

## 2.0 Maxwell's equations

This section presents a short review of Maxwell's equations and the wave equation. It is not intended to be a complete tutorial on the subject.

We start with understanding absorption with the classical harmonic oscillator model. Then, we list Maxwell's equations for absorbing media and derive the associated wave equation for dielectrics. The free-space wave equation is presented next. We conclude by discussing the frequency dependence of the refractive index, absorption and power flow.

### 2.1 Absorption

A classical description of absorption is the Lorentz model of molecular charge. Consider the charge distribution as shown in Figure 2.1, where an applied electric field  $U_0$  produces a dipole moment  $d$  from the positive and negative charge distribution. The positive charge is from the material nuclei, and the negative charge is from material electrons. At optical frequencies, separation of the charges results from the force of the applied field on either the ionic bonds, like with NaCl, or the electron cloud itself, like with Si and Ge. The induced dipole moment leads to a bound charge distribution in the material and the resulting *polarization*  $P = \gamma e x$ .

$P$  is determined by the displacement  $x$ , which in turn is governed by the forces acting on the charge distribution. Figure 2.1 shows a simple free-body diagram of a harmonic oscillator, where the positively charged nucleus is essentially at rest. Negatively charged electrons with mass  $m_e$  are bound to the nucleus by a spring with restoring force constant  $m_e \omega_0^2$ , a damper with restoring force constant  $2\xi m_e$ . The harmonic oscillator equation of motion for displacement  $x$  is

$$\frac{\partial^2 x}{\partial t^2} + \xi \frac{\partial x}{\partial t} + \omega_0^2 x = -U_0(t) / m_e \quad , (2.1)$$

where  $\xi$  is the damping constant,  $m_e$  is the electron mass,  $\omega = 2\pi c/\lambda$  is the radian frequency of the photon at wavelength  $\lambda$ ,  $\omega_0$  is the resonant radian frequency and  $e$  is the electronic charge. The solution of Eq. (2.1) is

$$x(t) = \frac{e^{-U_0(t) / m_e}}{(\omega_0^2 - \omega^2) + j\omega\xi} \quad . (2.2)$$

Equation (2.2) shows that  $P(t) = \gamma e x(t)$  is directly proportional to the applied electric field

$$P(t) = \gamma e^{-x(t)} = \frac{\gamma (e^-)^2 U_0(t) / m_e}{(\omega_0^2 - \omega^2) + j\omega\xi} = \gamma\zeta U_0(t) \quad , (2.3)$$

where  $\gamma$  is the concentration of molecules per cubic meter and

$$\zeta = \frac{(e^-)^2 / m_e}{(\omega_0^2 - \omega^2) + j\omega\xi} \quad (2.4)$$

is the *molecular polarizability* of the material. Dipoles generated from  $e_0(t)$  exhibit their own electric field in the material. The electric field generated inside the material from the ensemble of dipoles is  $NP(t)/\epsilon_0$ , where  $\epsilon_0$  is the permittivity of free space and  $N$  is a constant between 0 and 1.<sup>1</sup> The total electric field inside the material is then

$$U(t) = U_0(t) - NP(t) / \epsilon_0 \quad . (2.5)$$

Combination of Eqs. (2.3) and (2.5) produce

$$P(t) = \frac{\epsilon_0 \gamma \zeta}{\epsilon_0 - N \gamma \zeta} U(t) = \epsilon_0 \chi U(t) \quad , (2.6)$$

where  $\chi$  is the *linear dielectric susceptibility* of the material. Application of Gauss's Law results in definition of the *dielectric displacement*  $D$  such that

$$D(t) = \epsilon_0 U(t) + P(t) = \epsilon_0 (1 + \chi) U(t) = \epsilon_0 \epsilon_r U(t) \quad , (2.7)$$

where  $\epsilon_r$  is the *relative dielectric constant* of the material.

## 2.2 Application of absorption to Maxwell's equations

The effects of  $P(t)$  must be included in Maxwell's equations for a complete description of the field. For  $B(t) = \mu_0 H(t)$  and isotropic material,

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<sup>1</sup> C. Kittel, An Introduction to Solid State Physics, John Wiley and Sons, New York, (1976), p. 404.

$$\nabla \times \mathbf{U}(\mathbf{r}, t) = -\frac{\partial \mathbf{B}(\mathbf{r}, t)}{\partial t} = -\mu_0 \frac{\partial \mathbf{H}(\mathbf{r}, t)}{\partial t} \quad , (2.8)$$

$$\begin{aligned} \nabla \times \mathbf{H}(\mathbf{r}, t) &= \mathbf{J}(\mathbf{r}, t) + \frac{\partial \mathbf{D}(\mathbf{r}, t)}{\partial t} = \sigma \mathbf{U}(\mathbf{r}, t) + \varepsilon_0 \frac{\partial \mathbf{U}(\mathbf{r}, t)}{\partial t} + \frac{\partial \mathbf{P}(\mathbf{r}, t)}{\partial t} \\ &= \sigma \mathbf{U}(\mathbf{r}, t) + \varepsilon_0 (1 + \chi) \frac{\partial \mathbf{U}(\mathbf{r}, t)}{\partial t} \quad , \end{aligned} \quad (2.9)$$

$$\nabla \cdot \mathbf{D}(\mathbf{r}, t) = 0 \quad , \text{ and (2.10)}$$

$$\nabla \cdot \mathbf{B}(\mathbf{r}, t) = 0 \quad , (2.11)$$

where the spatial dependence  $\mathbf{r}$  is specifically included,  $\sigma$  is the conductivity of the homogeneous and source-free material and the variables represent macroscopic values inside the material.

### 2.3 The wave equation in absorbing media

Combination of Eqs. (2.8) and (2.9) yields the wave equation

$$\nabla \times \nabla \times \mathbf{U}(\mathbf{r}, t) = -\mu_0 \frac{\partial}{\partial t} \nabla \times \mathbf{H}(\mathbf{r}, t) = -\mu_0 \frac{\partial}{\partial t} \left[ \sigma \mathbf{U}(\mathbf{r}, t) + \varepsilon_0 (1 + \chi) \frac{\partial \mathbf{U}(\mathbf{r}, t)}{\partial t} \right] \quad . (2.12)$$

Application of the identity  $\nabla \times \nabla \times \mathbf{U} = \nabla(\nabla \cdot \mathbf{U}) - \nabla^2 \mathbf{U}$  yields

$$\begin{aligned} \nabla[\nabla \cdot \mathbf{U}(\mathbf{r}, t)] - \nabla^2 \mathbf{U}(\mathbf{r}, t) &= -\mu_0 \left[ \sigma \frac{\partial \mathbf{U}(\mathbf{r}, t)}{\partial t} + \varepsilon_0 (1 + \chi) \frac{\partial^2 \mathbf{U}(\mathbf{r}, t)}{\partial t^2} \right] \\ &= -\mu_0 \varepsilon_0 \left[ \frac{\sigma}{\varepsilon_0} \frac{\partial \mathbf{U}(\mathbf{r}, t)}{\partial t} + (1 + \chi) \frac{\partial^2 \mathbf{U}(\mathbf{r}, t)}{\partial t^2} \right] \quad . \end{aligned} \quad (2.13)$$

For  $\nabla \cdot \mathbf{U}(\mathbf{r}, t) = 0$ ,

$$\begin{aligned} -\nabla^2 \mathbf{U}(\mathbf{r}, t) &= -\mu_0 \varepsilon_0 \left[ \frac{\sigma}{\varepsilon_0} \frac{\partial \mathbf{U}(\mathbf{r}, t)}{\partial t} + (1 + \chi) \frac{\partial^2 \mathbf{U}(\mathbf{r}, t)}{\partial t^2} \right] \\ &= -\frac{1}{c^2} \left[ \frac{\sigma}{\varepsilon_0} \frac{\partial \mathbf{U}(\mathbf{r}, t)}{\partial t} + (1 + \chi) \frac{\partial^2 \mathbf{U}(\mathbf{r}, t)}{\partial t^2} \right] \quad , \end{aligned} \quad (2.14)$$

where  $c = 3 \times 10^8$  is the speed of light in a vacuum. For harmonic fields of the form  $\mathbf{U}(\mathbf{r}, t) = \mathbf{A}(\mathbf{r}, t) \exp(-j\omega t)$ ,

$$\begin{aligned} \nabla^2 \mathbf{U}(\mathbf{r}, t) + \frac{1}{c^2} \left[ \frac{\sigma}{\epsilon_0} (-j\omega) + (1 + \chi) \omega^2 \right] \mathbf{U}(\mathbf{r}, t) &= 0 \\ \nabla^2 \mathbf{U}(\mathbf{r}, t) + \frac{\omega^2}{c^2} \left[ (1 + \chi) - \frac{j\sigma}{\epsilon_0 \omega} \right] \mathbf{U}(\mathbf{r}, t) &= 0 \quad (2.15) \\ \nabla^2 \mathbf{U}(\mathbf{r}, t) + \frac{\omega^2 \epsilon_r}{c^2} \mathbf{U}(\mathbf{r}, t) &= 0 \quad . \end{aligned}$$

Notice that  $\epsilon_r$  now includes effects of the finite conductivity. If the electric field is of the form  $U(z, t) = A \exp[j(kz - \omega t)]$ ,  $\nabla^2 U(z, t) = -k^2 U(z, t)$ , and

$$k = k_r + k_i j = \frac{2\pi}{\lambda} \sqrt{\epsilon_r} \quad . (2.16)$$

Normally,  $k_r$  and  $k_i$  are written as

$$k_r = \frac{2\pi n}{\lambda} \quad , (2.17)$$

and

$$k_i = 2\pi \kappa / \lambda = \alpha / 2 \quad . (2.18)$$

The electric field in the material is

$$U(z, t) = A_0 \exp(-\alpha z / 2) \exp \left[ j \left( \frac{2\pi n}{\lambda} z - \omega t \right) \right] \quad , (2.19)$$

and

$$I(z) = \frac{1}{2} c \epsilon_0 n A_0^2 \exp(-\alpha z) \quad \text{Wm}^{-2}, (2.20)$$

where  $I(z)$  is the irradiance. Equation (2.20) shows that the irradiance exponentially decays with increasing  $z$ . Physically, photons are absorbed starting at the top surface ( $z = 0$ ) of the material. The change in irradiance  $\Delta I$  due to single-photon absorption as the beam passes through a thin slice  $\Delta z$  of material is given by Beer's law

$$\frac{\Delta I}{\Delta z} = -\alpha I \quad , (2.21)$$

where  $\alpha$  is the *linear absorption coefficient*. Irradiance decreases through  $\Delta z$  proportionally to the incident irradiance  $I$  and  $\alpha$ . Note that, with  $\sigma_s = 0$ , the real and imaginary parts of  $\epsilon_r$  determine  $\alpha$  and  $n$ . For example, if  $\epsilon_r$  is real and positive,  $\alpha = 0$ , and there is no absorption.

## 2.4 Free space wave equation

In free space,  $P = 0$ ,  $\nabla \cdot \mathbf{U}(\mathbf{r}, t) = 0$ ,  $\epsilon_r = 1$  and Maxwell's equations become:

$$\nabla \times \mathbf{U}(\mathbf{r}, t) = -\mu_0 \frac{\partial \mathbf{H}(\mathbf{r}, t)}{\partial t}, \quad (2.22)$$

$$\nabla \times \mathbf{H}(\mathbf{r}, t) = \epsilon_0 \mathbf{U}(\mathbf{r}, t), \quad (2.23)$$

$$\nabla \cdot \mathbf{D}(\mathbf{r}, t) = 0, \quad (2.24)$$

$$\nabla \cdot \mathbf{B}(\mathbf{r}, t) = 0, \quad (2.25)$$

Through application of the identity  $\nabla \times \nabla \times \mathbf{U} = \nabla(\nabla \cdot \mathbf{U}) - \nabla^2 \mathbf{U}$ , the wave equation becomes

$$\nabla^2 \mathbf{U}(\mathbf{r}, t) - \frac{1}{c^2} \frac{\partial^2 \mathbf{U}(\mathbf{r}, t)}{\partial t^2} = 0. \quad (2.26)$$

## 2.5 Single-photon absorption: The band model

The absorption process can also be thought of in terms of an energy-level diagram. The energy-level diagram is convenient, because it leads to a more complete understanding of the absorption process through the application of quantum physics. Figure 2.2 shows the energy level diagram between two states. The lower state is partially filled with carriers. The upper state is mostly empty. A single photon of enough energy can excite a carrier (either an electron or a hole) from the lower level to the upper level. Energy from the photon is passed from the photon into the material, and the photon is annihilated. In order to bridge the energy gap between the lower and upper energy state, the single-photon energy  $E_p = \hbar\omega$  must be equal to or greater than the energy gap  $E_g = \hbar\omega_{01}$ . That is,  $E_p \geq E_g$ . When the photon is extinguished in this way, we say that the photon is *absorbed*. If the photon energy is such that  $E_p \leq E_g$ , the photon passes through the material. If the material can be described as a collection of independent molecules with concentration  $\gamma$  molecules per cubic meter,  $\alpha$  is proportional to the *molecular linear absorption cross section*  $\sigma_{01}$  as<sup>2</sup>

<sup>2</sup> M. Schubert and B. Wilhelm, Nonlinear Optics and Quantum Electronics, John Wiley and Sons, New York, 1986.

$$\alpha = \sigma_{01}\gamma = \frac{|d_{01}|^2 \pi \omega_{10} \gamma}{nc\epsilon_0 \hbar} g_L(\omega - \omega_{10}) \quad \text{m}^{-1}, \quad (2.27)$$

where  $\omega = 2\pi c/\lambda$  is the radian frequency of the photon at wavelength  $\lambda$ ,  $\omega_{10} = E_g/\hbar$  is the resonant radian frequency associated with the gap,  $\hbar$  is Planck's constant,  $n$  is the refractive index,  $\epsilon_0$  is the permittivity of free space,  $c$  is the speed of light in a vacuum,  $d_{01}$  is the dipole moment and  $g_L$  is the line shape function given by

$$g_L(\omega - \omega_{10}) = \frac{1}{\pi} \frac{1/\tau_{10}}{(\omega - \omega_{10})^2 + 1/\tau_{10}^2}, \quad (2.28)$$

where  $\tau_{10}$  is the relaxation time.

## 2.6 Frequency dependence of the refractive index and absorption

Note that  $\alpha$  in both Eqs. (2.17) and (2.22) is a function of the photon frequency  $\omega$ . The basic functional dependence can be described with either the Lorentz molecule or the band-energy diagram. However, the band-energy diagram is more useful with real materials where multiple resonances are found. Examples of the index of refraction and absorption for BK7, a common optical glass, are shown on Fig. 2.3. Note the increase in absorption, which is shown as a decrease in transmission, and the increase in refractive index near the ultraviolet resonance.

## 2.7 Power flow and the Poynting vector

The units of electric field strength  $U$  are volts/meter, and the units of magnetic field strength  $H$  are amps/meter. Thus the product ( $U$  times  $H$ ) has units (volts amps)/(square meter) or watts per square meter. A quantity having these units is called a "power flux density". Since electromagnetic waves have  $U$  and  $H$  fields perpendicular to the direction of propagation, the Poynting vector  $\mathbf{S} = \mathbf{U} \times \mathbf{H}$  determines the direction of power flow. (For materials like uniaxial crystals, this discussion must be modified. However, we will not consider it further for this class.)