# X-Ray Data Booklet

## Section 5.5 USEFUL EQUATIONS

The following pages include a number of equations useful to x-ray scientists, either expanding on subjects covered in this booklet or addressing topics not covered here. The equations have been drawn from D. T. Attwood, *Soft X-Rays and Extreme Ultraviolet Radiation: Principles and Applications* (Cambridge Univ. Press, Cambridge, 1999) [http://www.coe.berkeley.edu/AST/sxreuv], and the equation numbers refer to that volume, which should be consulted for further explanation and discussion. That reference also expands on the discussions in this booklet on zone plate optics, synchrotron radiation, and other topics.

## General X-Ray Formulas

Wavelength and photon energy relationship:

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

Number of photons required for 1 joule of energy:

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

## X-Ray Scattering and Absorption

Thomson cross section for a free electron:

$$\sigma_e = \frac{8\pi}{3} r_e^2 \tag{2.45}$$

$$r_e = \frac{e^2}{4\pi\epsilon_0 mc^2} = 2.82 \times 10^{-13}\text{cm} \tag{2.44}$$

and $r_e$ is the classical electron radius.

Scattering cross section for a bound electron:

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

Rayleigh cross section ($\omega^2 \ll \omega_s^2$):

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

Scattering by a multi-electron atom:

$$\frac{d\sigma(\omega)}{d\Omega} = r_e^2 |f|^2 \sin^2\Theta \tag{2.68}$$

$$\sigma(\omega) = \frac{8\pi}{3} |f|^2 r_e^2 \tag{2.69}$$

where the complex atomic scattering factor represents the electric field scattered by an atom, normalized to that of a single electron:

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

For forward scattering or long wavelength this reduces to

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

Refractive index for x-ray radiation is commonly written * as

$$n(\omega) = 1 - \delta + i\beta = 1 - \frac{n_a r_e \lambda^2}{2\pi}(f_1^0 - i f_2^0) \qquad (3.9\,\&\,3.12)$$

where

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

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

Absorption length in a material:

$$\ell_{\text{abs}} = \frac{\lambda}{4\pi\beta} = \frac{1}{2 n_a r_e \lambda f_2^0(\omega)} \qquad (3.22\,\&\,3.23)$$

Mass-dependent absorption coefficient:

$$\mu = \frac{2 r_e \lambda}{A m_u} f_2^0(\omega) \qquad (3.26)$$

Atomic absorption cross section:

$$\sigma_{\text{abs}} = 2 r_e \lambda f_2^0(\omega) = A m_u \mu(\omega) \qquad (3.28a\&b)$$

Relative phase shift through a medium compared to a vacuum:

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

where $\Delta r$ is the thickness or propagation distance.

---

* The choice of $+i\beta$ is consistent with a wave description $E = E_0 \exp[-i(\omega t - kr)]$. A choice of $-i\beta$ is consistent with $E = E_0 \exp[i(\omega t - kr)]$.

Snell's law:

$$\sin\phi' = \frac{\sin\phi}{n} \tag{3.38}$$

Critical angle for total external reflection of x-rays:

$$\theta_c = \sqrt{2\delta} \tag{3.41}$$

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

Brewster's angle (or polarizing angle):

$$\phi_{\mathrm{B}} \simeq \frac{\pi}{4} - \frac{\delta}{2} \tag{3.60}$$

## Multilayer Mirrors

Bragg's law:

$$m\lambda = 2d\sin\theta \tag{4.6b}$$

Correction for refraction:

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

where $\bar{\delta}$ is the period-averaged real part of the refractive index.

$$\Gamma = \frac{\Delta t_{\mathrm{H}}}{\Delta t_{\mathrm{H}} + \Delta t_{\mathrm{L}}} = \frac{\Delta t_{\mathrm{H}}}{d} \tag{4.7}$$

## Plasma Equations

Electron plasma frequency:

$$\omega_p^2 = \frac{e^2 n_e}{\epsilon_0 m} \tag{6.5}$$

Debye screening distance:

$$\lambda_D = \left( \frac{\epsilon_0 \kappa T_e}{e^2 n_e^2} \right)^{1/2} \tag{6.6}$$

No. of electrons in Debye sphere:

$$N_D = \frac{4\pi}{3} \lambda_D^3 n_e \tag{6.7}$$

Electron cyclotron frequency:

$$\omega_c = \frac{eB}{m} \tag{6.8}$$

Maxwellian velocity distribution for electrons characterized by a single-electron temperature $\kappa T_e$:

$$f(\mathrm{v}) = \frac{1}{(2\pi)^{3/2} \mathrm{v}_e^3} \, e^{-\mathrm{v}^2/2\mathrm{v}_e^2} \tag{6.1}$$

where

$$\mathrm{v}_e = \left( \frac{\kappa T_e}{m} \right)^{1/2} \tag{6.2}$$

Electron sound speed:

$$a_e = \left( \frac{\gamma \kappa T_e}{m} \right)^{1/2} \tag{6.79}$$

Critical electron density:

$$n_c \equiv \frac{\epsilon_0 m \omega^2}{e^2} = 1.11 \times 10^{21} \; \frac{\mathrm{e/cm^3}}{\lambda^2(\mu\mathrm{m})} \tag{6.112a \& b}$$

Refractive index of plasma is

$$n = \sqrt{1 - \frac{n_e}{n_c}} \tag{6.114b}$$

Ratio of electron energy in coherent oscillations to that in random motion:

$$\left| \frac{\mathrm{v}_{\mathrm{os}}}{\mathrm{v}_e} \right|^2 = \frac{e^2 E^2}{m\omega^2 \kappa T_e} = \frac{I/c}{n_c \kappa T_e} \tag{6.131a}$$

$$\left| \frac{\mathrm{v}_{\mathrm{os}}}{\mathrm{v}_e} \right|^2 = \frac{0.021 I (10^{14}\ \mathrm{W/cm^2}) \lambda^2\ (\mu\mathrm{m})}{\kappa T_e (\mathrm{keV})} \tag{6.131b}$$

Spectral brightness of blackbody radiation within $\Delta\omega/\omega = 0.1\%\mathrm{BW}$:

$$B_{\Delta\omega/\omega} = 3.146 \times 10^{11} \left( \frac{\kappa T}{eV} \right)^3 \frac{(\hbar\omega/\kappa T)^3}{(e^{\hbar\omega/\kappa T} - 1)} \frac{\text{photons/sec}}{(\mathrm{mm})^2 (\mathrm{mr})^2 (0.1\%\mathrm{BW})} \tag{6.136b}$$

Photon energy at peak spectral brightness:

$$\hbar\omega\,|_{\mathrm{pk}} = 2.822 \kappa T \tag{6.137}$$

where $\kappa$ is the Boltzmann constant.

Stefan-Boltzmann radiation law (blackbody intensity at any interface):

$$I = \sigma T^4 \tag{6.141b}$$

where the Stefan-Boltzmann constant is

$$\sigma = \frac{\pi^2 \kappa^4}{60 c^2 \hbar^3} \tag{6.142}$$

With $\kappa T$ in eV:

$$I = \widehat{\sigma} (\kappa T)^4 \tag{6.143a}$$

where $\widehat{\sigma}$ is the modified Stefan-Boltzmann constant

$$\widehat{\sigma} = \frac{\pi^2}{60 \hbar^3 c^2} = 1.027 \times 10^5 \frac{\text{watts}}{\mathrm{cm}^2 (\mathrm{eV})^4} \tag{6.143b}$$

## Coherence

Longitudinal coherence length:*

$$\ell_{\rm coh} = \lambda^2/2\Delta\lambda \tag{8.3}$$

Spatial or transverse coherence (rms quantities):

$$d \cdot \theta = \lambda/2\pi \tag{8.5}$$

or in terms of FWHM values

$$d \cdot 2\theta|_{\rm FWHM} = 0.44\lambda$$

Spatially coherent power within a relative spectral bandwidth $\lambda/\Delta\lambda = N$ for an undulator with $N$ periods:

$$\bar{P}_{{\rm coh},N} = \frac{e\lambda_{\rm u} I}{8\pi\epsilon_0 d_x d_y \theta_x \theta_y \gamma^2} \cdot \left(\frac{\hbar\omega_0}{\hbar\omega} - 1\right) f(\hbar\omega/\hbar\omega_0) \tag{8.7c}$$

where $\hbar\omega_0$ corresponds to $K = 0$, and where

$$f(\hbar\omega/\hbar\omega_0) = \frac{7}{16} + \frac{5}{8}\frac{\hbar\omega}{\hbar\omega_0} - \frac{1}{16}\left(\frac{\hbar\omega}{\hbar\omega_0}\right)^2 + \ldots \tag{8.8}$$

When the undulator condition ($\sigma' \ll \theta_{\rm cen}$) is satisfied, the coherent power within a relative spectral bandwidth $\Delta\lambda/\lambda < 1/N$, is

$$\bar{P}_{{\rm coh},\lambda/\Delta\lambda} = \frac{e\lambda_{\rm u} I \eta (\lambda/\Delta\lambda) N^2}{8\pi\epsilon_0 d_x d_y} \cdot \left(1 - \frac{\hbar\omega}{\hbar\omega_0}\right) f(\hbar\omega/\hbar\omega_0)$$
$$(\sigma'^2 \ll \theta_{\rm cen}^2) \tag{8.10c}$$

where $\eta$ is the combined beamline and monochrometer efficiency.

---

* The factor of two here is somewhat arbitrary and depends, in part, on the definition of $\Delta\lambda$. Equation (26) on page 2-14 omits this factor. See Attwood, op.cit., for further discussion.

Spatially coherent power available from a laser is

$$P_{\text{coh}} = \frac{(\lambda/2\pi)^2}{(d_x\theta_x)\,(d_y\theta_y)} P_{\text{laser}} \tag{8.11}$$

where $P_{\text{laser}}$ is the total laser power.

Normalized degree of spatial coherence, or complex coherence factor:

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

The van Cittert-Zernike theorem for the complex coherence factor is

$$\mu_{\text{OP}} = \frac{e^{-i\psi}\int\int I(\xi,\eta)e^{ik(\xi\theta_x+\eta\theta_y)}\,d\xi\,d\eta}{\int\int I(\xi,\eta)\,d\xi\,d\eta} \tag{8.19}$$

For a uniformly but incoherently illuminated pinhole

$$\mu_{\text{OP}}(\theta) = e^{-i\psi}\frac{2J_1(ka\theta)}{(ka\theta)} \tag{8.27}$$

which has its first null ($\mu_{\text{OP}} = 0$) at $ka\theta = 3.832$, which for $d = 2a$ corresponds to $d \cdot \theta = 1.22\lambda$.

## EUV/Soft X-Ray Lasers

Growth of stimulated emission:

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

where $L$ is the laser length and $G$ is the gain per unit length. For an upper-state ion density $n_u$ and a density inversion factor $F(\leq 1)$

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

where the cross section for stimulated emission is

$$\sigma_{\text{stim}} = \frac{\lambda^3 A_{u\ell}}{8\pi c(\Delta\lambda/\lambda)} \tag{7.16}$$

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

where $A_{u\ell}$ is the spontaneous decay rate, $f_{\ell u}$ is the oscillator strength and $g_\ell/g_u$ is the ratio of degeneracy factors.

Laser wavelength scaling goes as $1/\lambda^4$:

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

Doppler-broadened linewidth:

$$\left.\frac{(\Delta\lambda)}{\lambda}\right|_{\text{FWHM}} = \frac{v_i}{c} = \frac{2\sqrt{2\ln 2}}{c}\sqrt{\frac{\kappa T_i}{M}} \tag{7.19a}$$

where $v_i$ is the ion thermal velocity, $\kappa T_i$ is the ion temperature, and $M$ is the ion mass. With $\kappa T_i$ expressed in eV and an ion mass of $2m_p Z$

$$\left.\frac{(\Delta\lambda)}{\lambda}\right|_{\text{FWHM}} = 7.68 \times 10^{-5}\left(\frac{\kappa T_i}{2Z}\right)^{1/2} \tag{7.19b}$$

## Lithography

Minimum printable line width:

$$L_\mathrm{w} = k_1 \frac{\lambda}{\mathrm{NA}} \tag{10.1}$$

where $k_1$ is a constant dominated by the optical system, but affected by pattern transfer processes.

Depth of focus:

$$\mathrm{DOF} = \pm k_2 \frac{\lambda}{(\mathrm{NA})^2} \tag{10.2}$$

Degree of partial coherence:

$$\sigma = \frac{\mathrm{NA}_\mathrm{cond}}{\mathrm{NA}_\mathrm{obj}} \tag{10.3}$$

where the subscript cond refers to the condenser or illumination optics, and obj refers to the objective lens of the reduction optics.

International Technology Road Map for Semiconductors

| | Years | | | |
|---|---|---|---|---|
| | 2005 | 2008 | 2011 | 2014 |
| 1:1 lines (nm) | 100 | 70 | 50 | 35 |
| Isolated lines (nm) | 65 | 45 | 30 | 20 |

http://www.sematech.org