

Chapter 2

Theoretical basis: dust, radiation and matter interactions

This chapter introduces the basic theoretical tools used in this thesis work.

The propagation of radiation in a dusty medium is described in section 2.1. The formal solution of radiative transfer problem in presence of dust is given, and applied to the case of dusty circumstellar envelopes. The methods developed in this section are then used in the following chapters to model the circumstellar environment of AGB stars.

Section 2.2 introduces the physics of interactions between dust matter and radiation. The optical properties of dust minerals are summarized, and discussed in term of the “opacities” characterizing astrophysical dust. These opacities are a basic component to compute the spectral properties of radiation emitted and absorbed by dust.

The last section finally examines the interactions between dust and other particles, namely the positive ions and the electrons of a plasma in which dust grains can be embedded. The survival of dust in this conditions is analyzed, and the effects of the dust-particles interactions are described from the point of view of the grain thermodynamics. The basic equations shown in this section are then used to study the behaviour of dust in the ICM.

2.1 Radiative transfer in a dusty medium

With the exceptions of refractory grains in meteorites, the only observables for the study of cosmic dust are in most cases the bolometric flux and the

spectral flux distribution coming from the dust medium. In these cases the solution of a radiative transfer problem is necessary to connect the observations with the physical and thermodynamical status of the dust.

In this section the general equation of radiative transfer is introduced, and discussed in the case of a dusty medium. The condition of local thermodynamical equilibrium, in which the dust radiative emission balances the energy input from all heating sources, is introduced, and a solution method for the problem in a spherically symmetric geometry is given.

The case of spherical symmetry and thermal equilibrium is the typical approximation used to describe dusty circumstellar envelopes, in which the only heating source is the radiation field generated from the central star. A more general problem, in which the interactions between dust and matter give a substantial contribution to the energy balance, and the thermodynamical equilibrium does not apply due to different timescales between the heating and cooling processes, is discussed separately in section 2.3.4.

2.1.1 Spectral intensities and flux units

The *spectral intensity* I_ν of a radiation field is defined as the amount of energy dE in the frequency beam $d\nu$ that, coming from the solid angle $d\Omega$, crosses the surface dA in the time dt :

$$I_\nu = \frac{dE}{d\nu dt d\Omega dA} \quad (2.1)$$

The integral over the solid angle of the normal component of the intensity I_ν with respect to the collecting area is called *spectral flux*, and is the quantity measured by astronomical detectors:

$$F_\nu = \int_{4\pi} I_\nu \cos \theta d\Omega \quad (2.2)$$

The *bolometric flux* is instead defined as the total collected flux over all frequencies, and is thus related to F_ν by the integral:

$$F_{bol} = \int_0^\infty F_\nu d\nu \quad (2.3)$$

Spectral fluxes are measured in units of $\text{erg cm}^{-2} \text{s}^{-1} \text{Hz}^{-1}$. A commonly adopted unit, called Jansky, is defined as:

$$1 \text{ Jy} = 10^{-23} \text{ erg cm}^{-2} \text{ s}^{-1} \text{ Hz}^{-1} \quad (2.4)$$

Fluxes are also expressed in *magnitudes*, which is a logarithmic scale unit based on the *zero point* flux of the standard star α Lyr:

$$m = -2.5 \log \left(\frac{F_\nu}{F_{\nu,0}} \right) \quad (2.5)$$

This system, which imitates the way the human retina perceives luminous fluxes, was introduced by Hipparchos in 120 B.C., and is still widely used.

To compute the flux emitted by a dust cloud, one has to solve the problem of how electromagnetic radiation propagated in the dusty medium. This is done by the “radiative transfer equation”, described in the following section.

2.1.2 The general equation of radiative transfer

Barionic matter and electromagnetic radiation interacts in three basic forms: absorption, scattering, and emission.

Consider a volume of material with cross section dA and length $d\ell$, which is illuminated by a radiation field of intensity I_ν . In case of absorption, an amount $dE^{(a)}$ of energy is removed from the incident flux, and converted into internal energy of the absorbing material. The amount of energy that is absorbed is proportional to the intensity I_ν , and the constant of proportionality is called *absorption opacity* $k_\nu^{(a)}$:

$$dE^{(a)} = k_\nu^{(a)} I_\nu d\nu dt d\Omega dA d\ell \quad (2.6)$$

In the case of scattering, the fraction of incident radiation that is removed is immediately reflected in the same wavelength bin but at different solid angle. The scattered radiation is also proportional to I_ν , and the constant of proportionality is called *scattering opacity* $k_\nu^{(\sigma)}$:

$$dE^{(\sigma)} = k_\nu^{(\sigma)} I_\nu d\nu dt d\Omega dA d\ell \quad (2.7)$$

In the case of emission, the material releases into the radiation field an energy $dE^{(\epsilon)}$, proportional to a quantity j_ν , called *emissivity*. The emitted energy is not necessarily proportional to the intensity I_ν , but rather depends on the physical characteristics of the emitting material, and its energetic state:

$$dE^{(\epsilon)} = j_\nu d\nu dt d\Omega dA d\ell \quad (2.8)$$

For the conservation of energy, the total variation of the incident flux in the solid angle $d\Omega$ is given by the difference between the emitted, absorbed and scattered energy:

$$dI_\nu = \frac{dE^{(\epsilon)} - dE^{(a)} - dE^{(\sigma)}}{d\nu dt d\Omega dA} \quad (2.9)$$

which gives the *general equation of radiative transfer*:

$$\frac{dI_\nu}{d\ell} = j_\nu - k_\nu I_\nu \quad (2.10)$$

In this equation $k_\nu = k_\nu^{(a)} + k_\nu^{(\sigma)}$ is the *total opacity*, that describes the interactions between radiation and matter at a microscopic level. By defining the *source function* S_ν as the ratio between the emissivity and the total opacity, one can rewrite the radiative transfer equation in the more usual form:

$$\frac{dI_\nu}{d\ell} = k_\nu (S_\nu - I_\nu) \quad (2.11)$$

The source function describes the interactions between matter and radiation at a macroscopic level; its general form for a dusty medium is given in the next section.

2.1.3 The source function for a dusty medium

The radiative transfer equation is more properly expressed in terms of a non dimensional quantity, called *optical depth* which is proportional to the total opacity integrated along an optical path \mathcal{P} :

$$d\tau_\nu = k_\nu d\ell \quad \Rightarrow \quad \tau_\nu = \int_{\mathcal{P}} k_\nu d\ell \quad (2.12)$$

By introducing the optical depth, the only term in the equation 2.11 which depends on the properties of the interacting matter is the source function S_ν :

$$\frac{dI_\nu}{d\tau_\nu} = S_\nu - I_\nu \quad (2.13)$$

With this change of variable, the radiative transfer equation can be formally solved in terms of the optical depth:

$$I_\nu(\mathcal{P}) = \underbrace{I_\nu(0) e^{-\tau_\nu(\mathcal{P})}}_{\text{background component}} + \underbrace{\int S_\nu(\tau'_\nu) e^{-[\tau'_\nu - \tau_\nu(\mathcal{P})]} d\tau'_\nu}_{\text{source component}} \quad (2.14)$$

where the *background component* gives the amount of incident radiation extinguished along the path \mathcal{P} , and the *source component* is the contribution to I_ν given by the emission and scattering of the interacting matter.

For a dusty medium, the source component can be split in two separate contributions, one relative to the dust emission, and one giving the total dust scattering:

$$S_\nu = \frac{j_\nu}{k_\nu} = \frac{j_\nu^{(\epsilon)} + j_\nu^{(\sigma)}}{k_\nu^{(a)} + k_\nu^{(\sigma)}} \quad (2.15)$$

If T_d is the dust temperature (generally a function of the heating sources, among which the radiation field itself), then the emission component is equal to the black body emission $B_\nu(T_d)$, multiplied by the efficiency factor given by the absorption opacity k_ν :

$$j_\nu^{(\epsilon)} = k_\nu^{(a)} B_\nu(T_d) \quad (2.16)$$

The scattering component, on the other end, is obtained by integrating the scattered radiation over the total solid angle:

$$j_\nu^{(\sigma)} = \frac{1}{4\pi} \int_{4\pi} k_\nu^{(\sigma)} I_\nu(\Omega') g(\Omega', \Omega) d\Omega' \quad (2.17)$$

where $g(\Omega', \Omega)$ is the angular phase function for coherent scattering from direction Ω' to direction Ω (see e.g. Mihalas, 1978).

By introducing the *albedo* $\varpi_\nu = k_\nu^{(\sigma)}/k_\nu$, the formal expression of the source function for a dusty medium becomes:

$$S_\nu = (1 - \varpi_\nu) B_\nu(T_d) + \frac{\varpi_\nu}{4\pi} \int_{4\pi} I_\nu(\Omega') g(\Omega', \Omega) d\Omega' \quad (2.18)$$

By substituting equation 2.18 in equation 2.13 the radiative transfer problem can in principle be solved, once the thermal structure of the dust is determined. In the next section this problem is discussed, in the simplified case in which dust and radiation are thermalized.

2.1.4 Dust in local thermodynamical equilibrium

The thermal state of a single dust grain is defined by the balance between its heating and cooling sources. In general, these two processes can have very different timescales, τ_{heat} and τ_{cool} . If $\tau_{cool} \ll \tau_{heat}$, the temperature of the grain is subjected to fluctuation in time. In this case a common temperature for the dust cannot be defined, since each grain, at any given moment in time, may have a different temperature. In this situation, common for dust in a hot plasma (like dust in the ICM or SN remnants), a *statistical distribution* of dust temperature have to be used.

If $\tau_{cool} \sim \tau_{heat}$, the grains in the cloud can reach an equilibrium temperature T_d , which is described by the balance between emitted and absorbed radiation. In this case, the dust is said to be in *local thermodynamical equilibrium*, or LTE. This equilibrium is described by the following equation, in which the left hand side is the total flux irradiated on all solid angles, and the right hand side is the total absorbed flux:

$$\int d\Omega \int k_\nu S_\nu d\nu = 4\pi \int k_\nu J_\nu d\nu \quad (2.19)$$

where J_ν is the average flux intensity over all solid angles:

$$J_\nu = \frac{1}{4\pi} \int I_\nu d\Omega \quad (2.20)$$

In the hypothesis in which radiative cooling is the only active process, the source function in equation 2.18 can be used to describe the LTE condition of a dust grain:

$$\int d\Omega \int k_\nu (1 - \varpi_\nu) B_\nu(T_d) d\nu = 4\pi \int k_\nu (1 - \varpi_\nu) J_\nu d\nu \quad (2.21)$$

where the scattering term is eliminated by the solid angle integration.

2.1.5 Scaling properties of radiative transfer

As described in Ivezić & Elitzur (1997), the radiative transfer equation for dusty media possesses a number of scaling properties, that can be used to simplify the modeling of dusty clouds, and the interpretation of the observational results.

The first of these properties is *scale invariance*. Consider a generic path \mathcal{P} , and the adimensional coordinate $y = \ell/R_1$ along the path, with R_1 an arbitrary length scale. Then equation 2.11 can be written as:

$$\frac{dI_\nu}{dy} = \tau_\nu(\mathcal{P}) \eta(y) [S_\nu(y) - I_\nu(y)] \quad (2.22)$$

where $\eta(y)$ is a dimensionless function describing the variations of the opacity with position:

$$\eta(y) = \frac{1}{\tau_\nu(\mathcal{P})} \cdot \frac{d\tau_\nu(y)}{dy} = \frac{k_\nu(y)}{\int k_\nu(y) dy} \quad (2.23)$$

Note that $\eta(y)$ generally depends on the wavelength, but if the optical properties of the individual absorbers do not change with position, this dependence disappears. In the case in which the relative abundance is constant along \mathcal{P} , then the function $\eta(y)$ reduces to the normalized dimensionless density:

$$\eta(y) = \frac{n_d(y)}{\int n_d(y) dy} \quad (2.24)$$

Equation 2.22 does not explicitly depend on quantities having the dimensions of length, since the absolute spatial scale has disappeared from the formulation of the problem, and is only necessary to express the total optical depth in terms of the physical size of the system. The properties of the radiation described by equation 2.22, are instead fully described by the adimensional variable y , showing that the problem is in fact scale invariant with respect to the spatial scale.

A second important property of the radiative transfer equation, is the way it scales with respect to the absolute normalization of the radiation intensity and flux. As shown in Ivezić & Elitzur (1997) for a dusty medium in LTE, if the only energy source is an external energy field I_ν^E , then the radiative transfer problem is fully specified by the temperature T_1 at the dust heated boundary, which defines the *scaling function*:

$$\Psi = \frac{4\sigma T_1^4}{F_1^E} \quad (2.25)$$

where

$$F_1^E = \int d\nu \int I_\nu^E \cos \theta d\Omega = \frac{L^E}{4\pi R_1^2} \quad (2.26)$$

is the bolometric flux at the heating boundary layer, produced by an external source of luminosity L^E , placed at a distance R_1 . In the case of circumstellar envelopes, T_1 is the temperature at the radius R_1 of the central cavity of

the envelope, $L_* = L^E$ is the parent star luminosity and F_1^E its bolometric flux.

In a system in which the position of the boundary layer is determined by the dust condensation (or sublimation) temperature T_{cond} (dust as close as possible to the hot external source), then the absolute scale of the bolometric flux is determined by the value of $T_1 = T_{cond}$, and the only relevant property of the input radiation is its adimensional spectral shape:

$$f_\nu^E = \frac{F_\nu^E}{\int F_\nu^E d\nu} \quad (2.27)$$

For a circumstellar dust envelope, the spectral energy distribution of the emitted radiation can be fully determined by specifying the spectral shape of the central stellar radiation, the optical depth τ_ν and the temperature T_1 at the inner envelope radius. This radius can either be the dust condensation radius for a system that is currently producing dust, or the radius of the central cavity in the case of a detached dust shell.

2.1.6 Solution for the spherically symmetric case

The solution of a radiative transfer problem is simplified in case of spherical symmetry, which makes it one-dimensional. For this reason, spherical symmetry is often adopted as an approximation for the real geometry. This is the case, for example, of dusty circumstellar envelopes: even though there are evidences for departures from spherical symmetry (see discussion in section 5), the quality of the data and the low spatial resolution of the images justify in most cases this kind of approximation.

The problem of radiative transfer for a spherical dusty shell was first developed by Rowan-Robinson (1980), which gave a solution method for this geometry. In this section we repeat his procedure, following the formalism developed by Ivezić & Elitzur (1997), in order to provide a description of the modeling procedure employed in the following chapters for AGB circumstellar envelopes.

In spherical symmetry the system is described by the radial adimensional coordinate y ; in the case of a dust shell, this coordinate can be defined to have the value $y = 1$ at the inner envelope boundary (so that T_1 is the inner temperature of the envelope). In this geometry, the optical depth along an optical path \mathcal{P} is described by the following integral (see figure 2.1):

$$\tau_\nu(y, \theta) = \tau_\nu^T \int_0^{y \cos \theta} \eta \left(\sqrt{u^2 + y^2 \sin^2 \theta} \right) du \quad (2.28)$$

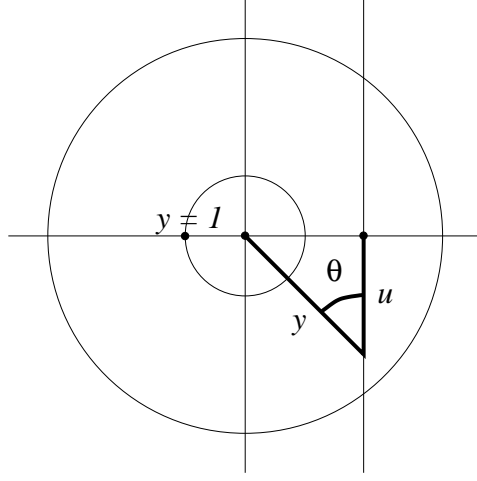


FIG. 2.1.— Geometry of a spherically symmetric dust envelope: y is the radial distance from the center of symmetry and u is the coordinate along the optical path intersecting the radial direction at an angle θ .

where τ_ν^T is the total optical depth along the radial direction:

$$\tau_\nu^T = \int_1^\infty k_\nu(y) dy \quad (2.29)$$

In this assumptions, the formal solution of the radiative transfer equation can be written as:

$$I_\nu(y, \theta) = I_\nu^E e^{-\tau(y)} \Theta \left[\frac{\theta_1^E}{y} - \theta \right] + I_\nu^d(y, \theta) \quad (2.30)$$

where Θ is the step function which limits the central star contribution only inside its angular size θ_1^E , and the last term is the dust component of the radiative intensity:

$$I_\nu^d = \int S_\nu(y', \theta) e^{-[\tau_\nu(y', \theta) - \tau_\nu(y, \theta)]} d\tau_\nu(y', \theta) \quad (2.31)$$

In a similar way, the angle averaged intensity, necessary to derive the dust thermal structure in the hypothesis of LTE, can be written as:

$$J_\nu(y) = \frac{F_1^E}{4\pi y^2} f_\nu^E e^{-\tau_\nu(y)} + J_\nu^d(y) \quad (2.32)$$

where J_ν^d is the dust diffuse average intensity, which is determined by the dust source function, and thus by the dust temperature. This last quantity require the solution of the LTE equation, that can be rewritten as:

$$k_P(T_d) T_d^4 = k_P(T_1) T_1^4 \frac{\int k_\nu (1 - \varpi_\nu) J_\nu(y) d\nu}{\int k_\nu (1 - \varpi_\nu) J_\nu(1) d\nu} \quad (2.33)$$

where $k_P(T)$ is the *Planck-averaged opacity* at the temperature T :

$$k_P(T) = \frac{\int k_\nu B_\nu(T) d\nu}{\int B_\nu(T) d\nu} \quad (2.34)$$

The flux scale Ψ , defined as $F_1 = 4\sigma T_1^4 \Psi$ can also be rewritten as a function of the angle averaged intensity $J_\nu(y)$; in the case of isotropic scattering, in which $g(\Omega', \Omega) = 1$:

$$\Psi = \frac{\int k_\nu f_\nu^E d\nu}{k_P(T_1)} \cdot \frac{1}{1 - \epsilon} \quad (2.35)$$

where

$$\epsilon = \frac{\int k_\nu (1 - \varpi_\nu) J_\nu^d(1) d\nu}{\int k_\nu (1 - \varpi_\nu) B_\nu(T_1) d\nu} \quad (2.36)$$

In the optically thin limit ($\tau_\nu \rightarrow 0$) the problem can be solved analytically:

$$\frac{k_P(T)}{k_P(T_1)} \left(\frac{T}{T_1} \right)^4 = \frac{1}{y^2} \quad , \quad \Psi = \frac{\int k_\nu f_\nu^E d\nu}{k_P(T_1)} \quad (2.37)$$

From this result, it is clear that the thermal structure and flux scale are fully determined by the spectral shape f_ν^E of the external energy source (the central star), and by the temperature T_1 of the inner shell boundary. If $k_\nu \propto \lambda^{-\beta}$, it is easy to find the well known result (first derived by Sopka et al., 1985):

$$T = T_1 y^{-\frac{2}{4+\beta}} \quad (2.38)$$

where $\beta \simeq 1-2$ for silicates and carbonaceous dust (Marengo et al., 1997).

In the case of an optically thick dust shell, the problem must be solved numerically, using an iterative method. By giving the optical properties k_ν and ϖ_ν of the dust, the initial temperature T_1 , the dust density distribution $\eta(y)$ and the spectral shape f_ν^E of the central star, one can solve equation 2.32 for $J_\nu(y)$, with the dust temperature derived from equation 2.33

and the flux scale given by equation 2.35. This method is applied in the public domain radiative code DUSTY (Ivezić et al., 1999), where an initial guess for the solution is provided by an analytical approximation, which is then iterated until convergence.

2.2 Interaction between dust and radiation

The interactions between dust grains and radiation, from a microscopic point of view, are described by the absorption and scattering opacities $k_\nu^{(a)}$ and $k_\nu^{(\sigma)}$. These two quantities are related to the electrical properties of the solid material of which the dust is made.

As discussed earlier, cosmic dust grains are in general amorphous conglomerates of crystalline materials. If the molecules and atoms that form the crystalline lattice are polar, their interactions with radiation are a consequence of Maxwell laws. In particular, part of the energy of an incident electromagnetic wave is absorbed by the dipoles in the lattice, and converted into internal energy associated to molecular and atomic vibrational states, or electronic population levels. Part of this internal energy is then emitted again, at characteristic frequencies of the material dipolar structure.

In this section the physics of the microscopic interactions between dust and radiation is reviewed. Since astronomical dust exists in the form of microscopic grains, its optical properties are best described by Mie theory, which allows to approximate the opacities of particulates with a rather simplified set of assumptions. The optical properties of bulk materials are instead derived by using the Kramers-Kronig relations, widely used in laboratory measurements of opacity from thin films of material. These methods are discussed in the last section.

2.2.1 The refractive index of solids

Consider a single oscillator of charge q and mass m in an electric field \vec{E} of harmonic frequency ω . In a dust grain this can be the case of a polar molecule, an ion in the lattice, or a free or bound electron. The equation of motion of the oscillator displacement around its rest position \vec{x} is:

$$\ddot{\vec{x}} + \gamma \dot{\vec{x}} + \omega_0^2 \vec{x} = \frac{q\vec{E}}{m} \quad (2.39)$$

where γ is a *damping* coefficient that counts for the “friction” opposed to the oscillator motion and ω_0 is the *natural frequency* of the oscillator (in a classical physics analogy, $m\omega_0^2$ would be the oscillator “spring constant”).

The induced dipolar moment $\vec{p} = q\vec{x}$ is derived by solving the differential equation 2.39:

$$\vec{p} = \frac{-q^2\vec{E}}{m} \cdot \frac{1}{(\omega_0^2 - \omega^2) - i\gamma\omega} = \alpha(\omega)\vec{E} \quad (2.40)$$

where $\alpha(\omega)$ is the *polarizability* $\alpha(\omega)$ of the oscillator:

$$\alpha(\omega) = \frac{-q^2}{m} \cdot \frac{1}{(\omega_0^2 - \omega^2) - i\gamma\omega} \quad (2.41)$$

The macroscopic polarizability \vec{P} of a medium made of N molecules per unit volume is $\vec{P} = N\alpha(\omega)\vec{E}$. From Maxwell equation the electric displacement of such material is $\vec{D} = \epsilon\vec{E} = \vec{E} + 4\pi\vec{P}$, where:

$$\epsilon = 1 + 4\pi N\alpha(\omega) \quad (2.42)$$

is the complex dielectric constant of the material. From equation 2.41 the dielectric constant can be expressed in terms of the natural frequency ω_0 and the dumping factor γ :

$$\epsilon = 1 + \frac{4\pi Nq^2}{m} \cdot \frac{1}{(\omega_0^2 - \omega^2) - i\gamma\omega} \quad (2.43)$$

With this formalism, ϵ is a complex function of ω , and can thus be decomposed in its real and imaginary part:

$$\epsilon' = 1 + \frac{4\pi Nq^2}{m} \cdot \frac{(\omega_0^2 - \omega^2)}{(\omega_0^2 - \omega^2)^2 + \gamma^2\omega^2} \quad (2.44)$$

$$\epsilon'' = \frac{4\pi Nq^2}{m} \cdot \frac{\gamma\omega}{(\omega_0^2 - \omega^2)^2 + \gamma^2\omega^2} \quad (2.45)$$

Figure 2.2 shows the behavior of the dielectric constant around a natural frequency ω_0 of the solid. The real part ϵ' in general *increases* with the frequency ω (*normal dispersion*). When $\omega \sim \omega_0$, however, the value of ϵ' *decreases* with ω and this is known as *anomalous dispersion*. The width of the anomalous dispersion is related to the value of γ : the larger the dumping coefficient of the oscillating dipole, the larger the anomalous dispersion region is. Similarly, the imaginary part ϵ'' has a peak for $\omega \sim \omega_0$, whose width is also related to γ . Since γ measures the efficiency of a medium to “dump” an incident electromagnetic field, e.g. to extract energy from it, it is related to the opacity of the material. The anomalous dispersion region

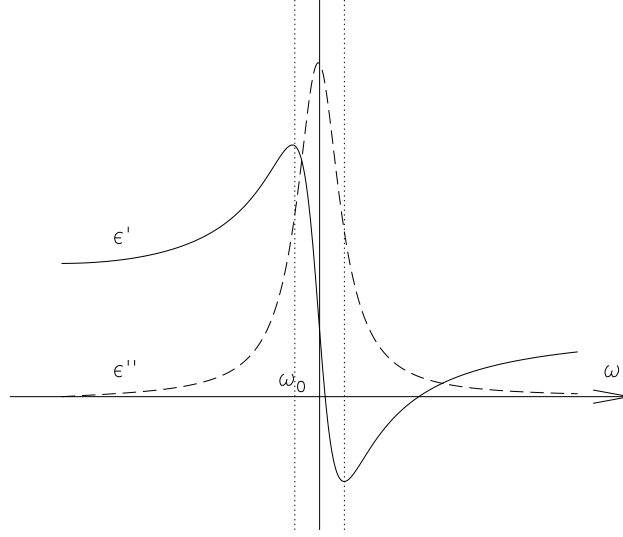


FIG. 2.2.— Real and imaginary part of the dielectric constant $\epsilon = \epsilon' + i\epsilon''$, plotted around the natural frequency ω_0 of the oscillating dipole

is where the absolute value of ϵ is larger, e.g. where the radiation is mostly absorbed. A material will thus be opaque at wavelengths close to its natural frequencies ω_0 , and the amount of opacity is related to the magnitude of γ .

To make this explicit, one can translate the dielectric constant in terms of the complex refractive index $\mathbf{n} = n + ik$, defined as ratio between the speed of the radiation in the vacuum and in the solid. By writing the incident radiation as an idealized harmonic wave with frequency ω and wavelength λ :

$$A = A_0 e^{i(\omega t + \frac{2\pi}{\lambda}x)} \quad (2.46)$$

the same radiation will propagate in the medium as:

$$\tilde{A} = A_0 e^{i(\omega t - \frac{2\pi}{\lambda}nx)} e^{-\frac{2\pi}{\lambda}kx} \quad (2.47)$$

The imaginary part k of the refraction index is thus responsible for the absorption of the incident radiation, while n is the optical refraction index related to the phase shift in the transmitted electromagnetic wave. By solving equation 2.39 with a solution in the form 2.47, one can derive the relation between \mathbf{n} and the complex refraction index ϵ :

$$\epsilon' = n^2 - k^2 = \Re[\mathbf{n}^2] \quad (2.48)$$

$$\epsilon'' = 2nk = \Im[\mathbf{n}^2] \quad (2.49)$$

The real and imaginary part of the refraction index, and the complex dielectric function, are thus complementary parameters describing the optical properties of a certain material. They depend on the atomic and molecular constants of the medium, and in particular on the natural frequencies and dumping factors of the dipolar oscillators. In general, a solid can have as many ω_0 and γ , as the number of its possible dipolar oscillators. These can be due to: (i) the orientation of polar molecules in the solid, (ii) the ionic polarization due to the relative movements of ions in the solid, and (iii) the electronic polarization due to the displacement of atomic electrons with respect to their nuclei. These three types of oscillators have different ω_0 , characteristic of separate regions of the electromagnetic spectrum. Solids with polar molecules will have absorption features at frequencies around $\sim 10^{11}$ Hz (millimetric wavelengths), ionic polarization will give rise to features at $\sim 10^{13}$ Hz (infrared), while electron displacement will have effects on the spectra at $\sim 10^{15}$ Hz (UV).

Since we are mainly interested to the properties of dust in the mid-IR, the optical constant of the grains at such wavelengths will be dominated by features related to the ionic vibrations in the dust lattice.

2.2.2 Mie Theory

Mie theory describes how spherical, homogeneous particles interact with electromagnetic radiation. It rests on the following assumptions:

- the only significant interactions are between single particles and radiation of arbitrary wavelength
- the frequency dependent optical constants (ϵ or \mathbf{n}) fully describe the optical properties of the particles
- the scattering of radiation from the particles is *elastic* (the wavelength of scattered radiation is the same as that of incident light)
- there is no systematic phase relation between the radiation scattered by the particles

- the medium in which the particles are distributed is *homogeneous* and *isotropic*

With Mie theory one can express the scattering and absorption opacities as a function of the optical constants. This is done by assuming the medium as made of N identical particles per unit volume, interacting with a radiation of intensity I_ν . From equations 2.6 and equation 2.7, the intensity of the absorbed and scattered radiation is:

$$I_\nu^{(a)} = k_\nu^{(a)} I_\nu \quad (2.50)$$

$$I_\nu^{(\sigma)} = k_\nu^{(\sigma)} I_\nu \quad (2.51)$$

The opacities $k_\nu^{(a)}$ and $k_\nu^{(\sigma)}$ are in general proportional to the number density and the geometrical cross section of the particles. The constants of this proportionality are the efficiencies of the particles material in absorbing and scattering the radiation, and are defined as:

$$Q_\nu^{(a)} = \frac{k_\nu^{(a)}}{\pi a^2 N} \quad (2.52)$$

$$Q_\nu^{(\sigma)} = \frac{k_\nu^{(\sigma)}}{\pi a^2 N} \quad (2.53)$$

By using Mie theory, the efficiencies $Q_\nu^{(a)}$ and $Q_\nu^{(\sigma)}$ can be written in terms of ϵ (see e.g. van de Hulst, 1957):

$$Q_\nu^{(a)} = \frac{8\pi a}{\lambda} \Im \left[\frac{\epsilon - 1}{\epsilon + 2} \right] \quad (2.54)$$

$$Q_\nu^{(\sigma)} = \frac{8}{3} \left(\frac{2\pi a}{\lambda} \right)^4 \Re \left[\frac{\epsilon - 1}{\epsilon + 2} \right] \quad (2.55)$$

2.2.3 Kramers-Kronig dispersion relations

For a bulk material, generally opaque to an incident radiation, a transmission spectra from which to measure \mathbf{n} (and thus $Q_\nu^{(a)}$ and $Q_\nu^{(\sigma)}$) is not always available. In this case, the only observable is the *reflectance power* R , that is the ratio between the incident and reflected intensity at wavelength ω :

$$R(\omega) = \frac{I_\nu^R}{I_\nu^I} \quad (2.56)$$

$R(\omega)$ is a wavelength dependent quantity related to the *reflectivity* $r(\omega)$, that gives the efficiency in which the electric field of an electromagnetic wave is reflected by the material:

$$E^R = r(\omega) E^I \quad (2.57)$$

As a complex quantity, $r(\omega)$ can be written in the form $r(\omega) = \rho(\omega)e^{i\theta(\omega)}$, where $\rho(\omega)$ is the magnitude of the reflectivity and $\theta(\omega)$ the phase shift between the reflected and incident wave. By solving the wave equation for E , one gets:

$$r(\omega) = \frac{1 - \mathbf{n}}{1 + \mathbf{n}} \quad (2.58)$$

Since $R(\omega) = r(\omega)r^*(\omega) = \rho^2(\omega)$, then:

$$R = \left| \frac{1 - \mathbf{n}}{1 + \mathbf{n}} \right| \quad (2.59)$$

thus allowing to express the real and imaginary part of the refraction index as a function of R and θ :

$$n = \frac{1 - R}{1 + R - 2\sqrt{R} \cos \theta} \quad (2.60)$$

$$k = \frac{-2\sqrt{R} \sin \theta}{1 + R - 2\sqrt{R} \cos \theta} \quad (2.61)$$

If R can be measured in the laboratory, θ is much more complex to obtain. A relation between $R(\omega)$ and $\theta(\omega)$ is however given by the Kramers-Kronig relations, which connect the real and imaginary part of any analytic function (see e.g. Jackson, 1962, p. 311). Using the Kramers-Kronig relations one can compute the value of $\theta(\omega)$ from the measured values of $R(\omega)$:

$$\theta(\omega) = \frac{-\omega}{\pi} \text{P} \int_0^\infty \frac{\ln R(\omega') - \ln R(\omega)}{\omega' - \omega} d\omega' \quad (2.62)$$

where P stands for the *principal part* of the integral.

2.2.4 Experimental determination of dust opacities

Mie theory and the Kramers-Kronig relations allow the determination of the optical constants of solids in an experimental setup, and can thus be used, in principle, to measure the opacity of cosmic dust in the laboratory. The problem, however, is the general unavailability of cosmic dust to perform

the experiments (given that the meteoritic dust grains cannot be isolated in the required quantities).

Astronomical spectra should then be used, and this is possible in the case of optically thin sources, when the main component of the observed spectra is either the extinguished background radiation (as for interstellar dust), or the thermal emission from a dusty envelope.

Consider the formal solution of the radiative transfer equation 2.14 for $\tau_\nu \ll 1$. In the first case (background component prevailing), the source function contribution can be neglected, and:

$$I_\nu(\mathcal{P}) \sim I_\nu(0) \tau_\nu(\mathcal{P}) \quad (2.63)$$

In the second case, instead, if the scattered radiation can be ignored (in a circumstellar envelope, the scattering contribution to the mid-IR spectra is usually less than 1%):

$$I_\nu(\mathcal{P}) \sim I_\nu(0) \tau_\nu(\mathcal{P}) + B_\nu(T_d) \tau_\nu(\mathcal{P}) \quad (2.64)$$

where T_d is the dust temperature in the region of the dust cloud where the radiation is emitted (the dust *photosphere*).

In both cases, the observed radiation intensity is proportional to the total optical depth of the dust. If the external source spectrum $I_\nu(0)$ and the dust continuum thermal radiation $B_\nu(T_d)$ can be modeled, the observed dust spectrum can be *rectified* in order to measure τ_ν directly from the data.

Once τ_ν is known, the total absorption efficiency $Q_\nu = Q_\nu^{(a)} + Q_\nu^{(\sigma)}$ is derived by equations 2.52 and 2.53:

$$Q_\nu = \frac{\tau_\nu}{\pi a^2 N D} \quad (2.65)$$

where N is the dust number density, and D the length of the optical path \mathcal{P} , estimated by the physical dimensions of the dust cloud (or the circumstellar envelope).

Once the absorption efficiency Q_ν is measured for a certain astronomical source, the comparison with laboratory spectra is necessary for the mineralogical identification of the dust, and to have a set of optical constants physically consistent. The laboratory measurement of opacity is made with one of the following procedures:

- measurements of refractive angles, which allow to derive the real part of the refractive index by use of Schnell's Law. A sample of high transparency is required.

- measurement of transmittance and reflectance at near normal incidence; the sample should also be quite transparent, but not as much as in the above case. The optical constants are then derived using Mie theory.
- measurements of reflectance at near-normal incident over a wide range of frequencies. The optical constants are derived by use of the Kramers-Kronig relations.
- ellipsometric techniques, which measures amplitude ratios and phase shifts directly, but are very difficult to use.
- measurements of reflectance for incident light of various polarization states and two oblique angles of incidence. This method is also difficult to perform, since it requires large sample surfaces, usually not available.

In practice, most of the “astronomical dust” opacities are derived by measuring the transmittance and reflectance of particulates embedded in a matrix of potassium bromide (KBr) that is supposedly transparent and linear for infrared measurements. This point, however, is controversial, since (Dorschner et al., 1978) found a wavelength shift between opacities measured with this method and from bulk material. The correction they introduced is widely used, but has recently been criticized on the basis of new measurements by (Speck, 1999).

To overcome these problems, many of the most recent opacities are now measured with the reflectance method, applied to thin films of bulk material enclosed in a diamond anvil.

2.3 Interaction between dust and matter

Even though most of the optical extinction and infrared emission of ISM and circumstellar envelopes is provided by dust, 99% of the total mass is due to the gaseous component of the circumstellar and interstellar medium. This is even more true for the ICM, where the presence of dust is uncertain, but large amounts of hot gas are responsible for the observed strong X ray emission. The interactions between dust grains and gas can in general give rise to physical and chemical modifications of the grains, and can play an important role in the dust thermodynamic and survival.

In circumstellar envelopes and molecular clouds, dust/gas interactions are responsible for the dynamics of mass loss around giant stars, and for

the chemical reactions that give rise to grain nucleation and growth. This processes are briefly discussed in chapter 4, in relation to the stellar winds of variable AGB stars.

This section focuses instead on the physical interactions mediated by the collisions of gaseous particles with the grains. If the kinetic energy of the colliding gas particles is high enough, compared with the energy density of the radiation, the heating processes of dust grains is dominated by such collisions, and the thermodynamical state of the dust can be very far from LTE. Grain charging and momentum transfer are also important, and should be considered when the dust is embedded in hot plasma, as in the case of SN remnants and ICM.

2.3.1 Grain charging

If the gas particles interacting with a grain are ionized, or can be ionized during the impact, then an electric charge can be transferred to the grain. The amount of the electric charge that builds up after several collisions can be very important, because determines the cross section of the grain with respect to impinging charged particles. Charging can also lead to the grain disintegration, when the accumulated charge is too high for the solid state forces that maintain the grain structure (Draine & Salpeter, 1979). Secondary particle emissions, electrons in negatively charged grains, or ions in grains with total positive charge, may however limit the total charge, thus preventing the grain destruction.

In steady state conditions, the total charge assumed in dust/ion collision is determined by the following equation:

$$\left(\frac{dQ}{dt}\right)_{tot} = \left(\frac{dQ}{dt}\right)_e + \sum_Z \left(\frac{dQ}{dt}\right)_Z = 0 \quad (2.66)$$

where the first term refers to the electronic components of the plasma, and the sum over Z is made over the positive ions. In the presence of ionizing radiation fields, a contribution $(dQ/dt)_{ph}$ due to photoelectric effects should also be taken into account, as can increase the positive charge of the grains, when the photoelectrons escape through the grain surface (see e.g. Spitzer, 1978).

In the case of hot plasma ($T \gtrsim 10^7$ K) the grains become transparent to electrons, and are charged positively. The efficiency of grain charging is however limited by secondary electron emission. As a result, the acquired dust electric potential is significantly smaller than the mean kinetic energy

of the gas particles ($q\mathcal{U}/kT \ll 1$), and the collisional cross section is thus simply given by the geometrical one (Dwek & Arendt, 1992).

2.3.2 Grain dynamics

Dust/gas collisions provide momentum transfer between dust grains and the gas. If θ is the incident angle in such a collision, the transferred momentum is:

$$\Delta p = \begin{cases} 2mv \cos \theta & \text{for elastic scattering} \\ mv \cos \theta & \text{for inelastic scattering} \end{cases} \quad (2.67)$$

The first case applies if the gaseous particle is reflected from the grain surface, while inelastic scattering occurs in case of absorption. If the trapped gas particle is subsequently emitted with a Maxwellian distribution of velocities at dust temperature, the final momentum can be larger than $mv \cos \theta$. This process is called *diffuse reflection* (Baines et al., 1965), and is more efficient when dust and gas temperatures are coupled and similar, as in dense molecular clouds.

In hot plasma, where the dust temperature is negligible with respect to the temperature of the gas, the momentum transfer in the release of the particle is very small, and $\Delta p \sim mv \cos \theta$. Then:

$$\frac{\Delta p_p}{\Delta p_e} \simeq \sqrt{\frac{m_p}{m_e}} \quad (2.68)$$

where m_p and m_e are the masses of the positive and negative charged particles (the latter are usually electrons, in which case most of the momentum transfer is due to the positive ions).

In circumstellar envelopes gas and dust are not coupled dynamically, and elastic reflection prevails, giving rise to the dragging force responsible for the envelope expansion in the winds of evolved stars (see chapter 4).

2.3.3 Grain destruction

The two main mechanisms for grain destruction are *thermal evaporation* and *sputtering*. The first process occurs when the grain temperature is high enough that the thermal energy kT_d of the surface atoms in the high energy tail of the kinetic distribution overcomes the lattice binding energy. In this process the grain cools down, preventing further evaporation. Only when T_d exceeds the dust sublimation temperature ($T_{subl} \simeq 1000$ K for carbonaceous

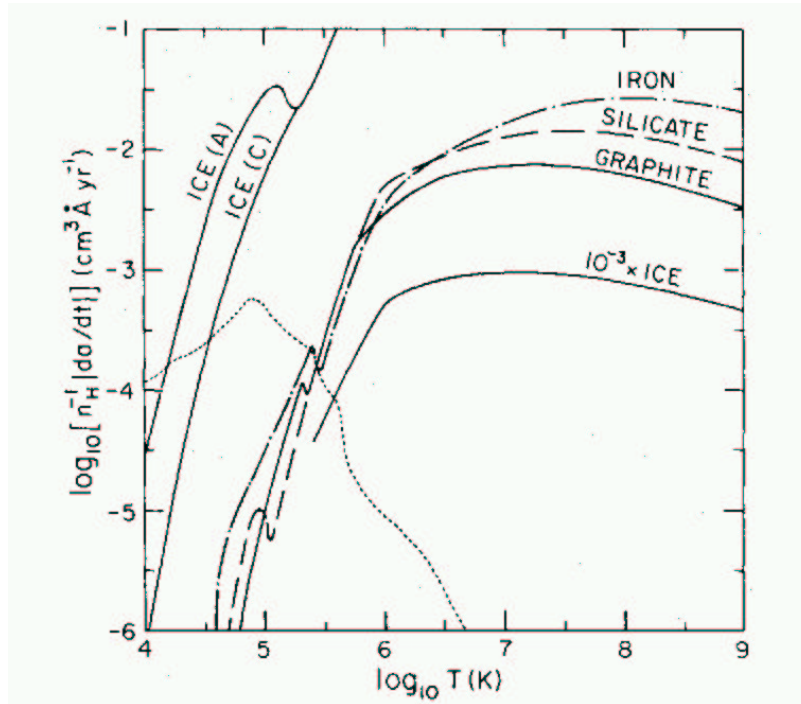


FIG. 2.3.— Sputtering rates for grains of different composition, as a function of gas kinetic temperature. From Draine & Salpeter (1979).

grains, and $\simeq 1500$ K for silicates), the grain completely evaporates in a short time.

Physical sputtering consists in the extraction of grain surface atoms by incident particles, primarily ions because of the larger energy and momentum transfers (Scalo et al., 1977). This process is to be distinguished from *chemical sputtering*, in which an incident particle bonds with a surface atom, creating an unstable molecule that eventually disintegrates, ejecting both particles from the grain (see e.g. Roth, 1983).

Dust sputtering is the main destructive process for dust in hot gas. It can be described as a cascade process, in which the incident particle first sets in motion a few target atoms, that in turn accelerate other atoms transferring enough energy to make them escape the grain. In the extreme cases in which all the atoms of the dust grain are involved, a complete evaporation takes place, and the grain is destroyed.

The sputtering lifetime is defined as the inverse of the rate in which a population of grains is depleted by sputtering, and is proportional to the

grain volume $V \propto a^3$ (the number of atoms to be removed) and inversely proportional to the grain cross section $\propto \pi a^2$ and gas density n_g :

$$\tau_{sputt} = \frac{1}{N} \left[\frac{dN}{dt} \right]^{-1} \propto \frac{V}{\pi a^2 n_g} \sim \frac{a}{n_g} \quad (2.69)$$

The sputtering rate in general depends on the grain composition and the kinetic temperature of the sputtering gas (see e.g. figure 2.3). If the temperature range is between 10^6 and 10^9 K this dependence can be ignored, and the following approximation is valid within a factor of 2 (Draine & Salpeter, 1979):

$$\tau_{sputt} \text{ (yr)} \simeq 10^6 \frac{a \text{ (\mu m)}}{n \text{ (cm}^{-3}\text{)}} \quad (2.70)$$

2.3.4 Grain thermodynamics

The energy deposited by incident particles in dust/gas collisions can dominate the dust grain thermodynamics if the gas kinetic energy is higher than the energy density of the ambient radiation field. This is typical for dust surviving in a hot plasma, subjected to electrons and ions collisions.

To evaluate the separate contribution of the positive and negative ions to the collisional heating of the dust grains, assume the plasma is thermalized to a temperature T . Then the individual ions of mass m have a Maxwellian energy and velocity distributions $f(E)$, and $v(E)$ respectively :

$$f(E) = \frac{2}{\sqrt{\pi}} \frac{E^{\frac{1}{2}}}{(kT)^{\frac{3}{2}}} e^{-\frac{E}{kT}} \quad (2.71)$$

$$v(E) = \int \left(\frac{2E}{m} \right)^{\frac{1}{2}} f(E) dE \quad (2.72)$$

The *heating rate* of a grain is proportional to the grain cross section, the gas density, and the average energy transfer of the collisions is:

$$H_{coll} = \pi a^2 n_g \int_0^\infty f(E) v(E) E \zeta(E) dE \quad (2.73)$$

where $\zeta(E)$ is the efficiency in which the energy of the ionic particle is transferred to the dust grain. In the case of incident electrons, this function is given by Dwek & Werner (1981):

$$\zeta(E) = \begin{cases} 1 & \text{for } E \lesssim E_* \\ 1 - \left[1 - \left(\frac{E_*}{E}\right)^{\frac{3}{2}}\right]^{\frac{2}{3}} & \text{for } E > E_* \end{cases} \quad (2.74)$$

This approximation reflects the idea that for impact energy lower than a critical value $E_*(\text{erg}) \simeq 3.7 \cdot 10^{-8} a^{2/3}(\mu\text{m})$ the electron energy is completely absorbed, while for higher energies the grains starts to become transparent to the impinging electrons.

By substituting the explicit form of the Maxwell distributions in equation 2.73, one obtains:

$$H_{coll} = \sqrt{\frac{8}{\pi m}} \frac{n_g}{(kT)^{3/2}} \int_0^\infty x^2 e^{-x} \zeta(E) dx \quad (2.75)$$

Notice that $H_{coll} \propto m^{1/2}$, and thus electron collisions prevails as heating sources of dust in a hot plasma. The average *time* between successive ion/grains collisions is defined as the reciprocal of the *collision rate*:

$$R_{coll} = \pi a^2 n_g \int_0^\infty v(E) f(E) dE \quad (2.76)$$

Since $\tau_{coll} = (R_{coll})^{-1} \propto m^{1/2}$, again electronic collisions due to the lower mass particle prevails.

If a grain is not evaporated by the energy input of an electron collision, its initial temperature is gradually restored by radiative cooling. The *radiative cooling rate* is given by the total flux irradiated by the dust grains, as in equation 2.19:

$$\Lambda_{rad}(T) = \int_0^\infty k_\nu B_\nu(T) d\nu \quad (2.77)$$

$$= 4\pi a^2 Q_P(T) \sigma T^4 \quad (2.78)$$

where $Q_P(T)$ is the *Planck averaged absorption efficiency* defined similarly to the Planck averaged opacity k_P in equation 2.34:

$$Q_P(T) = \int_0^\infty Q_\nu B_\nu(T) d\nu \quad (2.79)$$

The *radiative cooling time* τ_{cool} is defined as the total time needed by a grain to change its temperature from T_i to T_f :

$$\tau_{cool}(T_i, T_f) = \int_{T_i}^{T_f} \left| \frac{dT}{dt} \right|^{-1} dT \quad (2.80)$$

where

$$\frac{dT}{dt} = \frac{1}{c_V(T)} [H_0 - \Lambda_{rad}(T)] \quad (2.81)$$

is inversely proportional to the volume heat capacity of the grain material at the given temperature $c_V(T)$, and to the difference between the radiative cooling and the minimum heating rate H_0 provided by the background radiation field. This last term can in principle be expressed as a function of the temperature T_0 which the grain would have if in equilibrium with the ambient radiation field:

$$H_0 = 4\pi a^2 Q_P(T_0) \sigma T_0^4 \quad (2.82)$$

Note that if $H_0 \sim \Lambda_{rad}$ then the cooling time will be infinite, and the grains will be at the equilibrium temperature T_0 of the radiation field. This is the case, for example, of dust in circumstellar envelopes that is in LTE with the radiation (and T_0 is the local equilibrium dust temperature T_d). In the case of ICM dust, however, $\Lambda_{rad} \gg H_0$, and the main source of energy for the dust are the collisions with the electrons in the ICM plasma; the minimum temperature T_0 is defined as the temperature of the cosmic background radiation, or the equilibrium temperature that the dust would have with respect of the X-ray radiation emitted by the gas.

According to the ratio between the cooling and collision time, dust grains are in thermal equilibrium with the gas, or will oscillate between successive heating and cooling at each collision: in this case the thermal status of the dust is described by a statistical distribution of temperatures, in what is called a *stochastic heating* process. An example of stochastic heating is provided by dust in the ICM, and is discussed in chapter 6.