eV)	f_1^0	f_2^0	μ(cm^2/g)
30	1.071	5.292E+00	7.736E+04
70	19.38	4.732E+00	2.965E+04
100	14.02	1.124E+00	4.931E+03
300	4.609	1.568E+01	2.292E+04
700	31.41	1.819E+01	1.140E+04
1000	35.15	1.188E+01	5.210E+03
3000	35.88	1.366E+01	1.997E+03
7000	42.11	3.493E+00	2.189E+02
10000	41.67	1.881E+00	8.248E+01
30000	42.04	1.894E+00	2.769E+01







Edge Energies:							
K	19999.5 eV	L_1	2865.5 eV	M_1	506.3 eV	N_1	63.2 eV
		L_2	2625.1 eV	M_2	411.6 eV	N_2	37.6 eV
		L_3	2520.2 eV	M_3	394.0 eV	N_3	35.5 eV
				M_4	231.1 eV		
				M_5	227.9 eV		

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

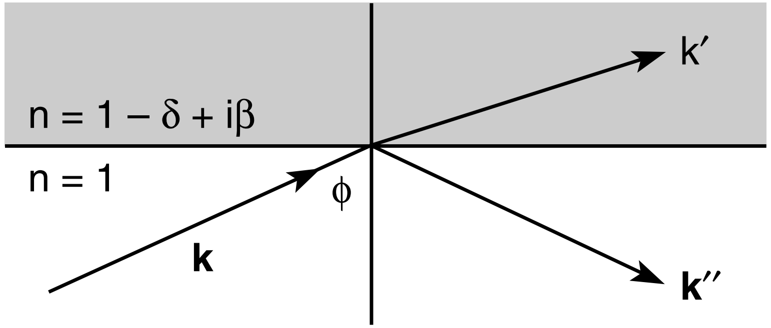
Complex Atomic Scattering Factors

$$f^0(\omega) = \sum_{s=1}^{Z} \frac{\omega^2}{\omega^2 - \omega_s^2 + i\gamma\omega} = f_1^0(\omega) - i f_2^0(\omega) \qquad \begin{matrix}(2.72)\\(2.79)\end{matrix}$$

which some write as

$$f(\omega) = Z - f_1(\omega) - i f_2(\omega)$$

Wave Propagation and Refractive Index at X-Ray Wavelengths



$$n(\omega) = 1 - \frac{n_a r_e \lambda^2}{2\pi}\left(f_1^0 - i f_2^0\right) \qquad (3.9)$$

$$n(\omega) = 1 - \delta + i\beta \qquad (3.12)$$

$$l_{\text{abs}} = \frac{\lambda}{4\pi\beta} \qquad (3.22)$$

$$\sigma_{\text{abs.}} = 2 r_e \lambda f_2^0(\omega) \qquad (3.28)$$

$$\Delta\phi = \left(\frac{2\pi\delta}{\lambda}\right)\Delta r \qquad (3.29)$$

$$\theta_c = \sqrt{2\delta} \qquad (3.41)$$

$$R_{s,\perp} \simeq \frac{\delta^2 + \beta^2}{4} \qquad (3.50)$$

$$\phi_B \simeq \frac{\pi}{4} - \frac{\delta}{2} \qquad (3.60)$$

The Wave Equation and Refractive Index

The transverse wave equation is

$$\left(\frac{\partial^2}{\partial t^2} - c^2\nabla^2\right)\mathbf{E}_T(\mathbf{r}, t) = -\frac{1}{\epsilon_0}\frac{\partial \mathbf{J}_T(\mathbf{r}, t)}{\partial t} \tag{3.1}$$

For the special case of forward scattering the positions of the electrons within the atom ($\Delta\mathbf{k} \cdot \Delta\mathbf{r}_s$) are irrelevant, as are the positions of the atoms themselves, n($\mathbf{r}$, t). The contributing current density is then

$$\mathbf{J}_0(\mathbf{r}, t) = -en_a \sum_s g_s \mathbf{v}_s(\mathbf{r}, t) \tag{3.2}$$

where n_a is the average density of atoms, and

$$\sum_s g_s = Z$$

The Wave Equation and Refractive Index (Continued)

The oscillating electron velocities are driven by the incident field **E**

$$\mathbf{v}(\mathbf{r}, t) = \frac{e}{m} \frac{1}{(\omega^2 - \omega_s^2) + i\gamma\omega} \frac{\partial \mathbf{E}(\mathbf{r}, t)}{\partial t} \qquad (3.2)$$

such that the contributing current density is

$$\mathbf{J}_0(\mathbf{r}, t) = -\frac{e^2 n_a}{m} \sum_s \frac{g_s}{(\omega^2 - \omega_s^2) + i\gamma\omega} \frac{\partial \mathbf{E}(\mathbf{r}, t)}{\partial t} \qquad (3.4)$$

Substituting this into the transverse wave equation (3.1), one has

$$\left(\frac{\partial^2}{\partial t^2} - c^2\,\nabla^2\right) \mathbf{E}_T(\mathbf{r}, t) = \frac{e^2 n_a}{\epsilon_0 m} \sum_s \frac{g_s}{(\omega^2 - \omega_s^2) + i\gamma\omega} \frac{\partial^2 \mathbf{E}_T(\mathbf{r}, t)}{\partial t^2}$$

Combining terms with similar operators

$$\left[\left(1 - \frac{e^2 n_a}{\epsilon_0 m} \sum_s \frac{g_s}{(\omega^2 - \omega_s^2) + i\gamma\omega}\right) \frac{\partial^2}{\partial t^2} - c^2\,\nabla^2\right] \mathbf{E}_T(\mathbf{r}, t) = 0 \qquad (3.5)$$

Refractive Index in the Soft X-Ray and EUV Spectral Region

Written in the standard form of the wave equation as

$$\left[\frac{\partial^2}{\partial t^2} - \frac{c^2}{n^2(\omega)}\nabla^2\right]\mathbf{E}_T(\mathbf{r}, t) = 0 \qquad (3.6)$$

The frequency dependent refractive index n(ω) is identified as

$$n(\omega) \equiv \left[1 - \frac{e^2 n_a}{\epsilon_0 m}\sum_s \frac{g_s}{(\omega^2 - \omega_s^2) + i\gamma\omega}\right]^{1/2} \qquad (3.7)$$

For EUV/SXR radiation ω^2 is very large compared to the quantity $e^2 n_a/\epsilon_0 m$, so that to a high degree of accuracy the index of refraction can be written as

$$n(\omega) = 1 - \frac{1}{2}\frac{e^2 n_a}{\epsilon_0 m}\sum_s \frac{g_s}{(\omega^2 - \omega_s^2) + i\gamma\omega} \qquad (3.8)$$

which displays both positive and negative dispersion, depending on whether ω is less or greater than ω_s. Note that this will allow the refractive index to be more or less than unity, and thus the phase velocity to be less or greater than c.

Refractive Index in the Soft X-Ray and EUV Spectral Region (continued)

$$n(\omega) = 1 - \frac{1}{2}\frac{e^2 n_a}{\epsilon_0 m}\sum_s \frac{g_s}{(\omega^2 - \omega_s^2) + i\gamma\omega} \qquad (3.8)$$

Noting that

$$r_e = \frac{e^2}{4\pi\epsilon_0 mc^2}$$

and that for forward scattering

$$f^0(\omega) = \sum_s \frac{g_s\omega^2}{\omega^2 - \omega_s^2 + i\gamma\omega}$$

where this has complex components

$$f^0(\omega) = f_1^0(\omega) - if_2^0(\omega)$$

The refractive index can then be written as

$$\boxed{n(\omega) = 1 - \frac{n_a r_e \lambda^2}{2\pi}\left[f_1^0(\omega) - if_2^0(\omega)\right]} \qquad (3.9)$$

which we write in the simplified form

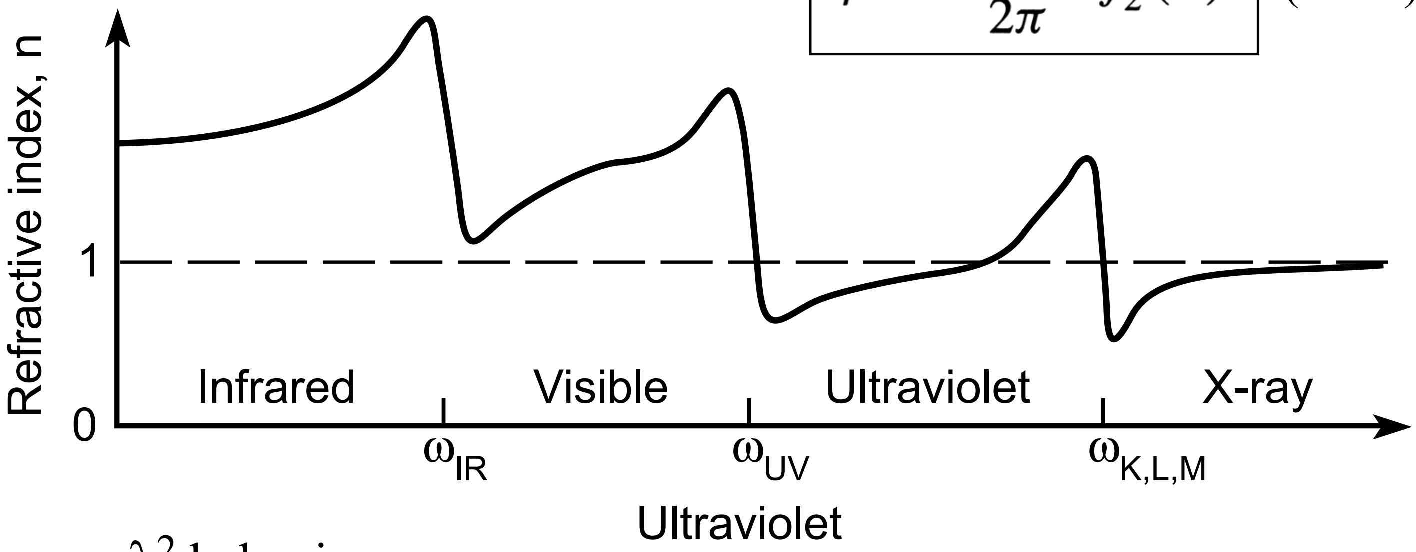
$$\boxed{n(\omega) = 1 - \delta + i\beta} \qquad (3.12)$$

Refractive Index from the IR to X-Ray Spectral Region

$$n(\omega) = 1 - \delta + i\beta \qquad (3.12)$$

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

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



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

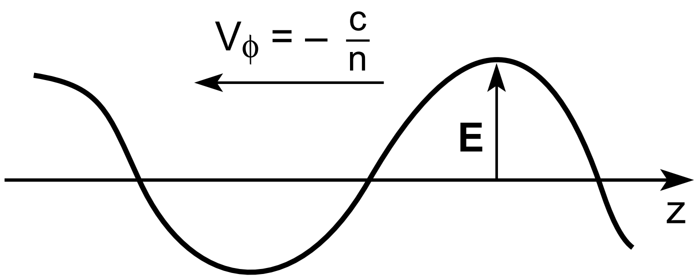
Phase Velocity and Refractive Index

The wave equation can be written as

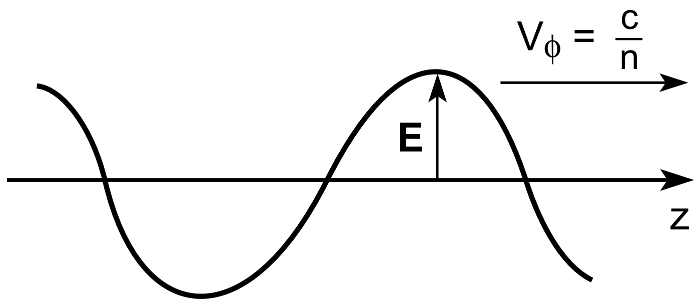
$$\left(\frac{\partial}{\partial t} - \frac{c}{n(\omega)}\nabla\right)\left(\frac{\partial}{\partial t} + \frac{c}{n(\omega)}\nabla\right)\mathbf{E}_{\mathrm{T}}(\mathbf{r}, t) = 0 \qquad (3.10)$$

The two bracketed operators represent left and right-running waves

$$\left(\frac{\partial}{\partial t} - \frac{c}{n}\frac{\partial}{\partial z}\right)E_x = 0 \qquad\qquad \left(\frac{\partial}{\partial t} + \frac{c}{n}\frac{\partial}{\partial z}\right)E_x = 0$$



Left-running wave



Right-running wave

where the phase velocity, the speed with which crests of fixed phase move, is not equal to c as in vacuum, but rather is

$$v_\phi = \frac{c}{n(\omega)} \qquad (3.11)$$

Phase Variation and Absorption of Propagating Waves

For a plane wave $$\mathbf{E}(\mathbf{r}, t) = \mathbf{E}_0 e^{-i(\omega t - \mathbf{k}\cdot\mathbf{r})} \tag{3.14}$$

in a material of refractive index n, the complex dispersion relation is

$$\frac{\omega}{k} = \frac{c}{n} = \frac{c}{1 - \delta + i\beta} \tag{3.15}$$

Solving for k

$$k = \frac{\omega}{c}(1 - \delta + i\beta) \tag{3.16}$$

Substituting this into (3.14), in the propagation direction defined by $\mathbf{k} \cdot \mathbf{r} = kr$

$$\mathbf{E}(\mathbf{r}, t) = \mathbf{E}_0 e^{-i[\omega t - (\omega/c)(1-\delta+i\beta)r]}$$

or

$$\mathbf{E}(\mathbf{r}, t) = \underbrace{\mathbf{E}_0 e^{-i\omega(t - r/c)}}_{\text{vacuum propagation}} \underbrace{e^{-i(2\pi\delta/\lambda)r}}_{\phi\text{-shift}} \underbrace{e^{-(2\pi\beta/\lambda)r}}_{\text{decay}} \tag{3.17}$$

where the first exponential factor represents the phase advance had the wave been propagating in vacuum, the second factor (containing $2\pi\delta r/\lambda$) represents the modified phase shift due to the medium, and the factor containing $2\pi\beta r/\lambda$ represents decay of the wave amplitude.

Intensity and Absorption in a Material of Complex Refractive Index

For complex refractive index n

$$\mathbf{H}(\mathbf{r}, t) = n\sqrt{\frac{\epsilon_0}{\mu_0}}\mathbf{k}_0 \times \mathbf{E}(\mathbf{r}, t) \tag{3.18}$$

The average intensity, in units of power per unit area, is

$$\bar{I} = |\bar{\mathbf{S}}| = \tfrac{1}{2}|\mathrm{Re}(\mathbf{E} \times \mathbf{H}^*)| \tag{3.19}$$

or

$$\bar{I} = \frac{1}{2}\mathrm{Re}(n)\sqrt{\frac{\epsilon_0}{\mu_0}}|\mathbf{E}|^2 \tag{3.20}$$

Recalling that

$$\mathbf{E}(\mathbf{r}, t) = \underbrace{\mathbf{E}_0 e^{-i\omega(t-r/c)}}_{\text{vacuum propagation}} \underbrace{e^{-i(2\pi\delta/\lambda)r}}_{\phi\text{-shift}} \underbrace{e^{-(2\pi\beta/\lambda)r}}_{\text{decay}} \tag{3.17}$$

$$\bar{I} = \frac{1}{2}\mathrm{Re}(n)\sqrt{\frac{\epsilon_0}{\mu_0}}|\mathbf{E}_0|^2 e^{-2(2\pi\beta/\lambda)r}$$

or

$$\bar{I} = \bar{I}_0 e^{-(4\pi\beta/\lambda)r} \tag{3.21}$$

the wave decays with an exponential decay length

$$\boxed{l_{\mathrm{abs}} = \frac{\lambda}{4\pi\beta}} \tag{3.22}$$

Absorption Lengths

$$\boxed{l_{\text{abs}} = \frac{\lambda}{4\pi\beta}} \tag{3.22}$$

Recalling that $\beta = n_a r_e \lambda^2 f_2^\circ(\omega)/2\pi$

$$l_{\text{abs}} = \frac{1}{2n_a r_e \lambda f_2^0(\omega)} \tag{3.23}$$

In Chapter 1 we considered experimentally observed absorption in thin foils, writing

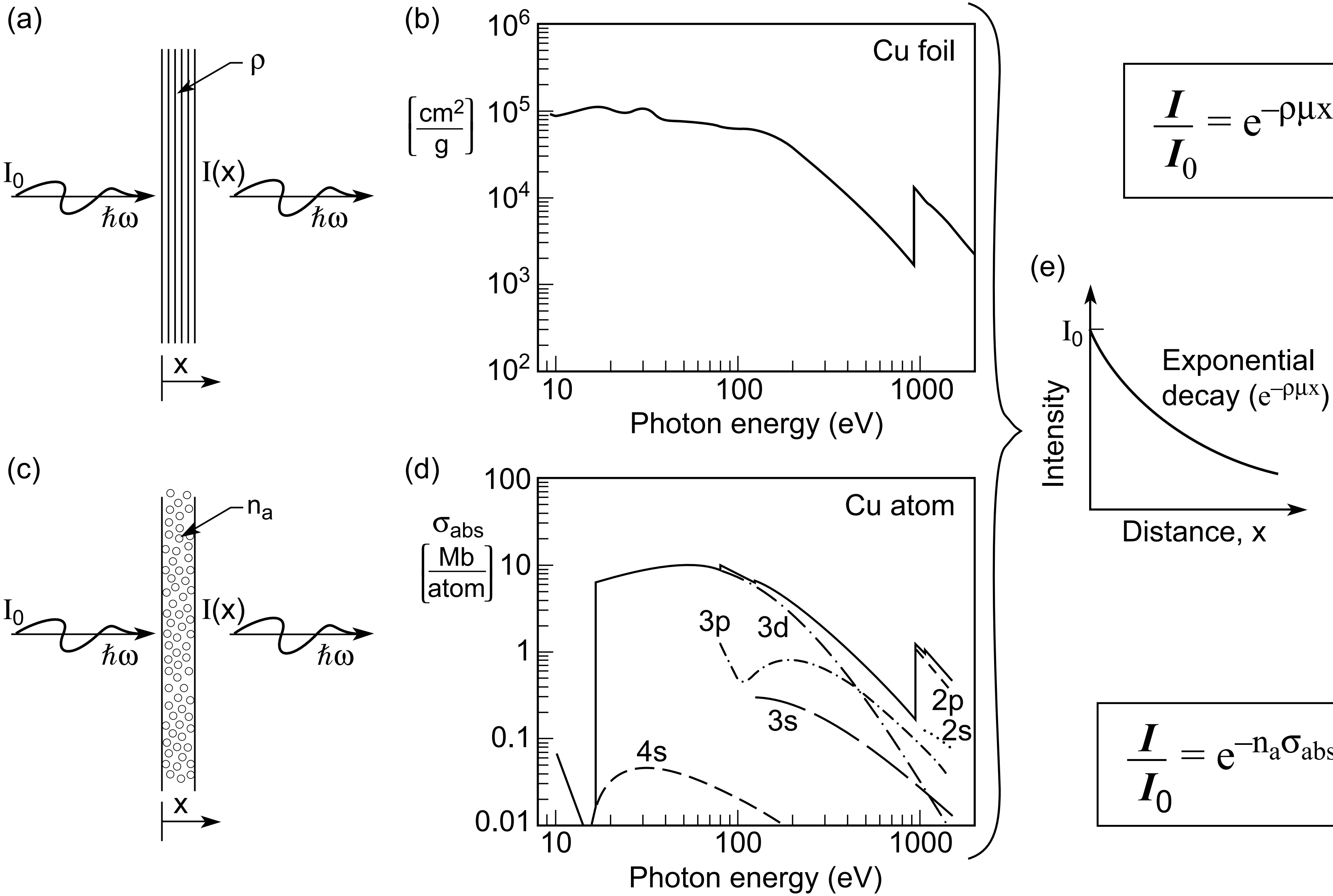
$$\frac{\bar{I}}{\bar{I}_0} = e^{-\rho\mu r} \tag{3.24}$$

where ρ is the mass density, μ is the absorption coefficient, r is the foil thickness, and thus $l_{\text{abs}} = 1/\rho\mu$. Comparing absorption lengths, the macroscopic and atomic descriptions are related by

$$\mu = \frac{2r_e\lambda}{Am_u} f_2^0(\omega) \tag{3.26}$$

where $\rho = m_a n_a = Am_u n_a$, m_u is the atomic mass unit, and A is the number of atomic mass units

Photoabsorption by Thin Foils and Isolated Atoms



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

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

Phase Shift Relative to Vacuum Propagation

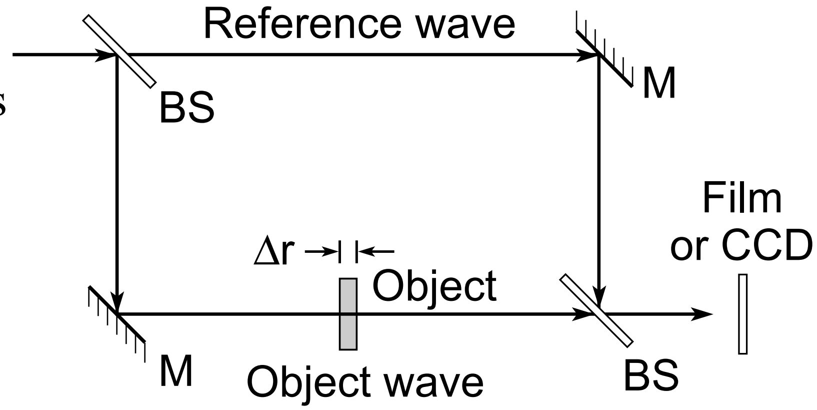
For a wave propagating in a medium of refractive index n = 1 – δ + iβ

$$\mathbf{E}(\mathbf{r}, t) = \underbrace{\mathbf{E}_0 e^{-i\omega(t-r/c)}}_{\text{vacuum propagation}} \underbrace{e^{-i(2\pi\delta/\lambda)r}}_{\phi\text{-shift}} \underbrace{e^{-(2\pi\beta/\lambda)r}}_{\text{decay}} \qquad (3.23)$$

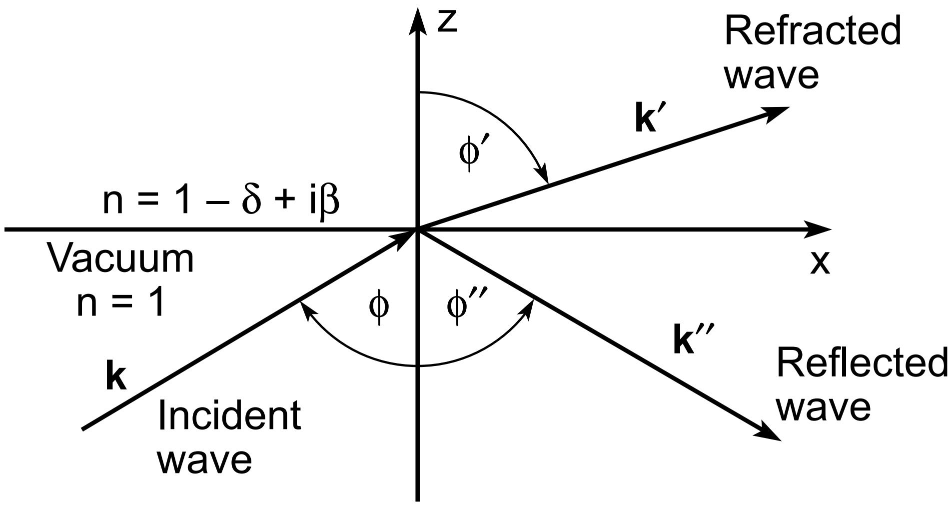
the phase shift Δϕ relative to vacuum, due to propagation through a thickness Δr is

$$\boxed{\Delta\phi = \left(\frac{2\pi\delta}{\lambda}\right)\Delta r} \qquad (3.29)$$

- Flat mirrors at short wavelengths
- Transmissive, flat beamsplitters
- Bonse and Hart interferometer
- Diffractive optics for SXR/EUV



Reflection and Refraction at an Interface



incident wave: $\mathbf{E} = \mathbf{E}_0 e^{-i(\omega t - \mathbf{k}\cdot\mathbf{r})}$ (3.30a)

refracted wave: $\mathbf{E}' = \mathbf{E}_0' e^{-i(\omega t - \mathbf{k}'\cdot\mathbf{r})}$ (3.30b)

reflected wave: $\mathbf{E}'' = \mathbf{E}_0'' e^{-i(\omega t - \mathbf{k}''\cdot\mathbf{r})}$ (3.30c)

(1) All waves have the same frequency, ω, and $|\mathbf{k}| = |\mathbf{k}''| = \dfrac{\omega}{c}$

(2) The refracted wave has phase velocity

$$V_\phi = \frac{\omega'}{k'} = \frac{c}{n} \text{ , thus } k' = |\mathbf{k}'| = \frac{\omega}{c}(1 - \delta + i\beta)$$

Boundary Conditions at an Interface

- **E** and **H** components parallel to the interface must be continuous

$$\mathbf{z}_0 \times (\mathbf{E}_0 + \mathbf{E}_0'') = \mathbf{z}_0 \times \mathbf{E}_0' \qquad (3.32a)$$

$$\mathbf{z}_0 \times (\mathbf{H}_0 + \mathbf{H}_0'') = \mathbf{z}_0 \times \mathbf{H}_0' \qquad (3.32b)$$

- **D** and **B** components perpendicular to the interface must be continuous

$$\mathbf{z}_0 \cdot (\mathbf{D}_0 + \mathbf{D}_0'') = \mathbf{z}_0 \cdot \mathbf{D}_0' \qquad (3.32c)$$

$$\mathbf{z}_0 \cdot (\mathbf{B}_0 + \mathbf{B}_0'') = \mathbf{z}_0 \cdot \mathbf{B}_0' \qquad (3.32d)$$

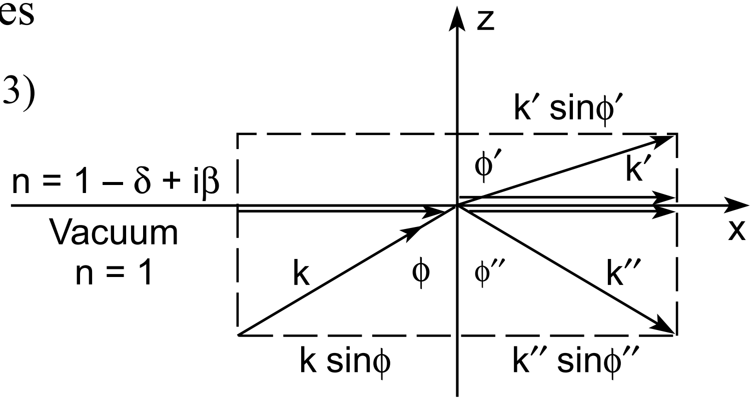
Spatial Continuity Along the Interface

Continuity of parallel field components requires

$$(\mathbf{k}\cdot\mathbf{x}_0 = \mathbf{k}'\cdot\mathbf{x}_0 = \mathbf{k}''_0\cdot\mathbf{x}_0) \quad \text{at } z = 0 \qquad (3.33)$$

$$k_x = k'_x = k''_x \qquad (3.34a)$$

$$k\sin\phi = k'\sin\phi' = k''\sin\phi'' \qquad (3.34b)$$



Conclusions:

Since k = k″ (both in vacuum)

$$\sin\phi = \sin\phi'' \qquad (3.35a)$$

$$\therefore \quad \boxed{\phi = \phi''} \qquad (3.35b)$$

The angle of incidence equals the angle of reflection

$$k\sin\phi = k'\sin\phi' \qquad (3.36)$$

$$k = \frac{\omega}{c} \quad \text{and } k' = \frac{\omega'}{c/n} = \frac{n\omega}{c}$$

$$\sin\phi = n\sin\phi'$$

$$\boxed{\sin\phi' = \frac{\sin\phi}{n}} \qquad (3.38)$$

Snell's Law, which describes refractive turning, for complex n.

Total External Reflection of Soft X-Rays and EUV Radiation

Snell's law for a refractive index of n $\simeq$ 1 – δ, assuming that β → 0

$$\sin\phi' = \frac{\sin\phi}{1-\delta} \qquad (3.39)$$

Consider the limit when $\phi' \rightarrow \frac{\pi}{2}$

$$1 = \frac{\sin\phi_c}{1-\delta}$$

$$\sin\phi_c = 1-\delta \qquad (3.40)$$

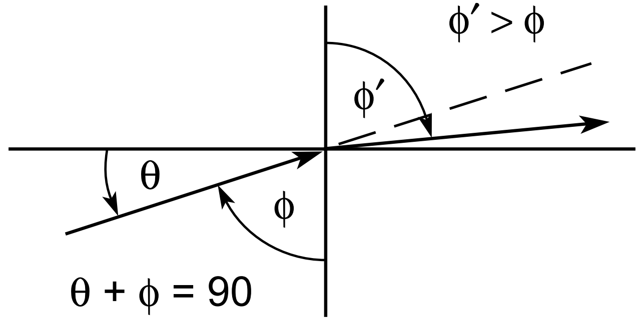
$$\sin(90^\circ - \theta_c) = 1-\delta$$

$$\cos\theta_c = 1-\delta$$

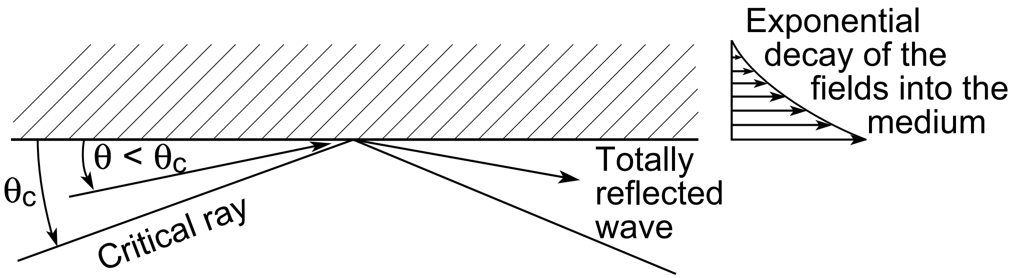
$$1 - \frac{\theta_c^2}{2} + \cdots = 1-\delta$$

$$\boxed{\theta_c = \sqrt{2\delta}} \qquad (3.41)$$

The critical angle for total external reflection.



Glancing incidence ($\theta < \theta_c$) and total external reflection



Total External Reflection (continued)

$$\boxed{\theta_c = \sqrt{2\delta}} \qquad (3.41)$$

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

$$\theta_c = \sqrt{2\delta} = \sqrt{\frac{n_a r_e \lambda^2 f_1^0(\lambda)}{\pi}} \qquad (3.42a)$$

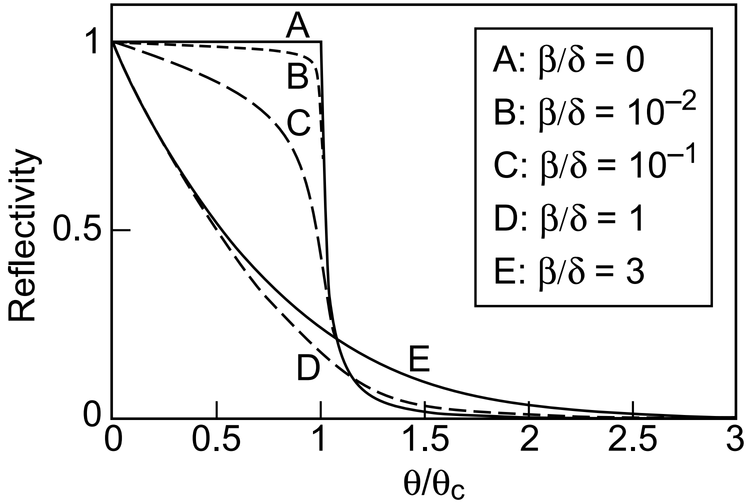
The atomic density n_a, varies slowly among the natural elements, thus to first order

$$\theta_c \propto \lambda\sqrt{Z} \qquad (3.42b)$$

where f_1^0 is approximated by Z. Note that f_1^0 is a complicated function of wavelength (photon energy) for each element.

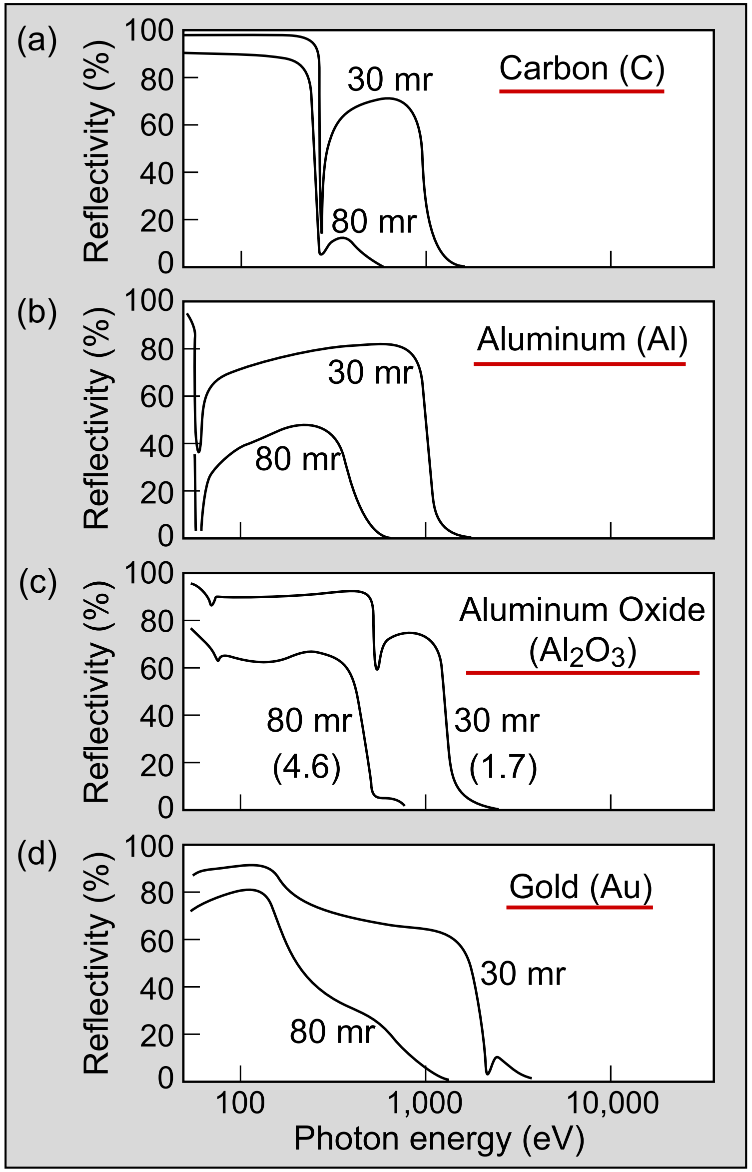
Total External Reflection with Finite Absorption

Glancing incidence reflection
as a function of β/δ



- finite β/δ rounds the sharp angular dependence
- cutoff angle and absorption edges can enhance the sharpness
- note the effects of oxide layers and surface contamination

. . . for real materials



(Henke, Gullikson, Davis)

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Reflection at an Interface (s-polarization)

E_0 perpendicular to the plane of incidence (s-polarization)

tangential electric fields continuous

$$E_0 + E_0'' = E_0' \qquad (3.43)$$

tangential magnetic fields continuous

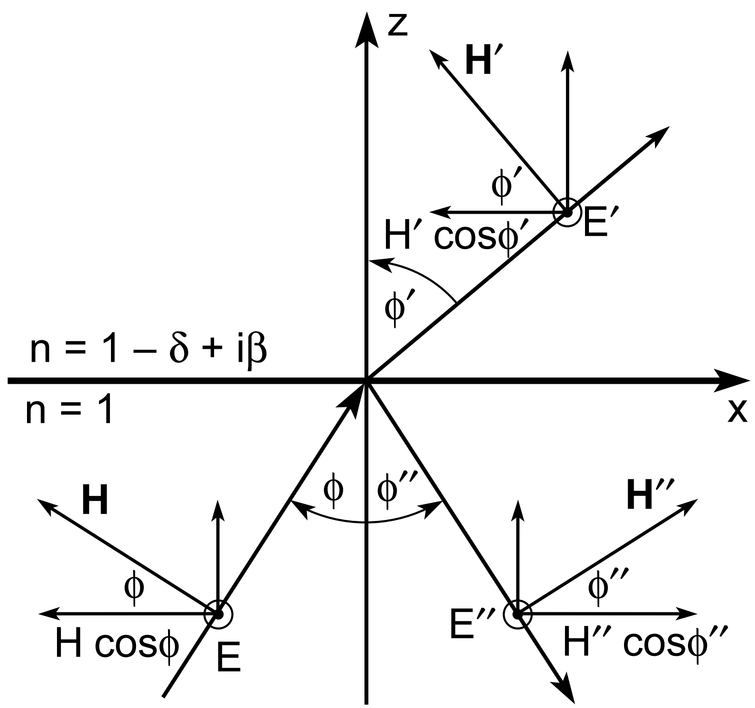
$$H_0 \cos\phi - H_0'' \cos\phi = H_0' \cos\phi' \qquad (3.44)$$

$$\mathbf{H}(\mathbf{r}, t) = n\sqrt{\frac{\epsilon_0}{\mu_0}}\mathbf{k}_0 \times \mathbf{E}(\mathbf{r}, t) \;\Rightarrow\; H = n\sqrt{\frac{\epsilon_0}{\mu_0}}E$$

$$\sqrt{\frac{\epsilon_0}{\mu_0}}E_0 \cos\phi - \sqrt{\frac{\epsilon_0}{\mu_0}}E_0'' \cos\phi = n\sqrt{\frac{\epsilon_0}{\mu_0}}E_0' \cos\phi'$$

$$(E_0 - E_0'')\cos\phi = nE_0' \cos\phi' \qquad (3.45)$$

Snell's Law: $\sin\phi' = \dfrac{\sin\phi}{n}$



Three equations in three unknowns (E_0', E_0'', ϕ') (for given E_0 and ϕ)

Reflection at an Interface (continued)

E_0 perpendicular to the plane of incidence (s-polarization)

$$\frac{E_0'}{E_0} = \frac{2\cos\phi}{\cos\phi + \sqrt{n^2 - \sin^2\phi}} \tag{3.47}$$

$$\frac{E_0''}{E_0} = \frac{\cos\phi - \sqrt{n^2 - \sin^2\phi}}{\cos\phi + \sqrt{n^2 - \sin^2\phi}} \tag{3.46}$$

The reflectivity R is then

$$R = \frac{\bar{I}''}{\bar{I}_0} = \frac{|\bar{\mathbf{S}}''|}{|\bar{\mathbf{S}}|} = \frac{\frac{1}{2}\mathrm{Re}(\mathbf{E}_0'' \times \mathbf{H}_0''^*)}{\frac{1}{2}\mathrm{Re}(\mathbf{E}_0 \times \mathbf{H}_0^*)} \tag{3.48}$$

With n = 1 for both incident and reflected waves,

$$R = \frac{|E_0''|^2}{|E_0|^2}$$

Which with Eq. (3.46) becomes, for the case of perpendicular (s) polarization

$$\boxed{R_s = \frac{\left|\cos\phi - \sqrt{n^2 - \sin^2\phi}\right|^2}{\left|\cos\phi + \sqrt{n^2 - \sin^2\phi}\right|^2}} \tag{3.49}$$

Normal Incidence Reflection at an Interface

Normal incidence ($\phi = 0$)

$$R_s = \frac{\left|\cos\phi - \sqrt{n^2 - \sin^2\phi}\right|^2}{\left|\cos\phi + \sqrt{n^2 - \sin^2\phi}\right|^2} \qquad (3.49)$$

$$R_{s,\perp} = \frac{|1-n|^2}{|1+n|^2} = \frac{(1-n)(1-n^*)}{(1+n)(1+n^*)}$$

For $n = 1 - \delta + i\beta$

$$R_{s,\perp} = \frac{(\delta - i\beta)(\delta + i\beta)}{(2-\delta+i\beta)(2-\delta-i\beta)} = \frac{\delta^2+\beta^2}{(2-\delta)^2+\beta^2}$$

Which for $\delta \ll 1$ and $\beta \ll 1$ gives the reflectivity for x-ray and EUV radiation at normal incidence ($\phi = 0$) as

$$\boxed{R_{s,\perp} \simeq \frac{\delta^2+\beta^2}{4}} \qquad (3.50)$$

Example: Nickel @ 300 eV (4.13 nm)
From table C.1, p. 433
$f_1^0 = 17.8$ $\quad f_2^0 = 7.70$
$\delta = 0.0124$ $\quad \beta = 0.00538$

$\Big\}\ R_\perp = 4.58 \times 10^{-5}$

Glancing Incidence Reflection (s-polarization)

$$R_s = \frac{\left|\cos\phi - \sqrt{n^2 - \sin^2\phi}\right|^2}{\left|\cos\phi + \sqrt{n^2 - \sin^2\phi}\right|^2} \qquad (3.49)$$

For $\quad \theta = 90^\circ - \phi \le \theta_c$

where $\quad \theta_c = \sqrt{2\delta} \ll 1$

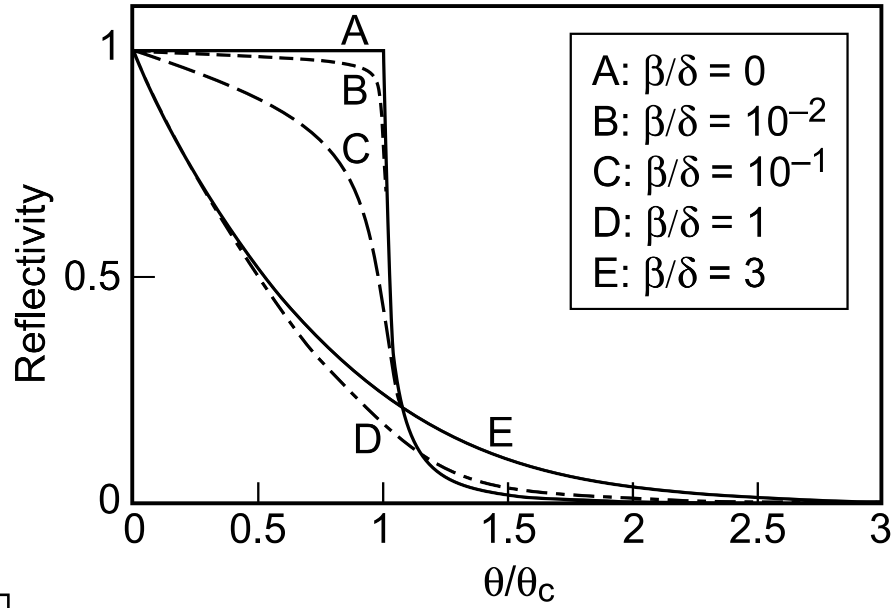
$$\cos\phi = \sin\theta \simeq \theta$$

$$\sin^2\phi = 1 - \cos^2\phi = 1 - \sin^2\theta \simeq 1 - \theta^2$$

For $n = 1 - \delta + i\beta$

$$n^2 = (1-\delta)^2 + 2i\beta(1-\delta) - \beta^2$$

$$R_{s,\theta} = \frac{\left|\theta - \sqrt{(\theta^2 - \theta_c^2) + 2i\beta}\right|^2}{\left|\theta + \sqrt{(\theta^2 - \theta_c^2) + 2i\beta}\right|^2} \qquad (\theta \ll 1)$$



E. Nähring, "Die Totalreflexion der Röntgenstrahlen", Physik. Zeitstr. XXXI, 799 (Sept. 1930).

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Reflection at an Interface (p-polarization)

E_0 parallel to the plane of incidence (p-polarization)

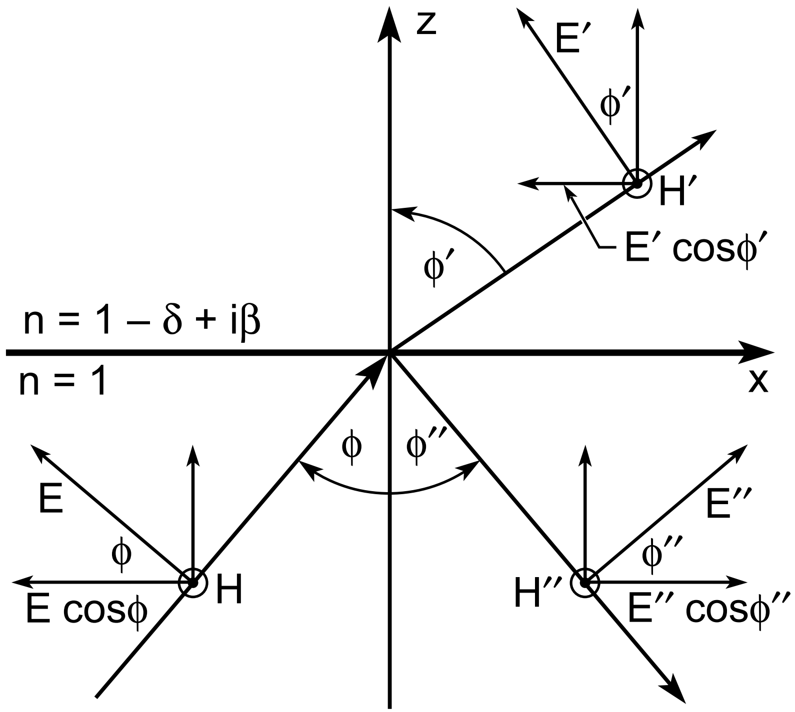
$$\frac{E_0''}{E_0} = \frac{n^2 \cos\phi - \sqrt{n^2 - \sin^2\phi}}{n^2 \cos\phi + \sqrt{n^2 - \sin^2\phi}} \tag{3.54}$$

$$\frac{E_0'}{E_0} = \frac{2n \cos\phi}{n^2 \cos\phi + \sqrt{n^2 - \sin^2\phi}} \tag{3.55}$$

The reflectivity for parallel (p) polarization is

$$R_p = \left|\frac{E_0''}{E_0}\right|^2 = \frac{\left|n^2 \cos\phi - \sqrt{n^2 - \sin^2\phi}\right|^2}{\left|n^2 \cos\phi + \sqrt{n^2 - \sin^2\phi}\right|^2} \tag{3.56}$$

which is similar in form but slightly different from that for s-polarization. For $\phi = 0$ (normal incidence) the results are identical.



Brewster's Angle for X-Rays and EUV

For p-polarization

$$R_p = \left| \frac{E_0''}{E_0} \right|^2 = \frac{\left| n^2 \cos\phi - \sqrt{n^2 - \sin^2\phi} \right|^2}{\left| n^2 \cos\phi + \sqrt{n^2 - \sin^2\phi} \right|^2} \qquad (3.56)$$

There is a minimum in the reflectivity where the numerator satisfies

$$n^2 \cos\phi_B = \sqrt{n^2 - \sin^2\phi_B} \qquad (3.58)$$

Squaring both sides, collecting like terms involving ϕ_B, and factoring, one has

$$n^2(n^2 - 1) = (n^4 - 1)\sin^2\phi_B$$

or

$$\sin\phi_B = \frac{n}{\sqrt{n^2 + 1}}$$

the condition for a minimum in the reflectivity, for parallel polarized radiation, occurs at an angle given by

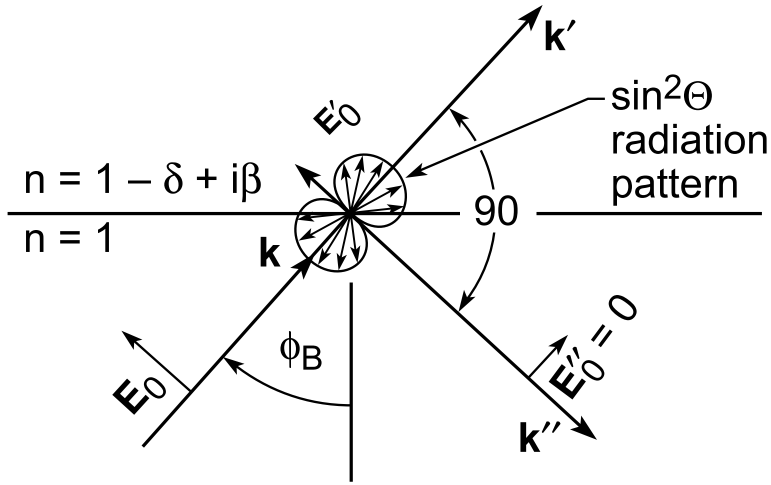
$$\tan\phi_B = n \qquad (3.59)$$

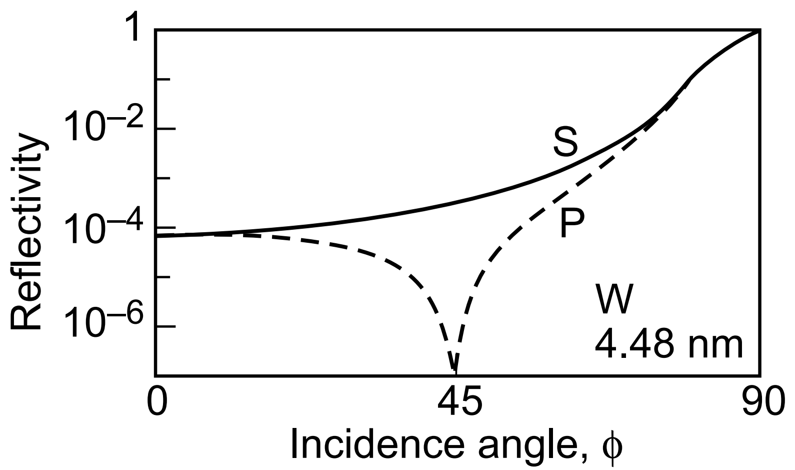
For complex n, Brewster's minimum occurs at

$$\tan\phi_B = 1 - \delta$$

or

$$\boxed{\phi_B \simeq \frac{\pi}{4} - \frac{\delta}{2}} \qquad (3.60)$$

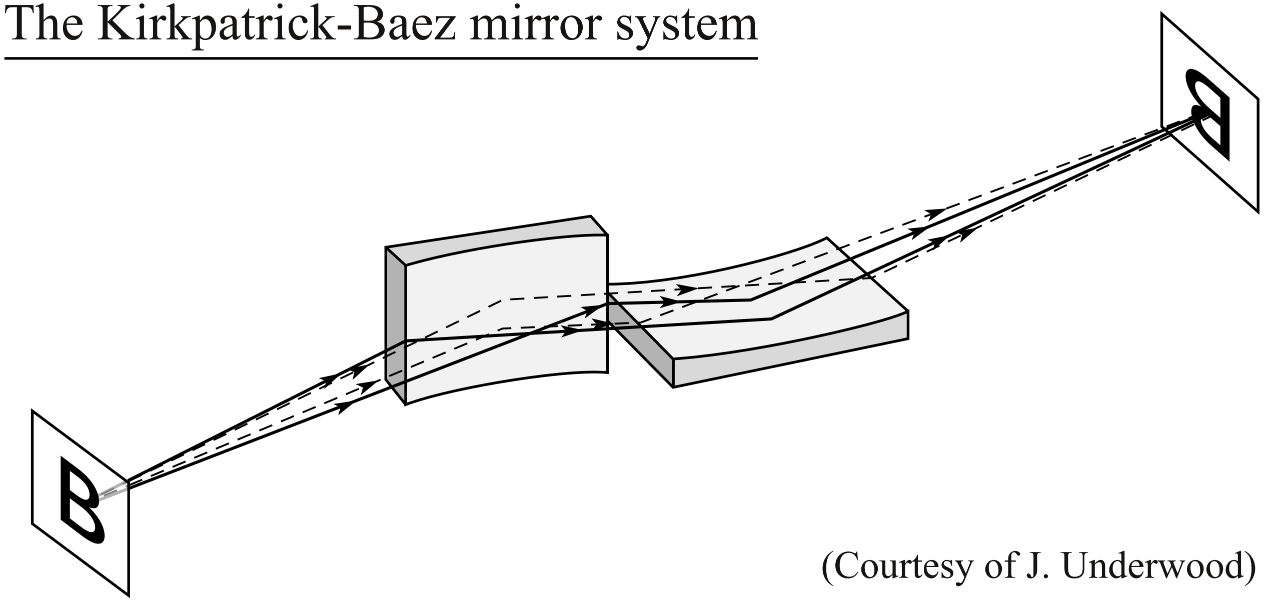




(Courtesy of J. Underwood)

Focusing with Curved, Glancing Incidence Optics

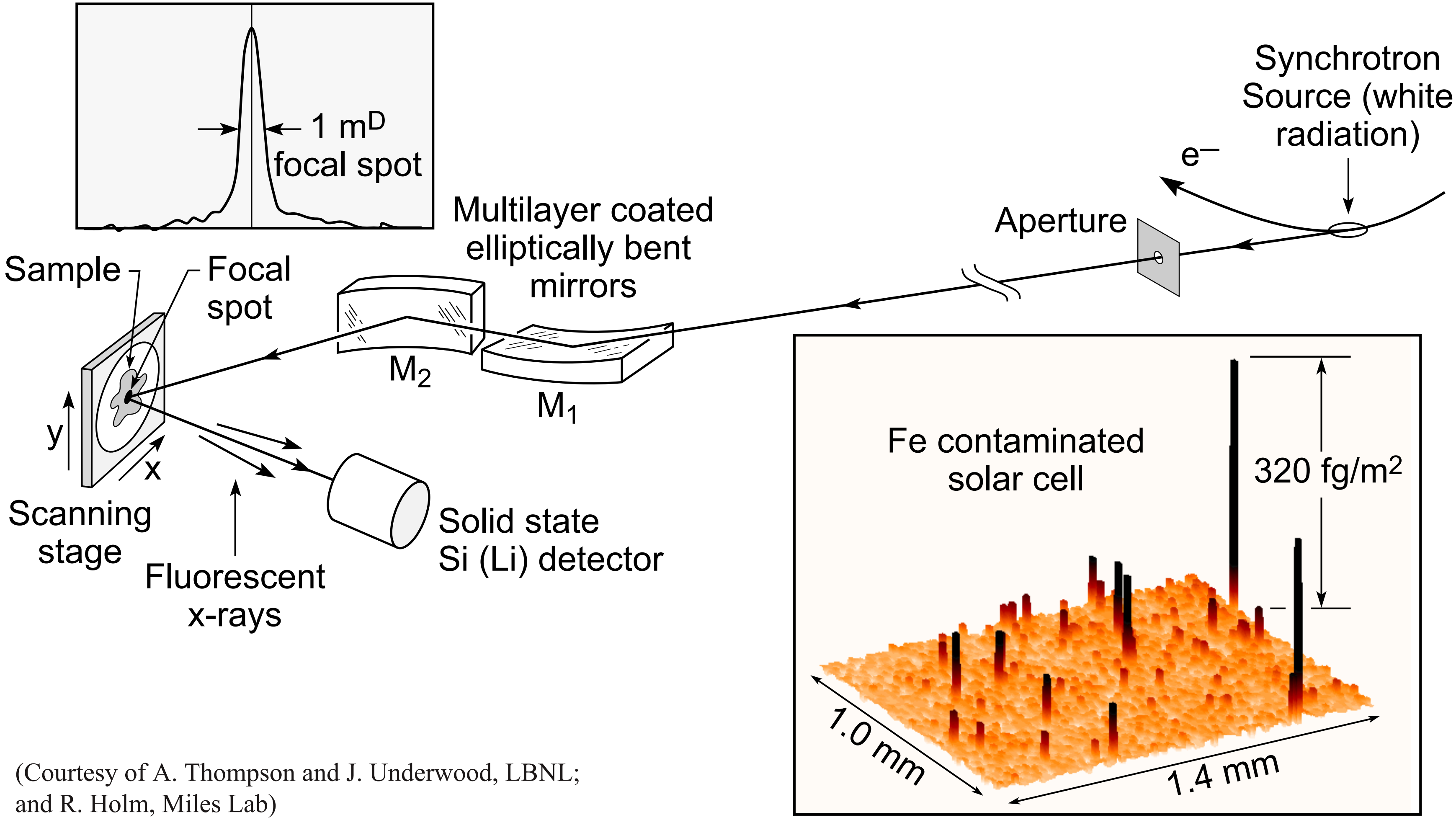
The Kirkpatrick-Baez mirror system



(Courtesy of J. Underwood)

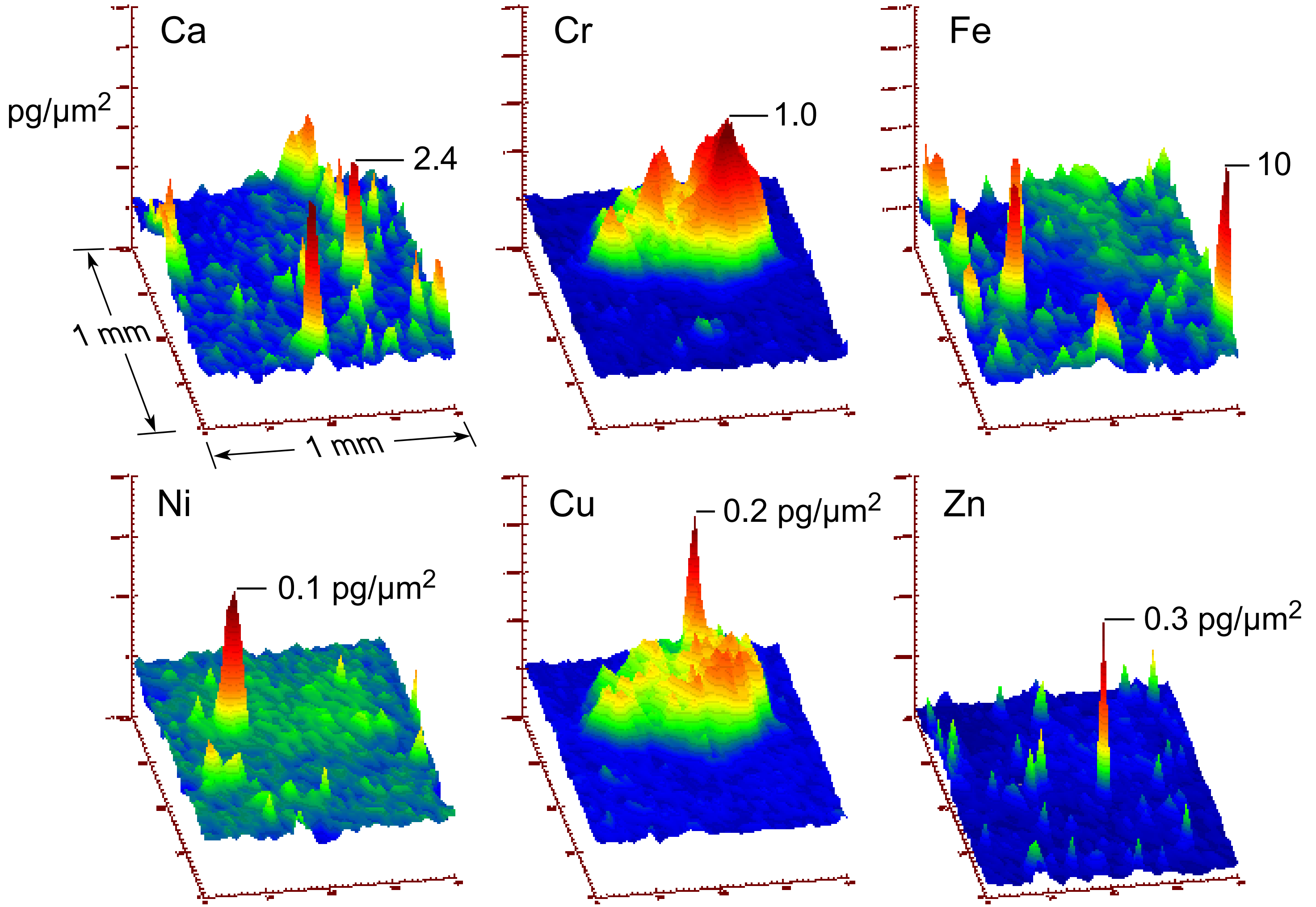
- Two crossed cylinders (or spheres)
- Astigmatism cancels
- Fusion diagnostics
- Common use in synchrotron radiation beamlines
- See hard x-ray microprobe, chapter 4, figure 4.14

Buried, Trace Amounts of Iron in a Defective Silicon Solar Cell



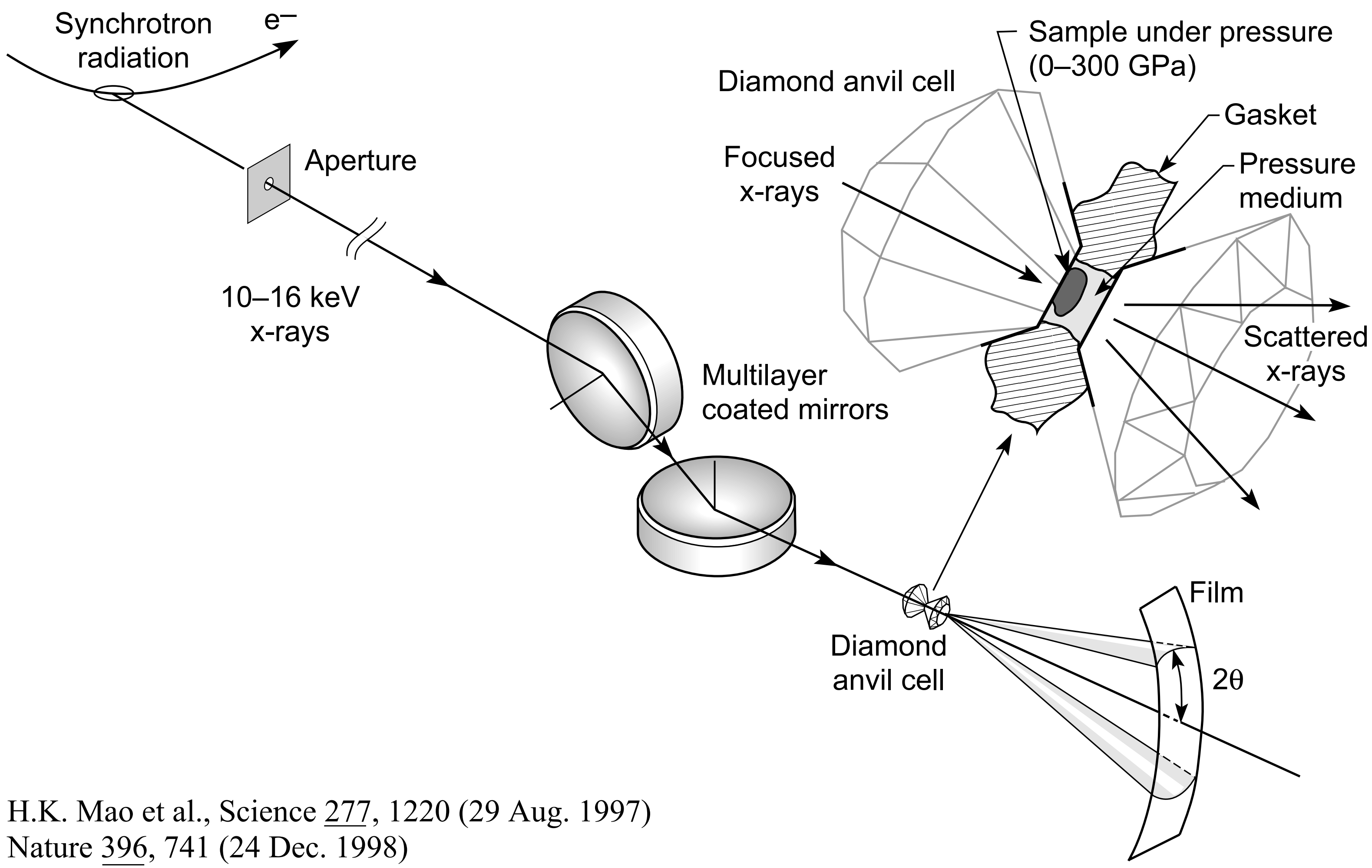
(Courtesy of A. Thompson and J. Underwood, LBNL; and R. Holm, Miles Lab)

Microprobe Analysis of Contaminated Soil



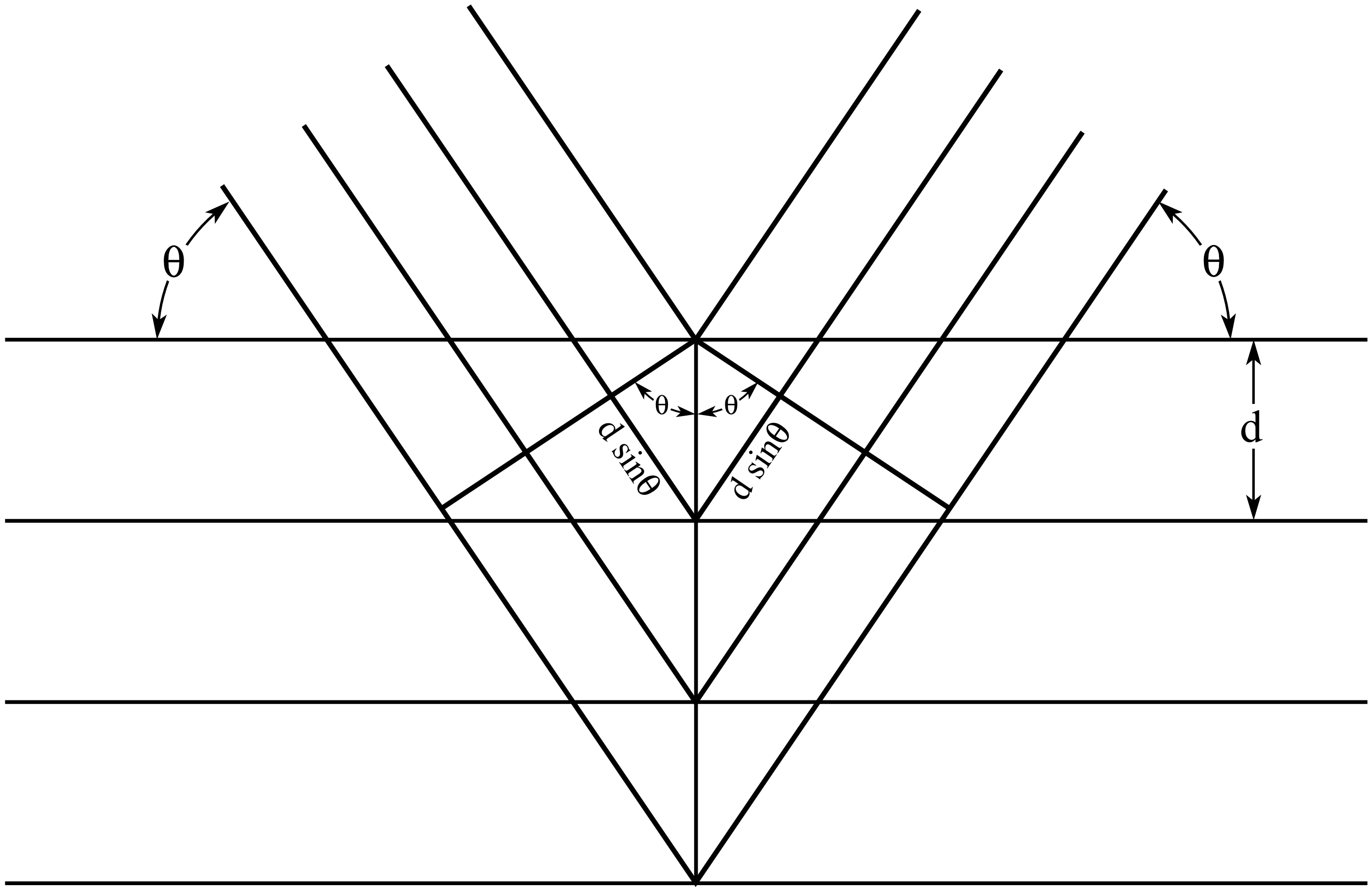
(Courtesy of T. Tokunaga; and A. Thompson, LBNL)

High Resolution X-Ray Diffraction Under High Pressure Using Multilayer Coated Focusing Optics



H.K. Mao et al., Science 277, 1220 (29 Aug. 1997)
Nature 396, 741 (24 Dec. 1998)

Bragg Scattering, or Diffraction, Seen as a Reflection from Crystal Planes



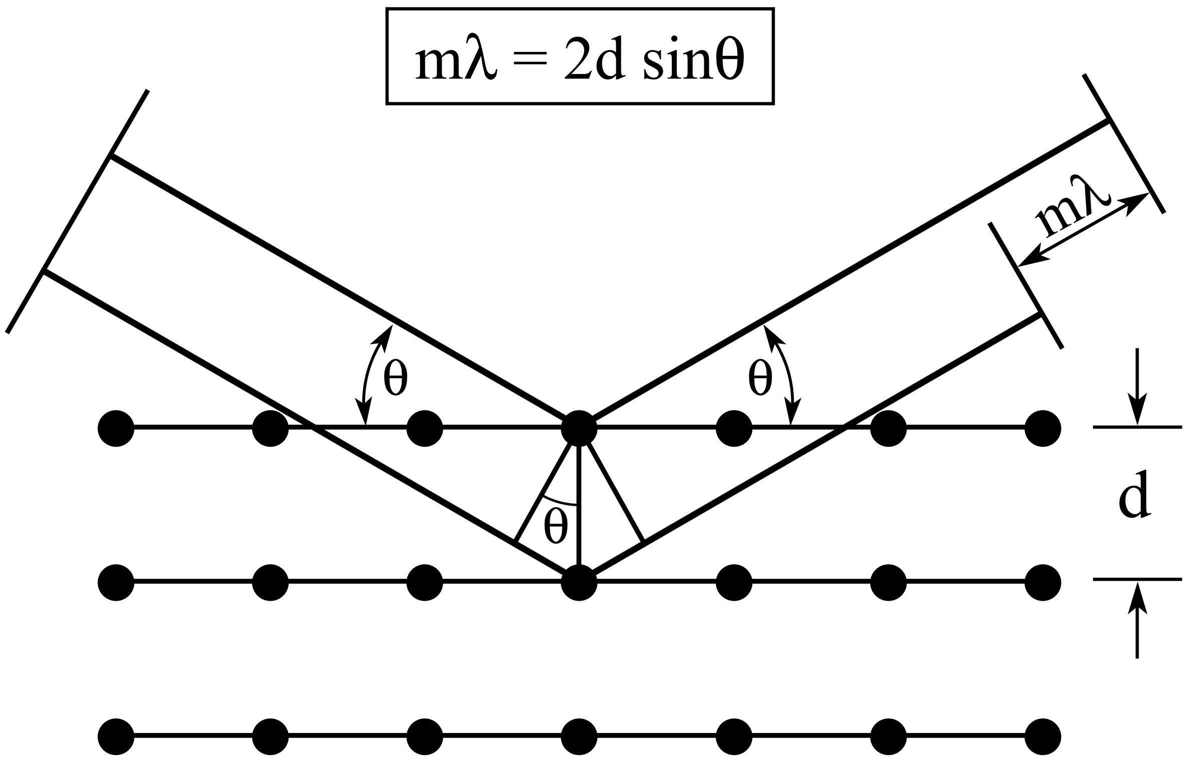
Constructive interference occurs when the additional path length is equal to an integral number of wavelengths:

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

(Bragg's Law)
(m = 1, 2, . . .)

R.B. Leighton, *Principles of Modern Physics* (McGraw-Hill, New York, 1959), section 12.4.

The Derivation of Bragg's Law



The path difference of radiation "reflecting" off sequential planes must be equal to an interger number of wavelengths.

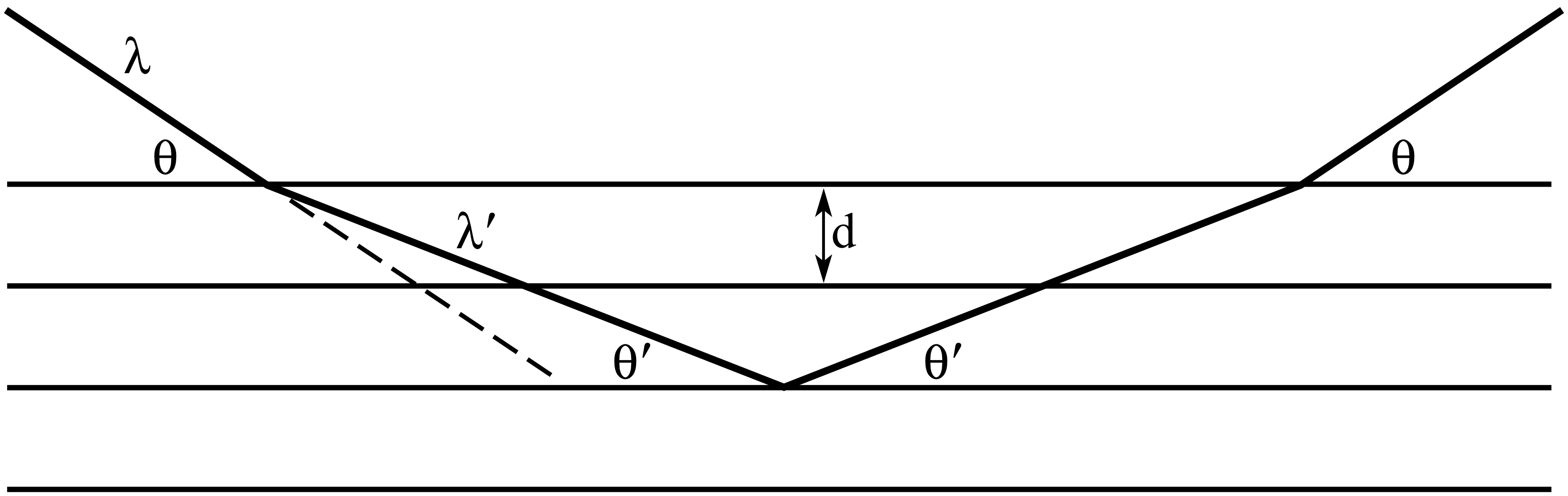
The angle θ is measured from the crystal plane, and the distance between planes is referred to as the "d-spacing".

From A.H. Compton and S.K. Allison, *X-Rays in Theory and Experiment* (D.Van Nostrand, New York, 1926), p.29.
Also see M. Siegbahn, *The Spectroscopy of X-Rays* (Oxford University Press, London, 1925), p.16.

X-Rays are Refracted Entering a Crystal

Refraction of x-rays at a crystal surface requires a small correction to the Bragg condition:

$$m\lambda = 2d\sin\theta\left(1 - \frac{4\bar{\delta}d^2}{m^2\lambda^2}\right)$$



R.B. Leighton, *Principles of Modern Physics* (McGraw-Hill, New York, 1959), p. 456.