Lorentz Oscillator Model of the Dielectric Function

by Dr. Colton, Physics 581 (last updated: Fall 2020)

Introduction: the dielectric function

The dielectric constant of a material, ϵ_r, also called the *relative permittivity*, describes how electric fields get partially screened inside dielectric materials. In general the applied electric fields could be oscillating (e.g. from electromagnetic waves), and the amount of screening will depend on the frequency of oscillation ω, making $\epsilon_r(\omega)$ more properly referred to as the *dielectric function* rather than a dielectric constant. The low frequency value can be written as $\epsilon_r(0)$ and the high frequency limit written as $\epsilon_r(\infty)$. Note that Kittel leaves off the subscript r's on all of these terms and just writes $\epsilon(\omega)$. That's a little non-standard; usually ϵ means the product $\epsilon_0\epsilon_r$.

On an atomic level, the screening occurs because bound electrons move a little bit in response to the fields to create an atomic dipole. If we assume there are N induced dipoles per volume in the material,[1] each possessing *dipole moment* **p**, then the dielectric function relates to the dipole moment through these equations:

$$\mathbf{P} = N\mathbf{p} \tag{1}$$

$$\mathbf{P} = \epsilon_0 \chi_e \mathbf{E} \tag{2}$$

$$\epsilon_r = 1 + \chi_e \tag{3}$$

P is the *polarization function*, describing the net dipole moment per volume, which could potentially vary with position (but we will assume it doesn't). χ_e is the *electric susceptibility* and like ϵ_r, it varies with ω. Eq. 1 is essentially the definition of the polarization function. Eq. 2 is one of the *constitutive equations* for linear isotropic dielectrics, which are the only type of dielectrics we'll consider here. Eq. 3 is the standard relationship between the susceptibility and the dielectric function.

Eqs. 1-3 can be combined to describe how the dielectric function depends on the atomic dipole moment p:

$$\epsilon_r = 1 + \frac{Np}{\epsilon_0 E} \tag{4}$$

As a separate matter, the dielectric function relates to the *index of refraction* n via:

$$n = \sqrt{\epsilon_r} \tag{5}$$

If there is a phase shift between a sinusoidal electric field and the polarization response described by Eq. 2, then we treat that mathematically by representing sine waves as complex exponentials and making χ_e a complex function. That in turn also makes both ϵ_r and n complex functions, through Eqs. 3 and 5.

For reasons that are beyond the scope of this handout, the real part of n governs refraction as per Snell's law, and the imaginary part of n (often labeled k, not to be confused with the wave vector k) governs absorption. I like the convention used by some authors to put a tilde above a variable to expressly indicate when quantities are complex, e.g. $\tilde{\epsilon}_r$ or $\tilde{n}$, but although I will do that frequently in this handout, I will likely not be 100% consistent. Both $\epsilon_r(\omega)$ and $\tilde{\epsilon}_r(\omega)$ refer to the same thing, namely the complex dielectric function.

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[1] I'm using N instead of n because n is used in Eq. 5 and beyond for the index of refraction.

Reflection at a boundary between two materials is governed by the *Fresnel equations*, which for normal incidence (i.e. light waves striking perpendicularly to the surface) at an air-solid boundary give us:

$$R = \left|\frac{n-1}{n+1}\right|^2 \tag{6}$$

where R is the reflectivity, namely the fraction of the optical power that is reflected, and we've approximated the index of refraction of air as 1. Here the *complex* index of refraction of the material must be used whenever the imaginary part of n is significant.

We will develop a model for $\epsilon_r(\omega)$ using Eq. 4, then will use the developed $\epsilon_r(\omega)$ function in Eqs. 5 and 6 to compare with experimental results of the reflectivity for several situations.

The Lorentz oscillator model

The Lorentz oscillator model, also known as the Drude-Lorentz oscillator model, involves modeling an electron as a driven damped harmonic oscillator. In this model the electron is connected to the nucleus via a hypothetical spring with spring constant C. The driving force is the oscillating electric field. An oscillating applied field gives rise to an oscillating dipole moment which (as we will see) is proportional to the field. We can then use that proportionality ratio p/E in Eq. 4 to yield an equation for $\epsilon_r(\omega)$.

The dipole moment of a pair of opposite charges is $p = q \times \text{separation distance}$. If we assume the nucleus to be stationary, the separation distance is equal to the position of the electron, x. We will use Newton's Second Law to obtain the position of the electron as a function of time.

Let's say the driving oscillating electric field at the location of the atom is $E = E_0 \cos(\omega t)$, which I will write as $\cos(-\omega t)$ so that it matches time dependence of a standard traveling EM wave, namely $\cos(kx - \omega t)$. As is standard, we will say that the damping force is proportional to the velocity, and is described by damping coefficient γ (units of γ chosen such that force $= \gamma m v$). The source of the damping force is not specified, but must be present so that the oscillations don't go infinite when the driving force is at the resonant frequency. Proceeding with Newton's Second Law, we have:

$$F_{net} = m\frac{d^2x}{dt^2}$$

$$F_{driving} + F_{spring} + F_{damping} = m\frac{d^2x}{dt^2}$$

$$qE_0\cos(-\omega t) - Cx - \gamma m\frac{dx}{dt} - m\frac{d^2x}{dt^2}$$

$$\frac{d^2x}{dt^2} + \gamma\frac{dx}{dt} + \frac{C}{m}x = \frac{qE_0}{m}\cos(-\omega t)$$

Let $\omega_0 = \sqrt{C/m}$ for notation (the spring's resonant frequency).

$$\frac{d^2x}{dt^2} + \gamma\frac{dx}{dt} + \omega_0^2 x = \frac{qE_0}{m}\cos(-\omega t) \tag{7}$$

Eq. 7 is therefore the driven damped harmonic equation of motion we need to solve. To solve it we'll use the physicist's favorite trick, which is to guess the form of the answer and plug it into the equation.

Guess $x = x_0 \cos(-\omega t + \phi)$ as solution → $\tilde{x} = x_0 e^{i\phi} e^{-i\omega t}$ in complex notation

$\tilde{x} = \tilde{x}_0 e^{-i\omega t}$ (the phase ϕ is lumped in with complex $\tilde{x}_0$)

Derivatives:

$$\frac{d\tilde{x}}{dt} = (-i\omega)\tilde{x}_0 e^{-i\omega t}$$

$$\frac{d^2\tilde{x}}{dt^2} = (-i\omega)^2\tilde{x}_0 e^{-i\omega t}$$

Plug into Eq. 7; also convert cosine into a complex exponential:

$$(-i\omega)^2\tilde{x}_0 e^{-i\omega t} + \gamma(-i\omega)\tilde{x}_0 e^{-i\omega t} + \omega_0^2\tilde{x}_0 e^{-i\omega t} = \frac{qE_0}{m} e^{-i\omega t}$$

Cancel the $e^{-i\omega t}$ factors:

$$\tilde{x}_0(-\omega^2 - i\omega\gamma + \omega_0^2) = \frac{qE_0}{m}$$

$$\tilde{x}_0 = \frac{qE_0}{m} \frac{1}{\omega_0^2 - \omega^2 - i\omega\gamma}$$

This is the amplitude of oscillation. The fact that it is complex just means there is a phase shift between the driving electric field and the response of the electron's motion. With the explicit time dependence added back in, we have:

$$\tilde{x} = \frac{qE_0}{m} \frac{1}{\omega_0^2 - \omega^2 - i\omega\gamma} e^{-i\omega t}$$

Therefore the oscillating dipole moment is:

$$\begin{aligned} \tilde{p} &= q\tilde{x} \\ &= \frac{q^2}{m} \frac{1}{\omega_0^2 - \omega^2 - i\omega\gamma} E_0 e^{-i\omega t} \\ &= \frac{q^2}{m} \frac{1}{\omega_0^2 - \omega^2 - i\omega\gamma} \tilde{E} \end{aligned}$$

Plugging in the ratio of p to E into Eq. 4, we arrive at the essential result of this model:

$$\epsilon_r = 1 + \frac{Nq^2}{m\epsilon_0} \frac{1}{\omega_0^2 - \omega^2 - i\omega\gamma}$$

The quantity $\frac{Nq^2}{m\epsilon_0}$ has units of frequency squared, and its square root is called the *plasma frequency* because it happens to also be the frequency a plasma will naturally oscillate at if the positive and negative charges in the plasma are offset from each other. Therefore

$$\omega_p = \sqrt{\frac{Nq^2}{m\epsilon_0}}$$

We can now write the dielectric function in a nice compact form to conclude this model:

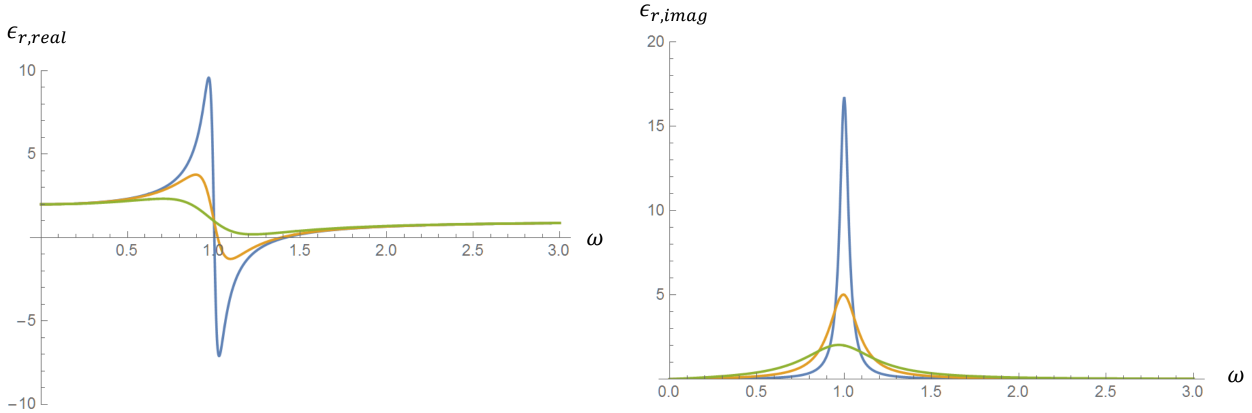
$$\boxed{\epsilon_r(\omega) = 1 + \frac{\omega_p^2}{\omega_0^2 - \omega^2 - i\omega\gamma}} \tag{8}$$

Note that even in this fairly straightforward model we arrived at a *complex* dielectric function, which leads to a complex index of refraction, which as stated above gives rise to refraction, absorption, and reflection. And more than that, it also predicts that the dielectric function (and hence index of refraction) will have frequency dependence: there is *dispersion*.

In situations where you have different types of electrons, e.g. electrons bound to different types of atoms, Eq. 8 can be modified to become a summation, with each term weighted by what is called the *oscillator strength* of the particular resonance. But I won't do that here.

Plots of the dielectric function

Here's what the real and imaginary parts of Eq. 8 look like as a function of ω, plotted with $\omega_p = \omega_0 = 1$ for simplicity; each of the two plots includes three values of γ: 0.06, 0.2, and 0.5. As the damping decreases, the peaks get narrower and taller.



Colton plot 1. Plots of $\epsilon_{r,real}$ and $\epsilon_{r,imag}$ for a material with an electronic resonance, plotted with $\omega_0 = 1$ and three different damping values.

Notice how whatever the damping constant might be, $\tilde{\epsilon}_r$ goes to a specific low frequency DC value, and to a different specific high frequency value. Those values can be obtained by using $\omega = 0$ and $\omega = \infty$ in Eq. 8.

Low frequency value:

$$\tilde{\epsilon}_r(0) = 1 + \frac{\omega_p^2}{\omega_0^2 - 0^2 - i0\gamma}$$

$$= 1 + \frac{\omega_p^2}{\omega_0^2}$$

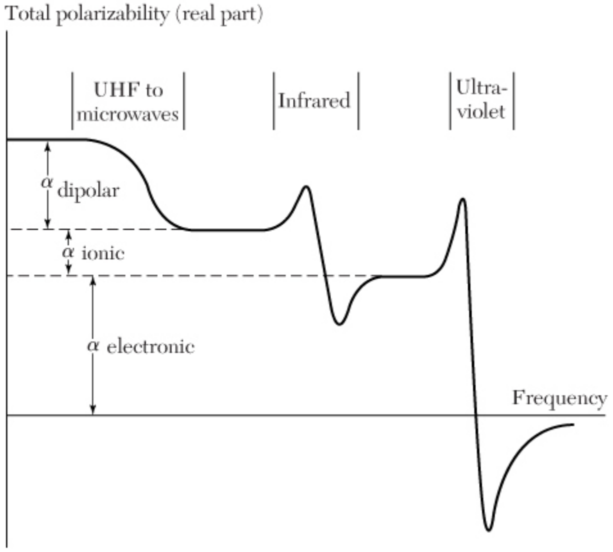
High frequency value:

$$\tilde{\epsilon}_r(\infty) = 1 + \frac{\omega_p^2}{\omega_0^2 - \infty^2 - i\infty\gamma}$$
$$= 1$$

The low and high frequency values are real numbers. It is only in the neighborhood of the resonance (ω close to ω_0) that the complex nature of the dielectric function is important.

The Lorentz model applied to insulating solids

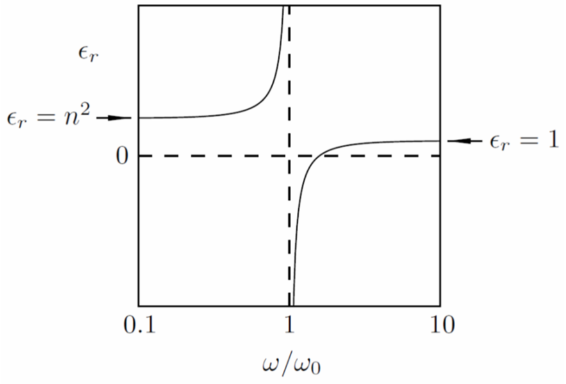
Kittel gives a plot describing how the real part of the polarizability, which is directly related to the dipole moment, of some representative solid changes with frequency. There are two resonances which each look similar to the Lorentz model plot above. One resonance is labeled "electronic" and occurs in the ultraviolet; the other is labeled "ionic" and occurs in the infrared.



Kittel, *Introduction to Solid State Physics*, Fig. 16-8. Schematic of the frequency dependence of the several contributions to the polarizability.

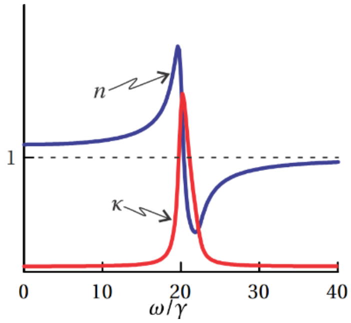
UV resonances: oscillations of electrons

The UV resonances most closely correspond to what I described in the model above: electrons on "springs" oscillating back and forth in response to an applied AC field. Here's a plot of $\epsilon_{r,real}$ from this model from Stokes, assuming a single resonance and no damping at all ($\gamma = 0$).



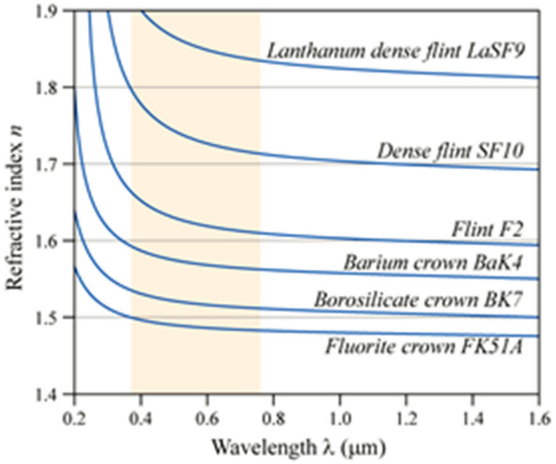
Stokes, *Solid State Physics for Advanced Undergraduate Students*, Fig. 16-5. The dielectric constant near the resonant frequency of the orbital electrons in a solid, using the Lorentz model with $\gamma = 0$. He is using the letter n to refer to the low frequency value of the index of refraction (i.e. rather than the frequency dependent index $n(\omega)$), which is not standard.

The Peatross and Ware textbook used for Physics 471 (Optics) also applies this model to solids and has a similar plot; in this case they plot the real and imaginary parts of $\tilde{n}$, labeled n and κ, respectively.



Peatross and Ware, *Physics of Light and Optics*, Fig. 2.6. Real and imaginary parts of the index of refraction for a Lorentz oscillator dielectric with $\omega_p = 10\gamma$ and $\omega_0 = 20\gamma$.

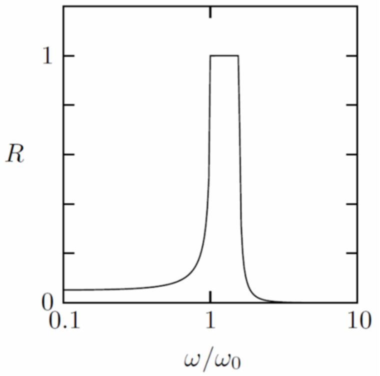
As mentioned, this resonance typically occurs in the UV. For visible light just below the resonance, the real part of n continually increases with frequency. This is called *normal dispersion* and is plotted (as a function of wavelength instead of frequency) for several types of glass in this plot from Wikipedia.



Wikipedia, *Dispersion (optics).* Index of refraction for several types of glass showing normal dispersion for visible light wavelengths.

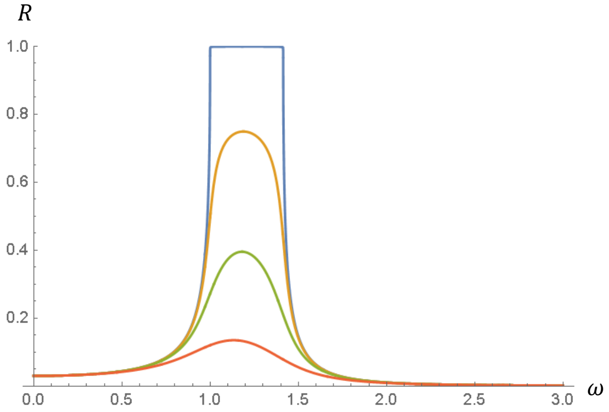
By contrast, right around the resonance, n decreases with frequency. This is called *anomalous dispersion* and is seen in many materials in the UV range.

The index of refraction directly impacts the reflectivity via Eq. 6. Stokes has plotted here how the reflectivity in insulators changes with frequency near the UV resonance, again assuming no damping. Insulators become highly reflective for frequencies just above ω_0!



Stokes, Fig. 16-6. The reflectivity near the resonant frequency of the orbital electrons in a solid, at normal incidence and with no damping, plotted for an air/insulator interface using the equations $\tilde{n} = \sqrt{\tilde{\epsilon}_r}$ and $R = \left|\frac{1-\tilde{n}}{1+\tilde{n}}\right|^2$.

Damping rounds out the corners and decreases the maximum reflectivity. Here's my own plot of R for several values of damping, namely $\gamma = 0$, 0.06, 0.2, and 0.5 (again with $\omega_p = \omega_0 = 1$ for simplicity).

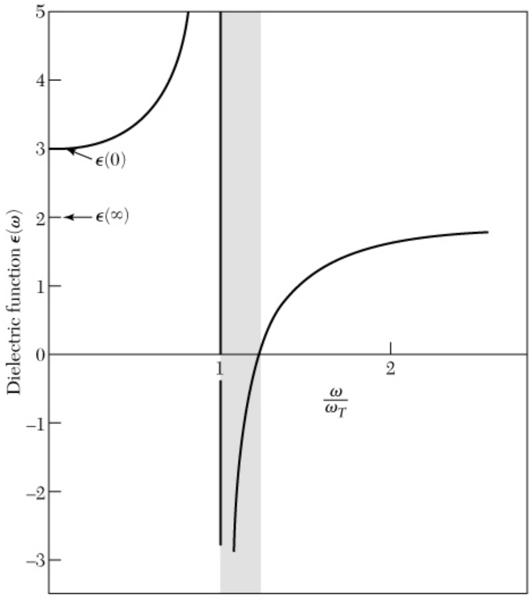


Colton plot 2. Plot of R for the UV resonance in an insulator, with $\omega_p = 1$ and four different damping values.

Infrared resonances: oscillations of ions

In ionic or partially ionic materials, the atoms themselves are charged and their interactions with neighboring atoms cause them to be anchored to their lattice spots as with a spring. The Lorentz oscillator model can therefore also be used to explain their behavior! The masses are much larger, so the resonant frequencies are much smaller. The relevant charge q is the ionic charge, which in general would be different than the charge of an electron, e. In partially ionic materials the ionic charge can even be fractional.

In the next figure, Kittel plots $\epsilon_{r,real}$ from the Lorentz model for such oscillating ions.



(a)

Kittel, Fig. 14.13a. The dielectric constant near the resonant frequency of the oscillating ions in a solid, using the Lorentz model with no damping and the small modifications described below.

The right hand side of this graph doesn't go to 1 as Eq. 8 would predict. This is a result of interaction between the high frequency end of the IR resonance with the low frequency end of the UV resonance and is normally just handled by arbitrarily changing the 1 in Eq. 8 to "$\epsilon(\infty)$"… but note that $\epsilon(\infty)$ of the IR resonance is the same as the $\epsilon(0)$ of the UV resonance. Eq. 8 therefore becomes:

$$\epsilon_r(\omega) = \epsilon_r(\infty) + \frac{\omega_p^2}{\omega_0^2 - \omega^2 - i\omega\gamma} \tag{9}$$

With that modification, $\epsilon_r(0) = \epsilon_r(\infty) + \frac{\omega_p^2}{\omega_0^2}$ instead of what it was for the UV resonances above.

Eq. 9 is actually usually written in terms of $\epsilon_r(0)$ and $\epsilon_r(\infty)$ instead of in terms of a plasma frequency. Recognizing that for this situation the natural spring resonance ω_0 occurs at the TO phonon frequency, ω_T,[2] we have:

$$\epsilon_r(\omega) = \epsilon_r(\infty) + \frac{\epsilon_r(0) - \epsilon_r(\infty)}{1 - \frac{\omega^2}{\omega_T^2} - \frac{i\omega\gamma}{\omega_T^2}} \tag{10}$$

A little bit of algebra suffices to show that Eqs. 9 and 10 are equivalent.

The TO frequency ω_T in Kittel's figure above is where ω crosses from positive infinity to negative infinity. The LO phonon frequency ω_L is defined to be the right hand side of the shaded region, namely the frequency where ϵ_r is zero as it crosses from negative to positive again. Exciting at the frequency of transverse optical

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[2] To quote Stokes pg 186: "The response of the ions to the driving force of the electric field will be greatest when their motion is… one of the natural lattice waves in the crystal. It is not difficult to identify the frequency at which this occurs. First of all, since the motion of the positive and negative ions is in opposite directions, the lattice wave belongs to the *optical branch* of the dispersion curves… Second, since the displacement of the ions is in a direction perpendicular to the direction of the wave vector, the lattice wave is *transverse*."

phonons causes a huge response to the dielectric function, but exciting at the frequency of longitudinal optical phonons causes no response at all because the electromagnetic waves are transverse.

As can be seen in plots below, electromagnetic waves with frequencies between ω_T and ω_L will not propagate at all in the medium but will instead have 100% reflectivity (if no damping). This is very similar to the large reflectivity in the UV resonance for frequencies just above ω_0, although the two effects are separated by several orders of magnitude!

We can obtain a useful equation by manipulating Eq. 10 as follows (assuming no damping). To start off, we use the fact that the dielectric function equals 0 when $\omega = \omega_L$.

$$0 = \epsilon_r(\infty) + \frac{\epsilon_r(0) - \epsilon_r(\infty)}{1 - \frac{\omega_L^2}{\omega_T^2}}$$

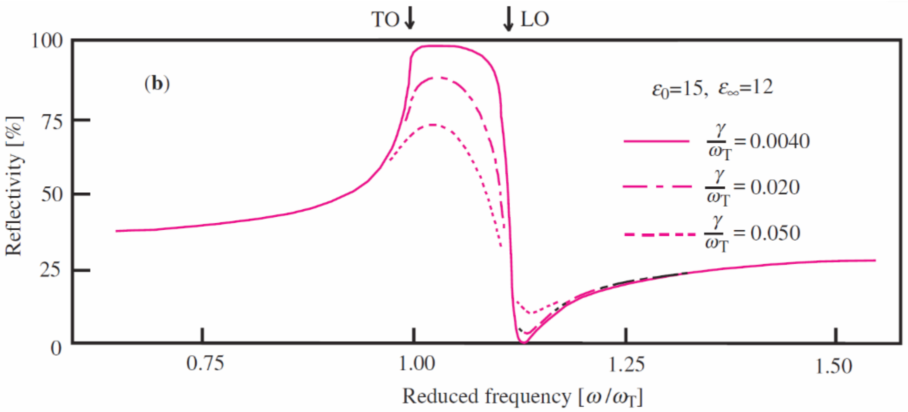
$$0 = \left(1 - \frac{\omega_L^2}{\omega_T^2}\right)\epsilon_r(\infty) + \epsilon_r(0) - \epsilon_r(\infty)$$

$$0 = -\frac{\omega_L^2}{\omega_T^2}\epsilon_r(\infty) + \epsilon_r(0)$$

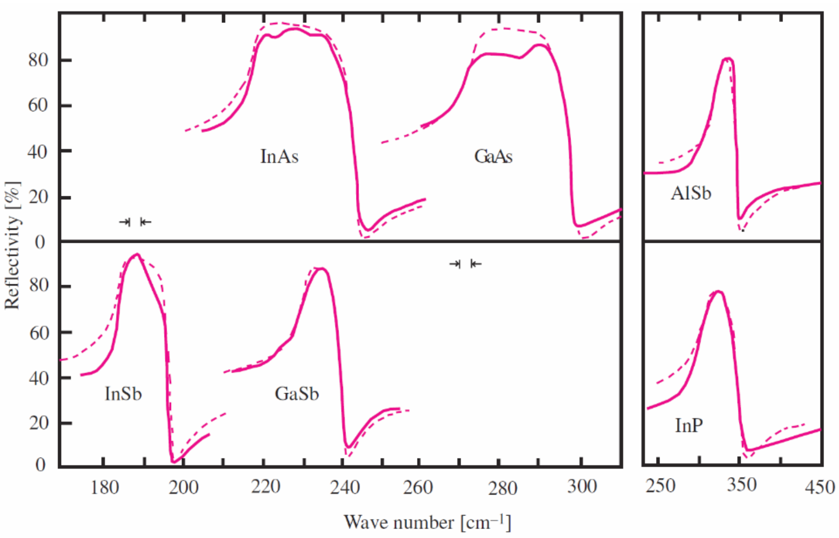
$$\frac{\omega_L^2}{\omega_T^2} = \frac{\epsilon_r(0)}{\epsilon_r(\infty)} \tag{11}$$

Eq. 11 is known as the LST relation (named for Lydane, Sachs, and Teller).

The semiconductor physics textbook by Yu and Cardona plots Eq. 10 for some arbitrary parameters, then uses it to fit some experimental measurements of IR reflectivity in real materials.

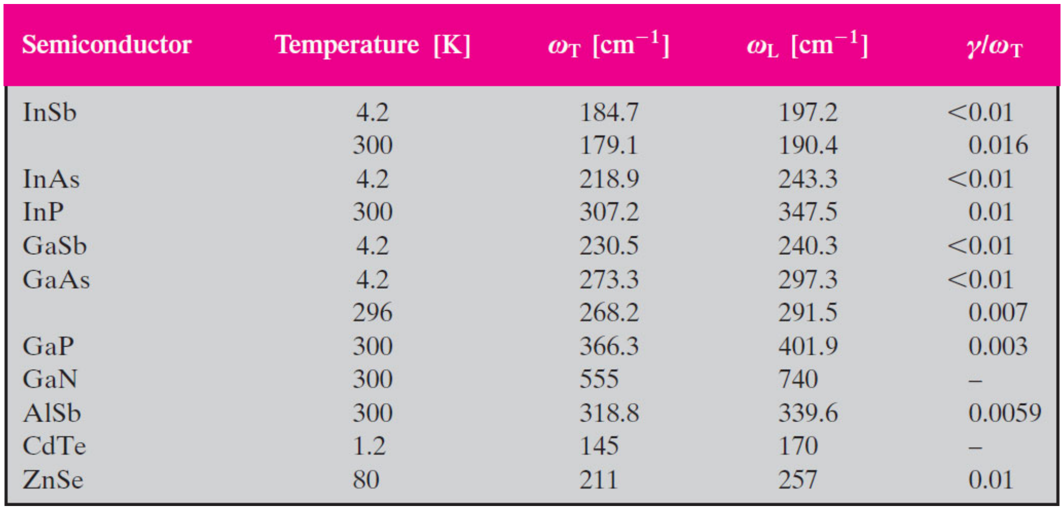


Yu & Cardona, *Fundamentals of Semiconductors*, Fig. 6.31(b). The infrared reflectivity from ionic oscillations, calculated from the Lorentz model with a few different values of damping.



Yu & Cardona, Fig. 6.32. Actual experimental reflectivity data (solid curves), and theoretical fits from the Lorentz model (dashed curves) using ω_T, ω_L, and γ as fitting parameters. The four plots on the left were measured at 4 K, the two on the right at 300 K.

Here's a table from the same book with experimental values for ω_T, ω_L, and γ for several materials obtained by fitting infrared reflectivity data like that.



Semiconductor	Temperature [K]	ω_T [cm^{-1}]	ω_L [cm^{-1}]	γ/ω_T
InSb	4.2	184.7	197.2	<0.01
	300	179.1	190.4	0.016
InAs	4.2	218.9	243.3	<0.01
InP	300	307.2	347.5	0.01
GaSb	4.2	230.5	240.3	<0.01
GaAs	4.2	273.3	297.3	<0.01
	296	268.2	291.5	0.007
GaP	300	366.3	401.9	0.003
GaN	300	555	740	–
AlSb	300	318.8	339.6	0.0059
CdTe	1.2	145	170	–
ZnSe	80	211	257	0.01

Yu & Cardona Table 6.5. The TO and LO phonon frequencies and the ratio of the damping constant γ to ω_T determined from lattice reflection spectra in several zinc-blende-type semiconductors and from Raman scattering.

Important note on units: As you can see, the *x*-axis of the Yu & Cardona, Fig. 6.32 plot is labeled "Wave number [cm^{-1}]". CAUTION: that is not what we've been calling the wave number! The wave number k, as we've been using it, would be labeled as rad/m or rad/cm. By contrast, when you see experimental data that is labeled "cm^{-1}", particularly with optical data like this, they nearly always mean $1/\lambda$ instead of $2\pi/\lambda$. I believe in the "olden days" k was originally defined as $1/\lambda$, and this has persisted in some settings (like this) even today. If you see a feature on a graph like this at, say, 185 cm^{-1}, you can convert it to regular wavelength like this: 185 cm^{-1} = 18500 m^{-1} $\rightarrow$ take inverse, λ = 5.405e-5 meters ≈ 54 µm.

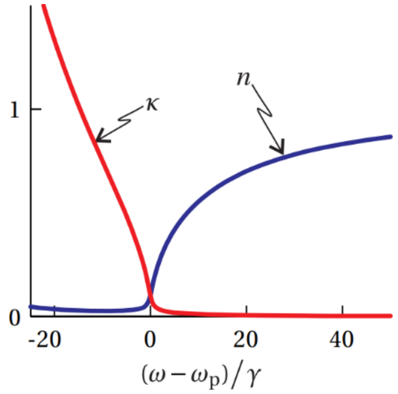
Similarly, in Yu & Cardona Table 6.5, the ω_T and ω_L values are given in terms of those same cm^{-1} units, rather than in actual units of ω. To get the actual ω's you could use $\frac{1}{\lambda} = \frac{f}{c}$ to solve for f (and hence ω).

The Lorentz model applied to metals

The fun doesn't stop! The valence electrons in metals are not anchored to their nuclei (no springs) but instead are free to move around the material. However, they still respond to electric fields and experience damping in the same way as the electrons in insulators for which we derived the Lorentz oscillator model above. Can we just set $\omega_0 = 0$ to account for no restoring forces? Yes we can! Setting $\omega_0 = 0$ in the Lorentz oscillator model (which, with no restoring forces is sometimes called the Drude model) trivially results in:

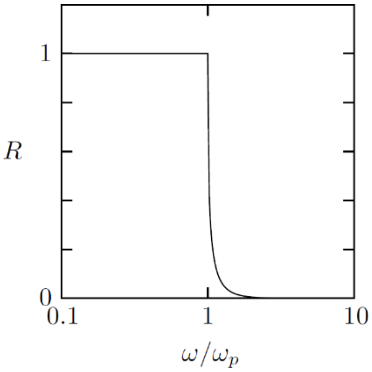
$$\tilde{\epsilon}_r(\omega) = 1 - \frac{\omega_p^2}{\omega^2 + i\omega\gamma} \tag{12}$$

Peatross and Ware also plot the real and imaginary parts of $\tilde{n}$ for this situation:

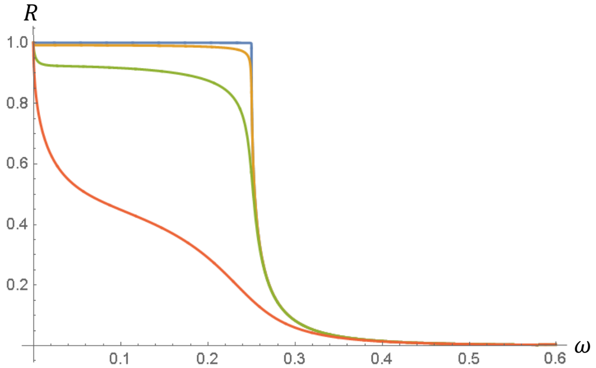


Peatross and Ware, Fig. 2.7. Real and imaginary parts of the index of refraction for a conductor with $\gamma = 0.02\ \omega_p$.

Stokes uses Eq. 12 (assuming $\gamma = 0$) to obtain $\tilde{n}$ and then R for normal incidence, which is plotted below. You can also see my own plot which includes some additional values of γ (I've arbitrarily set $\omega_p = 0.25$).



Stokes, Fig. 16-10. The reflectivity of metal near its plasma frequency, with no damping.



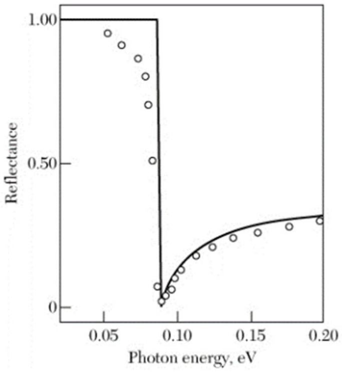
Colton plot 3. Plot of R for a metal with $\omega_p = 0.25$ and four different damping values: $\gamma = 0,\ 0.001,\ 0.01,\ 0.1$.

You can see that metals are highly reflective for frequencies below their specific plasma frequencies. In most metals the plasma frequency is in the UV; therefore they reflect visible light very efficiently. On the other hand, metals abruptly become very transparent for frequencies above the plasma frequency because the free electrons stop being able to respond to the oscillating electric field.

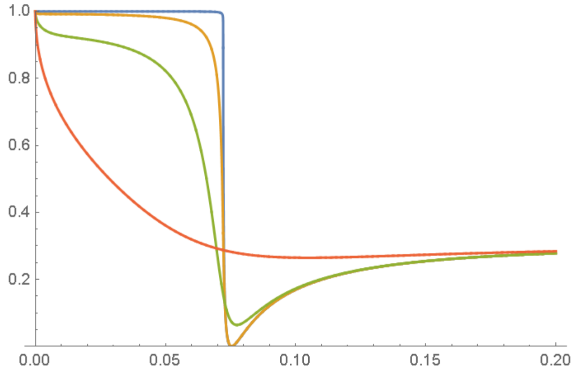
Finally, as with the IR resonances discussed above for ionic materials, in some metals the high frequency dielectric constant does not go to 1, so as before we will simply change the 1 in Eq. 12 to $\epsilon_r(\infty)$:

$$\tilde{\epsilon}_r(\omega) = \epsilon_r(\infty) - \frac{\omega_p^2}{\omega^2 + i\gamma\omega} \tag{13}$$

Here's a plot from Kittel using Eq. 13 to calculate and fit the reflectivity of indium antimonide (InSb), also with my own plot of R on the right. In my plot I've used $\epsilon_r(\infty) = 12$, $\omega_p = 0.25$, and four damping values: $\gamma = 0,\ 0.001, 0.01, 0.1$.



Kittel, Fig. 14.3. Experimental reflectivity of InSb (empty points), fitted with the Lorentz model with no damping (solid line). InSb is a narrow band gap semiconductor which acts fairly metallic at room temperature.



Colton plot 4. Plot of R with $\epsilon(\infty) = 12$, $\omega_p = 0.25$, and four different damping values. This plot makes it look like Kittel should have used some damping in the fit on the left to smooth out the sharp features in his solid line.

Notice how different Colton plot 4 looks compared to Colton plot 3, in terms of where the reflectivity dips, even though I have left $\omega_p = 0.25$. That's solely a result of adding in the $\epsilon(\infty)$ term to Eq. 13 compared to Eq. 12.