Dust: Optical Theory

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1. Introduction

Our investigations so far have focused on radiation absorbed and emitted by gas. However, the radiation we see from Galactic and extragalactic objects is absorbed by dust grains in the ISM, altering observed colors and line ratios, and in some cases obscuring objects entirely in the optical part of the spectrum.

Additionally, dust re-emits this energy in the infrared part of the spectrum. Infrared emission from dust can be a powerful diagnostic of the nature of interstellar dust, as well as telling us about sources of radiation that are completely obscured in the optical.

Our study of interstellar dust begins with the analysis of absorption, emission, and scattering by spherical particles. We will then discuss grain composition and the dielectric constant of typical materials. Advanced topics, such as grain asphericity, alignment, and polarization, emission from nanometer-size grains, and microwave emission, will be discussed in a subsequent lecture.

The major references here are:

§2: Your favorite E&M textbook

§3: Tielens, Ch. 5
and the classic paper:
Draine & Lee, ApJ 285, 89 (1984)

2. Optics of Spherical Grains

We consider processes involving grains of radius *a* and dielectric constant ε(ω). The dielectric constant is related to the electric susceptibility χ(ω) by:

$$\varepsilon(\omega) = 1 + 4\pi\chi(\omega);$$

in turn, the polarization (electric dipole moment per unit volume) of a material is given by **P**=χ**E**. The electric susceptibility is in general a complex function of frequency and is zero in vacuum.

A. ABSORPTION & SCATTERING: LONG-WAVELENGTH LIMIT

We first consider the case of wavelengths λ>>*a*. In this case, an incident electromagnetic wave corresponds to an externally applied electric field that is spatially uniform (over the size of the grain) but time-varying,

$$\mathbf{E}_{\text{ext}} \propto e^{-i\omega t}.$$

The polarization at position **x** within the grain is simply χ**E**(**x**), where **E**(**x**) is determined by integrating the electric field from a collection of electric dipoles:

$$\mathbf{E}(\mathbf{x}) = \mathbf{E}_{\text{ext}} - \nabla_{\mathbf{x}} \int_V \frac{\mathbf{x}-\mathbf{x}'}{|\mathbf{x}-\mathbf{x}'|^3} \cdot \mathbf{P}(\mathbf{x}')\,d^3\mathbf{x}'.$$

We are fortunate that the electric field introduced by a *uniform* polarization is:

$$\mathbf{E}_{\text{un}}(\mathbf{x}) = -\nabla_{\mathbf{x}} \int_V \frac{\mathbf{x}-\mathbf{x}'}{|\mathbf{x}-\mathbf{x}'|^3} \cdot \mathbf{P}\,d^3\mathbf{x}' = \nabla_{\mathbf{x}} \int_V (\mathbf{P}\cdot\nabla_{\mathbf{x}}) \frac{1}{|\mathbf{x}-\mathbf{x}'|}\,d^3\mathbf{x}' = (\mathbf{P}\cdot\nabla_{\mathbf{x}})\nabla_{\mathbf{x}} \int_V \frac{1}{|\mathbf{x}-\mathbf{x}'|}\,d^3\mathbf{x}'.$$

The last integral is the potential from a uniformly charged sphere with charge density ρ=1. Its gradient is (negative) the electric field of such a sphere, which by Gauss's law is −4π**x**/3 inside the sphere. Thus we see that the electric field from a sphere of uniform polarization is

$$\mathbf{E}_{\text{un}}(\mathbf{x}) = -\frac{4}{3}\pi\mathbf{P}.$$

We see that the dielectric sphere in a uniform external field has a solution for uniform polarization **P** where:

$$\mathbf{P} = \chi\mathbf{E} = \chi(\mathbf{E}_{\text{ext}} - \tfrac{4}{3}\pi\mathbf{P}),$$

or

$$\mathbf{P} = \frac{\chi}{1+\frac{4}{3}\pi\chi}\mathbf{E}_{\text{ext}}.$$

The overall dipole moment of the sphere is $(4/3)\pi a^3\mathbf{P}$, so the emitted (i.e. scattered) power is given by the dipole formula,

$$P_{\rm sc} = \frac{\omega^4}{3c^3}\left|\frac{4}{3}\pi a^3 \frac{\chi}{1+\frac{4}{3}\pi\chi}\mathbf{E}_{\rm ext}\right|^2 = \frac{\omega^4}{3c^3}\left|a^3\frac{\varepsilon-1}{\varepsilon+2}\mathbf{E}_{\rm ext}\right|^2 .$$

If we recall that the incident flux F is $c|\mathbf{E}_{\rm ext}|^2/8\pi$, we conclude that the cross section is

$$\sigma_{\rm sc} = \frac{8\pi a^6}{3\lambda^4}\left|\frac{\varepsilon-1}{\varepsilon+2}\right|^2 .$$

At long wavelengths, we see that the scattering cross section decreases rapidly as $\sim 1/\lambda^4$ (aside from possible issues with the dielectric constant) – this is the same physics as the Rayleigh blue-sky law.

We may also consider absorption. The power dissipation (in erg/cm^3/s) is given by the work done by the electric field on the dipoles:

$$W = \left\langle \mathbf{E}\cdot\dot{\mathbf{P}}\right\rangle = \frac{1}{2}\omega(\mathrm{Im}\,\chi)\,|\mathbf{E}|^2 = \frac{\omega\,\mathrm{Im}\,\varepsilon}{8\pi}|\mathbf{E}|^2 .$$

Integrating this over the sphere, we find an absorbed power

$$P_{\rm abs} = \frac{\omega a^3\,\mathrm{Im}\,\varepsilon}{6}|\mathbf{E}|^2 = \frac{\omega a^3\,\mathrm{Im}\,\varepsilon}{6}\left|\frac{3\mathbf{E}_{\rm ext}}{\varepsilon+2}\right|^2 .$$

The absorption cross section is then

$$\sigma_{\rm abs} = \frac{12\pi a^3\,\mathrm{Im}\,\varepsilon}{\lambda\,|\varepsilon+2|^2} .$$

At long wavelengths, $\lambda >> a$, we therefore see that the absorption will dominate unless the medium is lossless (ε nearly real).

B. ABSORPTION & SCATTERING: SHORT-WAVELENGTH LIMIT

For materials with modest dielectric constants (i.e. χ of order unity), one may estimate the large-angle scattering of radiation using geometric optics. Radiation falling within the geometric cross section $\sigma=\pi a^2$ is refracted or reflected at the grain surface, and is either scattered or absorbed depending on whether the optical depth through the grain ($\sim ka\ \mathrm{Im}\ \varepsilon$) is small or large.

An additional contribution to the cross section occurs due to diffractive effects. The presence of an obstruction causes small-angle scattering of radiation with a power equal to that that would have passed through the obstruction. This radiation is deflected through a typical angle $\theta \sim \lambda/a$, and the corresponding cross section is πa^2. Thus the total cross section is twice the geometrical value:

$$\sigma_{\rm tot} = 2\pi a^2.$$

At $\lambda << a$ the diffracted radiation can result in a "halo" appearing around a bright source, an effect observed in X-rays. As λ increases, the halo grows in size, until at $\lambda \sim a$ the diffraction pattern and geometrically refracted/reflected pattern merge into the dipole scattering pattern described previously.

C. THERMAL EMISSION

The radiation absorbed by a grain is re-emitted in the infrared. We are now in a position to understand the spectrum of emitted radiation.

We use the principle of detailed balance (again!) to compare the emission of a dust grain to absorption. If the grain has temperature $T_{\rm d}$, then in a blackbody of temperature $T_{\rm d}$ it must absorb an amount of radiation per unit frequency:

$$\frac{dP_{\rm abs}}{d\nu} = \frac{8\pi h\nu^3}{c^2}\frac{1}{e^{h\nu/kT_{\rm d}}-1}\sigma_{\rm abs}(\nu).$$

For practical cases the grains will have sizes up to ~0.5 μm and the radiation will emerge at wavelengths of many microns (due to the exponential factor); so we are in the long-wavelength limit and may write:

$$\frac{dP_{\rm abs}}{d\nu} = \frac{8\pi h\nu^3}{c^2}\frac{1}{e^{h\nu/kT_{\rm d}}-1}\frac{12\pi h a^3\,{\rm Im}\,\varepsilon}{\lambda\,|\varepsilon+2|^2} = \frac{192\pi^3 h a^3\nu^4}{c^3}\frac{1}{e^{h\nu/kT_{\rm d}}-1}\frac{{\rm Im}\,\varepsilon}{|\varepsilon+2|^2}.$$

The luminosity of the grain per unit frequency, L_ν, must be equal to this:

$$L_\nu = \frac{192\pi^3 h a^3\nu^4}{c^3}\frac{1}{e^{h\nu/kT_{\rm d}}-1}\frac{{\rm Im}\,\varepsilon}{|\varepsilon+2|^2}.$$

The grain will reach an equilibrium temperature when its total luminosity $L = \int L_\nu\, d\nu$ is equal to the amount of radiation absorbed.

3. Grain Properties

Next we consider the composition of dust grains and their likely dielectric constants. Our attention will then turn to their thermal balance.

A. MATERIALS

Clearly dust grains must be made primarily out of the abundant elements. The most abundant 10 elements (for solar composition) by number are:[1]

H	1
He	0.085
O	0.00049
C	0.00027
Ne	0.000085
N	0.000068
Mg	0.000040
Si	0.000032
Fe	0.000032
S	0.000013

While the true ISM abundances are not solar, the pattern is representative. The most abundant elements (H and He) do not by themselves form solids under reasonable conditions, although H may be incorporated into molecules if combined with heavy elements. Of the metals, by far the most abundant are C and O. Ne does not participate in chemistry, and we will return to N later, but the subsequent metals (Mg, Si, Fe) do form solid minerals with oxygen (the silicates).

Clearly many materials can be made out of these elements. The main cases that we will consider here, since they are observed in the diffuse ISM phases, are:

- *Carbonaceous material*: Ordinary carbon is found in the form of graphite, which consists of honeycomb-like sheets of carbon atoms bonded to three others in a hexagonal pattern. The sheets are held together by van der Waals forces. Carbonaceous material may also consist largely of small honeycomb-like units but with impurities, defects, etc. rather than pure graphite sheets (soot!). The smallest carbonaceous grains are the **polycyclic aromatic hydrocarbons** (PAHs). As their name suggests, these are really molecules. The PAHs are characterized by honeycomblike[2] carbon skeletons with hydrogen atoms bonded around the exterior.

- *Silicate minerals*: These are minerals consisting of Si atoms bonded in a tetrahedral pattern to 4 O atoms. There are many ways to connect these tetrahedral structures to each other. For example, the tetrahedral structures may share oxygen atoms, forming networks (O:Si = 2:1), long chains (O:Si = 3:1), or individual units (O:Si = 4:1). In the latter cases, the dangling oxygen

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[1] Asplund, Grevesse, Sauval, & Scott, ARA&A 47:481 (2009)

[2] In a planar hydrocarbon, the $2p_z$ orbitals of the carbons can mix with each other, such that the energy eigenstates are complicated linear combinations of these orbitals. The hydrocarbon is considered aromatic when the electrons occupying these levels can arrange themselves to give a lower energy (and hence greater stability) than one would expect by counting double bonds. Such structures often, but not always, involve hexagons.

atoms carry a single negative charge, and must be balanced by the incorporation of positive ions (e.g. Mg^{2+}, Fe^{2+}), leading to olivines (stoichiometry $Mg_xFe_{2-x}SiO_4$) or pyroxenes (stoichiometry $Mg_xFe_{1-x}SiO_3$). The silicate minerals may either be **crystalline** or **amorphous**; while crystalline silicates are observed in circumstellar material, the silicate content of ISM dust appears to be amorphous (narrow crystalline mid-IR features not observed).

In special environments, one may consider other grain materials: diamond, Si, SiC, Fe, iron oxides, etc., and in some cases there is evidence for these. In cold, dense environments, IR absorption spectroscopy also shows that **ice mantles** (including H_2O) have condensed onto grain surfaces.

B. DIELECTRIC CONSTANTS: GENERAL PROPERTIES

The dielectric constant of a material is a function of frequency. It consists of a real part (conservative) and an imaginary part (dissipative). Both are needed to compute optical properties. However, it is a remarkable fact that the *functions* Re $\chi(\omega)$ and Im $\chi(\omega)$ encode precisely the same information, thereby allowing us to infer all optical properties of a material from its absorption Im $\chi(\omega)$. This is because of causality: electric polarization **P** is caused by the electric field **E**, and the cause must precede the effect. In particular, if E_x is a δ-function at time t=0, then the polarization at any other time is:

$$P_x(t) = \int_{-\infty}^{\infty} \chi(\omega) e^{-i\omega t} d\omega .$$

Since **P** is real, we may write this as:

$$P_x(t) = \int_{-\infty}^{\infty} [\mathrm{Re}\,\chi(\omega)\cos\omega t + \mathrm{Im}\,\chi(\omega)\sin\omega t] d\omega .$$

This has to be zero for t<0. Therefore,

$$\int_{-\infty}^{\infty} \mathrm{Re}\,\chi(\omega)\cos\omega t d\omega = -\int_{-\infty}^{\infty} \mathrm{Im}\,\chi(\omega')\sin\omega' t d\omega' \text{ for } t<0.$$

For t>0, we may write the same equation but with $-t$:

$$\int_{-\infty}^{\infty} \mathrm{Re}\,\chi(\omega)\cos\omega t d\omega = \int_{-\infty}^{\infty} \mathrm{Im}\,\chi(\omega')\sin\omega' t d\omega' \text{ for } t>0.$$

In either case,

$$\int_{-\infty}^{\infty} \mathrm{Re}\,\chi(\omega)\cos\omega t d\omega = \mathrm{sgn}\, t \int_{-\infty}^{\infty} \mathrm{Im}\,\chi(\omega')\sin\omega' t d\omega' .$$

Now we note that since **P** and **E** are real, the susceptibility function satisfies χ(−ω)=χ*(ω), so Re χ is even and Im χ is odd. Therefore, the left-hand side is the Fourier transform of Re χ. We may thus use the inverse transform,

$$\operatorname{Re}\chi(\omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \operatorname{sgn} t\left[\int_{-\infty}^{\infty} \operatorname{Im}\chi(\omega')\sin\omega' t\, d\omega'\right]\cos\omega t\, dt,$$

To go further, we introduce σ→0 as an infintesimal parameter,

$$\operatorname{Re}\chi(\omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-\sigma|t|} \operatorname{sgn} t\left[\int_{-\infty}^{\infty} \operatorname{Im}\chi(\omega')\sin\omega' t\, d\omega'\right]\cos\omega t\, dt,$$

so that we are justified in performing the integral over *t*:

$$\int_{-\infty}^{\infty} e^{-\sigma|t|} \operatorname{sgn} t \sin\omega' t \cos\omega t\, dt = \frac{\omega'+\omega}{(\omega'+\omega)^2+\sigma^2} + \frac{\omega'-\omega}{(\omega'-\omega)^2+\sigma^2}.$$

This gives (using the oddness of Im χ to combine the two terms)

$$\operatorname{Re}\chi(\omega) = \frac{1}{\pi}\int_{-\infty}^{\infty} \operatorname{Im}\chi(\omega')\frac{\omega'-\omega}{(\omega'-\omega)^2+\sigma^2}\, d\omega'.$$

If we take the limit as σ→0, the integral becomes a *principal part*:

$$\operatorname{Re}\chi(\omega) = \frac{1}{\pi}\mathrm{PP}\int_{-\infty}^{\infty} \frac{\operatorname{Im}\chi(\omega')}{\omega'-\omega}\, d\omega',$$

where PP indicates that one is to exclude a region |ω’-ω|<ς from the integration region, and take the limit as ς→0. An analogous relation (swapping Re with Im and introducing a − sign) allows one to go from Re χ to Im χ.

It is possible to express the same equation in terms of only the positive frequencies using the oddness of Im χ:

$$\begin{aligned} \operatorname{Re}\chi(\omega) &= \frac{2}{\pi}\mathrm{PP}\int_{0}^{\infty} \frac{\omega'\operatorname{Im}\chi(\omega')}{\omega'^2-\omega^2}\, d\omega' \\ \operatorname{Im}\chi(\omega) &= -\frac{2\omega}{\pi}\mathrm{PP}\int_{0}^{\infty} \frac{\operatorname{Re}\chi(\omega')}{\omega'^2-\omega^2}\, d\omega' \end{aligned}.$$

These are called the **Kramers-Kronig relations**. With the help of the Kramers-Kronig relations, we need only specify Im χ(ω).

An interesting law can be obtained for the behavior of Im χ(ω). At very high frequencies (*h*ν >> binding energy of inner-shell electrons) where the electrons are essentially free particles, the position of an electron as a function of time is $\mathbf{x} = e\mathbf{E}/m_e\omega^2$, so the susceptibility must become:

$$\chi(\omega) \to -\frac{n_{\rm e,tot}e^2}{m_{\rm e}\omega^2}.$$

Matching this to the Kramers-Kronig relation implies

$$\int_0^\infty \omega' \,\mathrm{Im}\,\chi(\omega')\,d\omega' = \frac{\pi n_{\rm e,tot}e^2}{2m_{\rm e}}.$$

This is a "sum rule" that tells us that the total absorption at all frequencies must be related to the number of electrons.

C. DIELECTRIC CONSTANTS: SPECIFIC MATERIALS

Usually, the absorption can be described by several kinds of features:

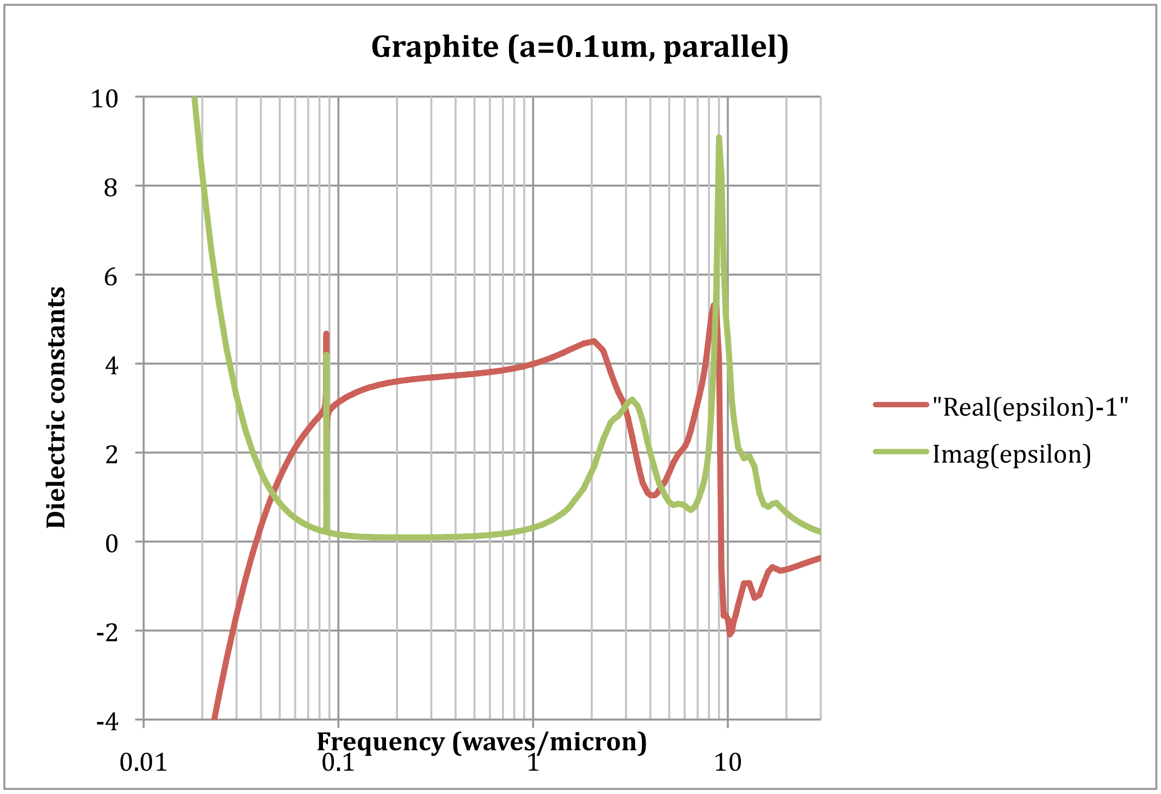
- *Electronic excitations*: Absorption occurs at frequencies corresponding to the energy differences between electronic energy levels. A common example is that in graphite sheets, electrons can be excited from the occupied π band (where the wave function changes phase by <90° between neighboring C atoms) to the π* band (where the wave function changes phase by >90°). A pileup of such transitions occurs at ~2200 Å, although in graphite the highest energy levels of the π band and the lowest of the π* band overlap, so that there is absorption even in the optical (hence the black color).
- *Vibrational modes*: The mid-infrared contains the typical vibration frequencies associated with the stretching and bending of atomic bonds. Silicates in particular have resonances at 10 μm (Si–O stretch) and 18 μm (O–Si–O bend). PAHs have a variety of modes associated with the carbon skeleton and the hydrogen atoms; for single molecules, however, the notion of a "dielectric constant" is not quite appropriate.
- *Conductors*: Free electrons in conductors (graphite, metals) imply a polarization that is the integral of the applied electric field, or alternatively $\mathrm{Im}\,\chi(\omega) \to 1/(\rho\omega)$ where ρ is the resistivity (Ohm's law).

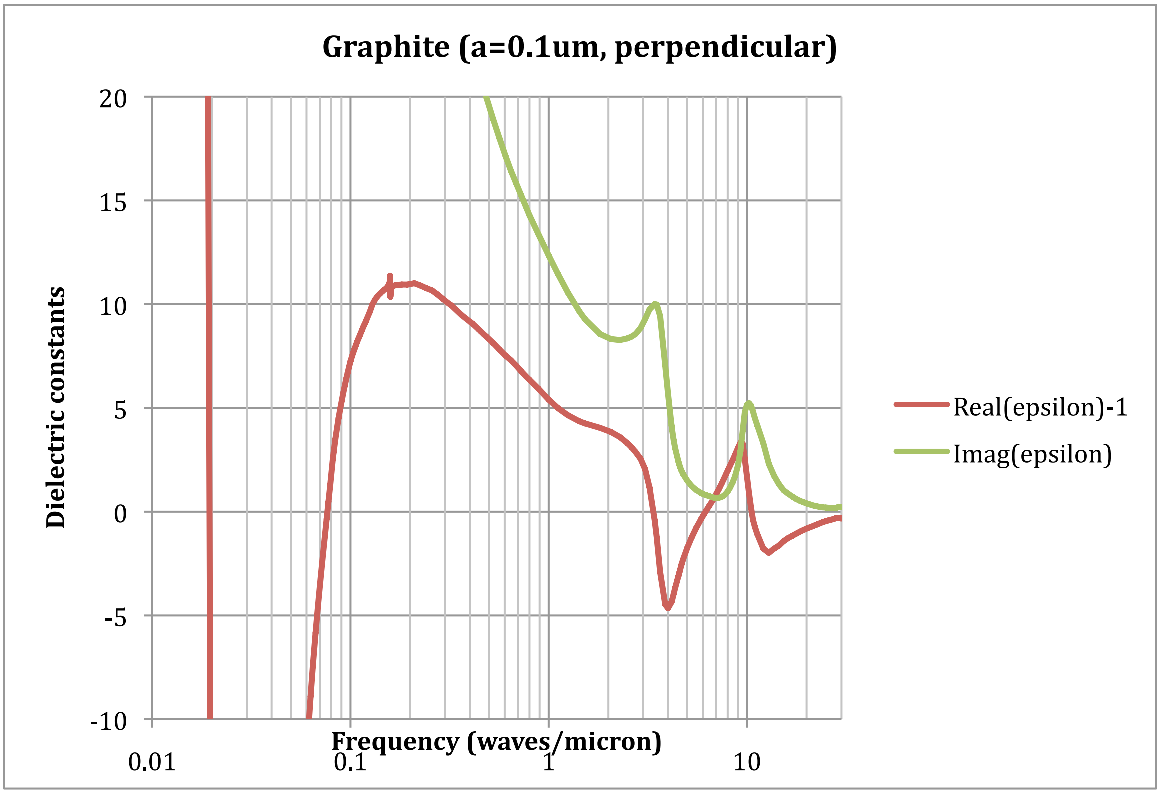
Some specific functions can be found on Bruce Draine's website: (see link from class page)

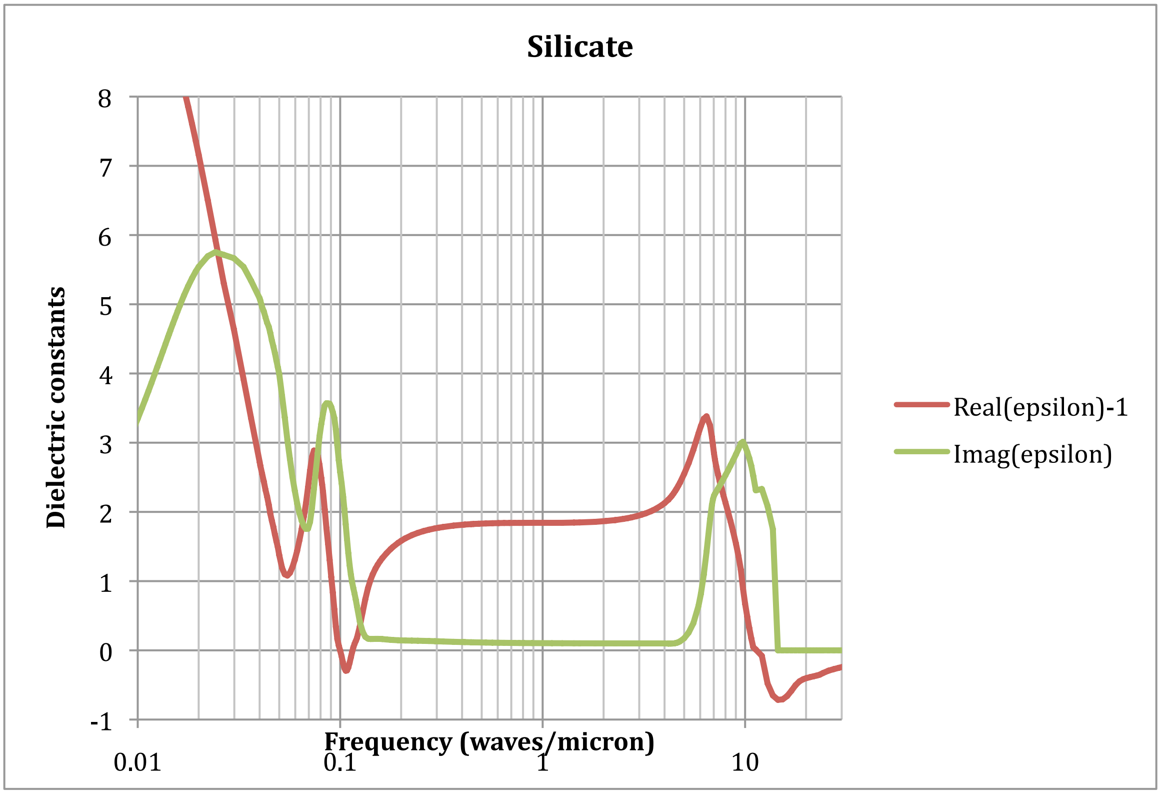
http://www.astro.princeton.edu/~draine/dust/dust.diel.html

The physics is discussed in Draine & Lee, ApJ 285, 89 (1984) although there have been some updates since then.

Some plots:


Graphite (a=0.1um, parallel)
Dielectric constants
10
8
6
4
2
0
-2
-4
Frequency (waves/micron)
0.01
0.1
1
10
"Real(epsilon)-1"
Imag(epsilon)


Graphite (a=0.1um, perpendicular)
Dielectric constants
20
15
10
5
0
-5
-10
Frequency (waves/micron)
0.01
0.1
1
10
Real(epsilon)-1
Imag(epsilon)


Silicate
Dielectric constants
8
7
6
5
4
3
2
1
0
-1
0.01
0.1
1
10
Frequency (waves/micron)
Real(epsilon)-1
Imag(epsilon)