Appendix B X-ray waves in media: further details

This appendix from www.cambridge.org/Jacobsen is an online extension of the book *X-ray Microscopy*. In it, we provide additional details on the refractive index for both visible light and for X rays, thus supplementing the discussion of Section 3.3.1 in the book.

One of the great triumphs of classical physics was the unification by Scottish physicist James Clerk Maxwell of several electromagnetic phenomena. However, the compact notation we have today for four equations isn't due to Maxwell, who had a set of 20 equations; our modern form of Maxwell's equations is actually the result of the self-taught Oliver Heaviside, who reformulated Maxwell's work using vector calculus [Hunt 1991a]. What might be called the Maxwell–Heaviside equations combine Faraday's law for how changing magnetic fields can induce voltages, Ampére's law for how currents and changing electric fields can produce magnetic fields, and Gauss' law for how electric charges produce electric fields (Gauss' law would also predict how magnetic monopoles, if they existed, would be expected to produce magnetic fields) into the following:

$$\text{Faraday: } \vec{\nabla} \times \vec{E} = -\frac{\partial \vec{B}}{\partial t} \tag{B.1}$$

$$\text{Ampère: } \vec{\nabla} \times \vec{B} = \mu_m(\vec{J} + \epsilon\frac{\partial \vec{E}}{\partial t}) \tag{B.2}$$

$$\text{Gauss (electric): } \vec{\nabla} \cdot \vec{E} = \frac{\rho}{\epsilon} \tag{B.3}$$

$$\text{Gauss (magnetic): } \vec{\nabla} \cdot \vec{B} = 0, \tag{B.4}$$

where $\vec{\nabla}\times$ is the *curl* and $\vec{\nabla}\cdot$ the *divergence*, ϵ is the electric permittivity, and μ_m is the magnetic permeability. In most cases of interest to us, the current density $\vec{J}$ is equal to an applied electric field $\vec{E}$ multiplied by the conductivity σ; this relationship is called Ohm's law, and you probably know it as $I = (1/R)V$. When Ohm's law applies, we can write Ampère's law as

$$\vec{\nabla} \times \vec{B} = \sigma\mu_m\vec{E} + \mu_m\epsilon\frac{\partial \vec{E}}{\partial t}, \tag{B.5}$$

though the electrical current term is not needed when considering dielectric media.

When an electric field is applied to a nonconducting material, some of the energy of the field can go into displacing electron orbitals slightly with respect to their nuclei, as was shown in Fig. 3.14. This leads to an average dipole moment per atom, or bulk polarization $\vec{P}$ of the material. For typical electric fields in most materials, this is related to the applied electric field E in a linear fashion, giving

$$\vec{P} = \epsilon_0 \chi_e \vec{E}, \tag{B.6}$$

involving the following parameters:

$$\text{permittivity of free space} \equiv \epsilon_0 = 8.85 \times 10^{-12}\ \mathrm{C}^2/\mathrm{N} \cdot \mathrm{m}^2 \tag{B.7}$$

$$\text{electric susceptibility} \equiv \chi_e \tag{B.8}$$

$$\text{permittivity} \equiv \epsilon = \epsilon_0(1 + \chi_e) \tag{B.9}$$

$$\text{dielectric constant} \equiv K = \epsilon/\epsilon_0 = (1 + \chi_e). \tag{B.10}$$

Dielectric constants are tabulated in a variety of places (see for example [Weast 1975]); gases tend to have values of $\chi_e \sim 10^{-3}$ while solids and liquids tend to have $\chi_e \sim 1$–8, though some materials have even larger values. At larger electric fields, the relationship between polarizability P and applied electric field E can become nonlinear, and eventually electric breakdown can occur.

When a magnetic field is applied to a material, it may affect the alignment of the magnetic dipole moments of individual nuclei. For non-ferromagnetic materials, the relationships between the magnetism M, the applied magnetic field B, and the auxiliary field H are:

$$\vec{M} = \chi_m \vec{H} \tag{B.11}$$

$$\vec{B} = \mu_0(\vec{H} + \vec{M}) = \mu_0(1 + \chi_m)\vec{H}, \tag{B.12}$$

involving the following parameters:

$$\text{magnetic susceptibility} \equiv \chi_m \tag{B.13}$$

$$\text{permeability} \equiv \mu_m = \mu_0(1 + \chi_m) \tag{B.14}$$

$$\text{permeability of free space} \equiv \mu_0 = 4\pi \times 10^{-7}\ \mathrm{N} \cdot \mathrm{C}^2/\mathrm{s}^2. \tag{B.15}$$

Note that $\chi_m < 0$ for diamagnetic materials (values of $\chi_m \approx -10^{-5}$ are common), and $\chi_m > 0$ for paramagnetic materials (values of 10^{-5} are common except for lanthanides, which have values more like 10^{-2}).

With these properties for nonconducting, electrostatically neutral, linear media in hand, the Maxwell–Heaviside equations can be manipulated [Griffiths 1989] to give wave equations for electric and magnetic fields:

$$\nabla^2 \vec{E} = \mu_m \epsilon \frac{\partial^2 \vec{E}}{\partial t^2} \tag{B.16}$$

$$\nabla^2 \vec{B} = \mu_m \epsilon \frac{\partial^2 \vec{B}}{\partial t^2} \tag{B.17}$$

This gives rise to a plane wave equation (Eq. 3.31) of

$$\vec{E} = \mathrm{Re}\left[\vec{E}_0 e^{-i(\vec{k}\cdot\vec{z} - \omega t)}\right] \tag{B.18}$$

for the electric field, with a similar expression for the magnetic field. If we insert this plane wave expression into the electric field wave equation (Eq. B.16), we find

$$k^2 = \mu_m \epsilon \omega^2. \tag{B.19}$$

for the relationship between the wave number k and the angular frequency ω.

We can now treat the propagation of electromagnetic waves in the material in a way similar to what we outlined for the driven, damped harmonic oscillator model described in Section 3.3 (see e.g., [Griffiths 1989, Sec. 9.4.3]). The sum of forces on an oscillation mode lead to an equation of motion for the oscillator [Griffiths 1989, c.f. Eq. 9.155] of

$$\begin{aligned} m_e \ddot{x} &= F_{\text{tot}} = F_{\text{binding}} + F_{\text{damping}} + F_{\text{driving}} \\ &= -m_e \omega_0^2 x - m_e \gamma \dot{x} + q\, E_0 e^{i\omega t}, \end{aligned} \tag{B.20}$$

which we see takes on the form shown in Eq. 3.47. In a steady state, the mode oscillates at the driving frequency, or

$$x(t) = \tilde{x} e^{i\omega t}, \tag{B.21}$$

where $\tilde{x}$ can be a complex number to allow for phase shifts. Inserting the expression of $x(t)$ from Eq. B.21 into Eq. B.20, we obtain

$$\begin{aligned} -m_e \omega^2 \tilde{x} e^{i\omega t} &= -m_e \omega_0^2 \tilde{x} e^{i\omega t} - i m_e \gamma \omega \tilde{x} e^{i\omega t} + q E_0 e^{i\omega t} \\ \tilde{x} m_e \left[(\omega_0^2 - \omega^2) + i\gamma\omega \right] &= q E_0 \\ \text{or } \tilde{x} &= \frac{q/m_e}{(\omega_0^2 - \omega^2) + i\gamma\omega} E_0. \end{aligned} \tag{B.22}$$

This displacement of the electron from its normal position relative to the positively charged nucleus leads to the atom having a small dipole moment (Fig. 3.14) of

$$\tilde{p}(t) = q\, x(t) = q \tilde{x} e^{i\omega t} = \frac{q^2/m_e}{(\omega_0^2 - \omega^2) + i\gamma\omega} E_0 e^{i\omega t}. \tag{B.23}$$

We can then go from a single oscillation mode's induced dipole moment to consider the volume polarization P. We will assume that an atom has a number of oscillation modes indexed by j, each with their own weighting g_j, resonance frequency ω_j, and damping coefficient γ_j. The complex volume polarization $\tilde{P}$ of the material is then given by [Griffiths 1989, Eq. 9.159]

$$\tilde{P} = \frac{n_a e^2}{m_e} \left(\sum_j \frac{g_j}{(\omega_j^2 - \omega^2) + i\gamma\omega} \right) E_0 e^{i\omega t}. \tag{B.24}$$

From this, we obtain a complex value for the electric susceptibility $\tilde{\chi}_e = \tilde{P}/(\epsilon_0 E_0)$ of

$$\tilde{\chi}_e = \frac{n_a e^2}{m_e \epsilon_0} \sum_j \frac{g_j}{(\omega_j^2 - \omega^2) + i\gamma_j \omega}, \tag{B.25}$$

where again ω is the driving frequency and ω_j represents the various oscillation mode resonance frequencies.

Let us return to our solution for the wave equation for plane electric waves. We found in Eq. B.19 that the wave vector k could be expressed as $k = \sqrt{\mu_m \epsilon}\,\omega$. We now define the index of refraction n as the ratio of the wave vector in our medium relative to the wave vector in free space, or

$$n \equiv \frac{k}{k_0} = \frac{\sqrt{\mu_m \epsilon}\,\omega}{\sqrt{\mu_0 \epsilon_0}\,\omega} = \sqrt{(1+\chi_m)(1+\chi_e)}, \tag{B.26}$$

where we have used $\epsilon = \epsilon_0(1+\chi_e)$ from Eq. B.9, and $\mu_m = \mu_0(1+\chi_m)$ from Eq. B.14. Since we saw in the discussion below Eq. B.14 that χ_m tends to be $\lesssim 10^{-4}$ for many materials, and in Section B.3 we saw that the magnetic fields associated with electromagnetic waves are weak, we'll drop the χ_m term. Even though we also saw that static electric field values of χ_e can be in the range 1–8 for many solids, for electromagnetic waves there is a weaker response so we'll assume that we can make the approximation $(1+\chi_e)^{-1/2} \simeq 1-\chi_e/2$. We can then go from Eqs. B.25 and B.26 to find [Griffiths 1989, Eq. 9.170]

$$\begin{aligned} n &= 1 + \frac{n_a e^2}{2m_e \epsilon_0} \sum_j \frac{g_j}{(\omega_j^2 - \omega^2) + i\gamma_j\omega} \\ &= 1 - \frac{n_a e^2}{2m_e \epsilon_0} \sum_j \frac{g_j}{(\omega_j^2 - \omega^2)^2 + \gamma_j^2\omega^2} \left[(\omega^2 - \omega_j^2) + i\gamma_j\omega\right], \end{aligned} \tag{B.27}$$

where in the second line (Eq. B.27, which is the same as Eq. 3.60) we have multiplied top and bottom by $(\omega_j^2 - \omega^2) - i\gamma_j\omega$. From this, we can separate the refractive index into real and imaginary parts:

$$\mathrm{Re}[n] = 1 - \frac{n_a e^2}{2m_e \epsilon_0} \sum_j \frac{(\omega^2 - \omega_j^2)\, g_j}{(\omega_j^2 - \omega^2)^2 + \gamma_j^2\omega^2} \tag{B.28}$$

$$\mathrm{Im}[n] = -\frac{n_a e^2}{2m_e \epsilon_0} \sum_j \frac{\gamma_j\omega\, g_j}{(\omega_j^2 - \omega^2)^2 + \gamma_j^2\omega^2}. \tag{B.29}$$

The real and imaginary parts impart separate effects on a wavefield ψ:

$$\begin{aligned} \psi(\vec{x},t) &= \psi_0 \exp[-i(n\vec{k_0}\cdot\vec{x} - \omega t)] \\ &= \psi_0 \exp[-i(\vec{k_0}\cdot\vec{x} - \omega t)] \cdot \\ &\qquad \exp[-i\,\mathrm{Re}[n-1]\,\vec{k_0}\cdot\vec{x}]\,\exp[\mathrm{Im}[n]\,\vec{k_0}\cdot\vec{x}]. \end{aligned} \tag{B.30}$$

That is, the real part of the refractive index Re$[n-1]$ describes the phase change of a wave propagating through the medium relative to vacuum, while the imaginary part Im$[n]$ describes attenuation or amplification of the wave.

B.1 The low-frequency limit: the visible-light refractive index

In Section 3.3.2 we described a rather important property of the optical response of materials: plasmon excitations set the great dividing line between the low- and high-frequency forms of the general refractive index expressions of Eq. B.28 and B.29. Let us then consider the term $(\omega_j^2 - \omega^2)$ in the limit that the driving frequency ω is well below the frequency of the preponderance of oscillation modes in the material, or $\omega \ll \omega_j$. In this case, the driving-frequency-dependent damping forces of $m_e \gamma \dot{x}$ (Eq. B.20) are small because ω^2 is small, so we can write

$$\frac{1}{(\omega_j^2 - \omega^2)} = \frac{1}{\omega_j^2}\left(1 - \frac{\omega^2}{\omega_j^2}\right)^{-1} \simeq \frac{1}{\omega_j^2}\left(1 + \frac{\omega^2}{\omega_j^2}\right). \tag{B.31}$$

We can then write the expression from Eq. B.28 of Re[n] as [Griffiths 1989, Eq. 9.173]

$$\mathrm{Re}[n] \simeq 1 + \left(\frac{n_a e^2}{2 m_e \epsilon_0} \sum_j \frac{g_j}{\omega_j^2}\right) + \omega^2 \left(\frac{n_a e^2}{2 m_e \epsilon_0} \sum_j \frac{g_j}{\omega_j^4}\right), \tag{B.32}$$

which is Eq. 3.61, and which (as noted in Eq. 3.62) can be written as $n = 1 + A(1 + B/\lambda^2)$ or alternatively as $n = 1 + A + C\omega^2$. This leads to a phase velocity of

$$v_p \equiv \frac{\omega}{k} = \frac{c}{n} = \frac{c}{1 + A + C\omega^2}, \tag{B.33}$$

which, for positive A and C, clearly leads to a phase velocity that is below c (see also the Cauchy form in Eq. 3.62). The group velocity is defined as

$$v_g \equiv \frac{d\omega}{dk}. \tag{B.34}$$

From Eq. 3.56 we have $\omega/k = n/c$, which we can rearrange as $\omega c = nk$ and differentiate:

$$\begin{aligned} d[\omega\, n(\omega)] &= d[ck] \\ d\omega \cdot n(\omega) + \omega \cdot d[n(\omega)] &= c\, dk \\ d\omega \cdot n(\omega) + d\omega \cdot \omega \cdot \frac{d[n(\omega)]}{d\omega} &= c\, dk \\ d\omega\Big[n(\omega) + \omega \frac{dn(\omega)}{d\omega}\Big] &= c\, dk \\ \frac{d\omega}{dk} &= \frac{c}{n(\omega) + \omega \frac{dn(\omega)}{d\omega}}. \end{aligned} \tag{B.35}$$

This lets us calculate the group velocity v_g using

$$v_g \equiv \frac{d\omega}{dk} = \frac{c}{n(\omega) + \omega \frac{dn(\omega)}{d\omega}}. \tag{B.36}$$

We can then use $d[1 + A + C\omega^2] = 2C\omega$ for $dn(\omega)/d\omega$ to find the group velocity for visible light to be

$$v_g \equiv \frac{d\omega}{dk} = \frac{c}{n(\omega) + \omega \frac{dn(\omega)}{d\omega}} = \frac{c}{(1 + A + C\omega^2) + \omega(2C\omega)}, \tag{B.37}$$

which again is less than c. Thus we conclude that both the phase and group velocities for visible light in refractive media are below the speed of light c in vacuum.

B.2 The high-frequency limit: the x-ray refractive index

We have seen above that the refractive index expression we have derived yields the expected results for visible light in the low-frequency limit. However, we wish to cross the great plasmon frequency divide and reach the promised land of the high-frequency limit, which is flowing with milk, honey, and X rays!

We therefore return to the refractive index expression of Eq. B.27, and consider its form with low damping $\gamma_j \to 0$ and at high driving frequencies ω well beyond most resonant frequencies ω_j, or $\omega_j^2 \ll \omega^2$ (since most ω_j frequencies are near the plasmon frequency, or at ~30 eV photon energies). We can then reduce Eq. B.27 as follows:

$$\begin{aligned} n &= 1 - \frac{n_a e^2}{2m_e\epsilon_0}\sum_j \frac{g_j}{(\omega^2-\omega_j^2)^2+\gamma_j^2\omega^2}\left[(\omega^2-\omega_j^2)+i\gamma_j\omega\right] \\ &\simeq 1 - \frac{n_a e^2}{2m_e\epsilon_0}\frac{1}{\omega^2}\sum_j g_j\,(1+i\gamma_j/\omega), \end{aligned} \tag{B.38}$$

Now $\omega = 2\pi c/\lambda$, and the classical radius of the electron in SI units is

$$r_e \equiv \frac{1}{4\pi\epsilon_0}\frac{e^2}{m_e c^2} = 2.818\times10^{-15}\ \text{m}. \tag{B.39}$$

We also can define

$$\alpha \equiv \frac{r_e}{2\pi}n_a \tag{B.40}$$

so Eq. B.38 can be written as

$$n \simeq 1 - \alpha\lambda^2(f_1 + if_2), \tag{B.41}$$

which is Eq. 3.65. In arriving at this, we have used

$$f_1 + if_2 = \sum_j g_j\,(1 + i\frac{\gamma_j}{2\pi c}\lambda). \tag{B.42}$$

We therefore see that Eq. B.41 reproduces Eq. 3.65. Now the sum of all oscillation modes should tend toward the number of electrons, or $\sum_j g_j \to Z$, and we also see from Eq. B.42 that the imaginary part f_2 should decline relative to the real part at least as steeply as the inverse of x-ray energy. We thus have a good basis for expecting

$$f_1 \to Z, \tag{B.43}$$

and f_2 declining at higher energies relative to f_1, which is the behavior seen in Fig. 3.16 (leading to the linear absorption coefficient scaling with energy of Eq. 3.77).

The phase velocity of X rays in media is found using Eq. 3.56 of $v_p = c/n$ to be

$$v_p = \frac{c}{1-\delta} = c(1-\delta)^1 \simeq c(1+\delta), \tag{B.44}$$

where we have used the binomial expansion; this gives Eq. 3.72. The group velocity v_g expression of Eq. B.36 can be calculated using $\tilde{f} = (f_1 + if_2)$ and

$$\frac{dn}{d\omega} = \frac{d[1-\alpha'\tilde{f}\omega^{-2}]}{d\omega} = +2\alpha'\tilde{f}\omega^{-3}, \tag{B.45}$$

to arrive at

$$\begin{aligned} v_g &= \frac{c}{n(\omega) + \omega\dfrac{dn(\omega)}{d\omega}} = \frac{c}{(1-\alpha'\tilde{f}\omega^{-2}) + \omega(+2\alpha'\tilde{f}\omega^{-3})} \\ &= \frac{c}{1+\alpha'\tilde{f}\omega^{-2}} \\ &\simeq c(1-\alpha'\tilde{f}\omega^{-2}) \\ \text{or } v_g &= \simeq c(1-\delta), \end{aligned} \tag{B.46}$$

where in the last step we use Eq. 3.69 and the fact that $f_2 \ll f_1$ at higher x-ray energies. This is how we arrive at the result shown in Eq. 3.73. We therefore see (to our relief!) that the group velocity for X rays traveling in media is less than the speed of light, even though the phase velocity is greater than c. One must imagine that Einstein must have realized this even though he didn't comment on it [Einstein 1918], as noted above Eq. 3.73.

B.3 Electric and magnetic field strength

Since electromagnetic wave propagation depends on electric and magnetic material properties, how big are the electric and magnetic fields? Let's consider the mean electric $\langle E\rangle$ and magnetic $\langle B\rangle$ field values produced by a monochromatic beam with an irradiance of $I_E = 6\times10^7$ W/m^2 (this corresponds to a 5 mW visible-light laser beam focused to a 10 μm spot, or a flux of $\Phi = 10^{10}$ photons/s of 300 eV soft X rays focused into a 100 nm spot). The resulting mean field values are given by the Poynting vector as

$$\langle E\rangle = (\tfrac{\mu_m}{\epsilon})^{1/4}\ \sqrt{I_E} = 1.5\times10^5 \text{ volts/m} \tag{B.47}$$

$$\langle B\rangle = (\mu_m^3\epsilon)^{1/4}\ \sqrt{I_E} = 5.0\times10^{-4} \text{ tesla.} \tag{B.48}$$

Thus, we see that the electric field is rather high (air sparks under a static field of about 8×10^5 V/m), while the magnetic field is rather small (only 50 times greater than that of the Earth), which leads us to predict that the dielectric constants of materials will dominate their optical properties. (Only in the case of magnetic circular dichroism do magnetic effects become significant in x-ray interactions; this was discussed in Section 9.1.4.) While $\langle E\rangle$ will usually have more of an effect than $\langle B\rangle$ in electromagnetic wave propagation, the $\langle E\rangle$ field is still relatively gentle. Consider the electric field within an atom, where we have electrons bound by energies of ~10 eV and atoms of size ~0.1 nm; this gives $\langle E\rangle \simeq 10^{11}$ V/m. At the lower intensities of interest to us, the fact that the electric field is relatively weak means that most materials respond linearly (rather than nonlinearly) to electromagnetic waves, thus justifying our assumption of linearity in $\vec{P} = \epsilon_0\chi_e\vec{E}$.