The processing and evolution of dust in Herbig Ae/Be systems.

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Citation for published version (APA):
Chapter 2

Dust physics, radiative transfer and spectral analysis

In this chapter, we will discuss details of the physical processes taken into account in our models of circumstellar dust environments. We will assume that the gas opacities are much smaller than the dust opacities and can be ignored. Essentially, the physical processes fall into three categories. First, the temperatures that dust particles adopt. Second, the spatial distribution of the dust. Third, the composition and grain structure of the dust particles.

Also, we will discuss the extent to which observations can constrain models of circumstellar dust. This is an important point as fitting of SEDs may give ambiguous results when trying to determine the properties and spatial distribution of circumstellar solid state material.

2.1 Radiative transfer

In our models we assume that the flux of photons emitted by the central star can be absorbed and re-emitted or scattered by solid state particles in the ambient medium. We assume that in the dust medium the energy in the radiation field is conserved, i.e. no other sources or sinks of energy are present, such as viscous processes or shocks. The constraint of radiative equilibrium determines the equilibrium temperature of the dust particles. We start with introducing some basic equations of radiation transfer, leading to a discussion of the temperature determination of the dust.

In arbitrary geometry the equation of transfer is given by

\[
\left[ \frac{1}{c} \frac{\partial}{\partial t} + \frac{\partial}{\partial s} \right] I_\nu(r, t, \hat{s}) = \eta_\nu(r, t, \hat{s}) - \chi_\nu(r, t, \hat{s}) I_\nu(r, t, \hat{s})
\]  

(2.1)

where \( c \) denotes the speed of light and \( I_\nu(r, t, \hat{s}) \) is the specific intensity of radiation at position \( r \), traveling in direction \( \hat{s} \), with frequency \( \nu \), at time \( t \). The emission and extinction of energy by dust grains is given by the coefficients \( \eta_\nu \) and \( \chi_\nu \), respectively. The extinction coefficient can be split in two contributions, namely

\[
\chi_\nu(r, t, \hat{s}) = \kappa_\nu(r, t, \hat{s}) + \sigma_\nu(r, t, \hat{s})
\]  

(2.2)

where \( \kappa_\nu \) is the absorption coefficient and \( \sigma_\nu \) is the scattering coefficient. We assume that the radiation field is time-independent and the thermal emissivity and scattering are
isotropic. Then Eq. (2.1) reduces to
\[
\frac{dI_v(r, \hat{s})}{ds} = -\chi_v(r)[I_v(r, \hat{s}) - S_v(r)]
\]
(2.3)
where we have introduced the generic source function
\[
S_v(r) \equiv \frac{\eta_v(r)}{\chi_v(r)}
\]
(2.4)
\[
= \frac{[\kappa_v(r)B_v(r) + \sigma_v(r)f_\nu(r)]}{[\kappa_v(r) + \sigma_v(r)]}.
\]
Here \(B_v\) is the Planck function and \(f_\nu\) defines the mean intensity of radiation
\[
f_\nu(r) = \frac{1}{4\pi} \int I_v(r, \hat{s})d\Omega
\]
(2.5)
which is the specific intensity averaged over all solid angles. It is because of the assumption of isotropic thermal emission and scattering that the source function can be written in the form of Eq. (2.4). The second equality in Eq. (2.4) is only valid when the grain material can be represented by a unique grain temperature \(T\). In general, this will not be the case, as size, shape and composition of the particles may result in different absorption properties and consequently, different grain temperatures. In this more general case, the thermal emissivity is given by
\[
\eta_v(r) \equiv \sum_i \kappa_{vi}(r)B_v(T_i(r))
\]
(2.6)
where \(i\) labels the different grain components.

Integration of Eq. (2.3) over all solid angles and all frequencies, and substitution of the generic source function yields for each grain component
\[
\nabla \cdot \mathcal{F}(r) = 4\pi \int_0^{\infty} \kappa_v(r)[B_v(T(r)) - f_\nu(r)]d\nu = 0
\]
(2.7)
where \(\mathcal{F}(r)\) is the frequency integrated flux. The monochromatic flux, from which the frequency integrated flux is derived, is defined as
\[
\mathcal{F}_\nu(r) = \oint I_v(r, \hat{s})(n \cdot \hat{s})d\Omega
\]
(2.8)
such that \(\mathcal{F} \cdot d\mathbf{S}\) gives the net rate of radiant energy flow accross an arbitrarily oriented surface \(d\mathbf{S} = \hat{s}dS\).

Eq. (2.7) gives the local representation of the constraint of radiative equilibrium. It states that the total amount of energy that is absorbed, per second, per unit volume \((4\pi \int_0^{\infty} \kappa_v f_\nu d\nu)\) equals the total amount of energy that is emitted in the same time interval, from the same volume element \((4\pi \int_0^{\infty} \kappa_v B_v d\nu)\). Note that the scattering extinction
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does not feature in this equation, which is to be expected as scatterings do not affect the energy contents of a volume element in any way. A global representation of radiative equilibrium can be derived from the total flux. Assuming e.g. spherical coordinates, such that the divergence of the total flux can be written as $\frac{1}{r^2} \frac{\partial(r^2 J)}{\partial r}$, one finds

$$4\pi r^2 J(r) = \text{constant} = L \quad (2.9)$$

where $L$ is the luminosity of the star.

2.1.1 An optically thin medium

To give an impression of what to expect for the temperatures of dust grains, we derive the temperature structure in an optically thin medium. In this type of medium the intensity incident on the grains is unattenuated star light, i.e. extinction processes can be neglected. Let us assume the radiation incident on the grains is star light with a uniform intensity $I^* = B_\nu(T_*)$, i.e. represented by a Planck function at a stellar surface temperature $T_*$. For the mean intensity at distance $r$ from the star one then finds

$$J_\nu(r) = W(r)B_\nu(T_*) \quad (2.10)$$

where $W(r)$ is the geometrical dilution factor

$$W(r) = \frac{1}{2} \left\{ 1 - \sqrt{1 - \left( \frac{R_*}{r} \right)^2} \right\}, \quad (2.11)$$

which in this case may be interpreted as being the solid angle subtended by the central star, as seen from distance $r$, over the total solid angle. Simple physical reasoning (or substitution) yields $W(R_*) = 1/2$, while at distances $r \gg R_*$, $W(r) = 1/4(R_*/r)^2$.

Now let us assume that the absorption cross section of a specific spherical dust grain is given by

$$C_{\text{abs,}\nu} = \pi a^2 Q_{\text{abs,}\nu} = \pi a^2 Q_{\nu} \left( \frac{\nu}{\nu_0} \right)^p \quad (2.12)$$

where $a$ is the radius of the grain and $Q_{\text{abs,}\nu}$ is the efficiency factor of absorption (see also Sect. 2.3.2). The absorption coefficient $\kappa_\nu$ is recovered by multiplying Eq. (2.12) with the particle number density. Substitution of the above three formulae in Eq. (2.7) yields

$$T(r) = \left[ W(r) \right]^{1/(p+4)} T_* \quad r \gg R_* \quad \left( \frac{1}{4} \right)^{1/(p+4)} \left( \frac{R_*}{r} \right)^{2/(p+4)} T_* \quad (2.13)$$

for the temperature distribution of the grains. In case $p = 1$, it follows that $T(r) \propto r^{-4/3}$. Note that for this description of $Q_{\text{abs,}\nu}$ the grain temperature is independent of grain size. This need not to be so in a more general case.
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In an optically thin medium, the actual spatial distribution of the dust is not relevant in so far that only \( M_{\text{dust}}(r)dr \), the total dust mass in the radial distance interval \((r, r + dr)\), needs to be specified. The quantity that determines the dust emission is therefore the distribution of mass over temperature, i.e. \( M_{\text{dust}}(T)dT \), and we will use this diagnostics in several chapters of this thesis. The monochromatic flux at a distance \( d \), can be expressed in the mass over temperature distribution as

\[
\mathcal{F}_\nu(d) = \frac{1}{4\pi d^2} \int_{T_{\text{min}}}^{T_{\text{max}}} \eta_\nu'(T) M_{\text{dust}}(T) dT = \frac{1}{4\pi d^2} \int_{T_{\text{min}}}^{T_{\text{max}}} \kappa_\nu'(T) B_\nu(T) M_{\text{dust}}(T) dT,
\]

where \( T_{\text{min}} \) and \( T_{\text{max}} \) denote the minimum and maximum temperatures that grains can assume, \( \eta_\nu' \) the thermal emissivity per unit mass and \( \kappa_\nu' = \kappa_\nu/\rho \) the mass absorption coefficient where \( \rho \) denotes the density of the medium. In Herbig Ae/Be (HAEBE) stars, the maximum temperature of grains may be identified with the temperature at which they evaporate when coming too close to the central star. If this evaporation temperature is denoted by \( T_{\text{evap}} \), then the radius at which this occurs is given by

\[
r_{\text{evap}} = R_* \left( 1 - 2 \left( \frac{T_{\text{evap}}}{T_*} \right)^{p-4} \right)^{1/2} \frac{R_*}{2} \left( \frac{T_{\text{evap}}}{T_*} \right)^{-(p-4)/2}.
\]

A typical upper limit for the temperature of refractory dust grains is \( T_{\text{evap}} = 1500 \) K. For a HAEBE star with \( T_* = 9000 \) K and \( R_* = 2.5R_\odot \), this yields \( r_{\text{evap}} = 22R_* \) or 0.5 AU. Inside this region no dust can exist. In addition, chemical reactions can set limits on the maximum or minimum temperature of grains (see Sect. 2.2.3).

As discussed in Chapter 1, there is growing evidence for circumstellar disks in HAEBE systems. However, the spectra of the HAEBE systems studied in this thesis show evidence for a prominent optically thin dust component. Since the emission of such a component only depends on \( M_{\text{dust}}(T) \), we can use Eq. (2.14) independent of geometry to fit the spectra. Furthermore, part of the circumstellar dust in HAEBE systems may be distributed in a more or less spherical shell. For instance, a remnant low density halo may be left from the Class I phase (cf. Fig 1.1). Also, hydrodynamical effects may create an inner halo or 'puffed up' inner region of which the density may roughly be represented by a spherical distribution of material. For the systems discussed in this thesis, spherically optically thick dust distributions can be ruled out by observations. For instance, the central stars in these systems are bright and hardly reddened. For the studies presented in this thesis a full radiative transfer calculation for a spherical geometry is therefore not required. For that reason, we will not discuss computational methods used to solve the radiative transfer equation for a spherical geometry.

2.1.2 Radiative transfer in axisymmetric geometry

As pointed out previously, one expects the dust in HAEBE systems to be distributed in a disk-like geometry. If we assume translational symmetry in the \( z \)-direction of a Cartesian
coordinate system, transfer equation (2.3) can be written as

\[
\frac{dI_\nu(r,\hat{s})}{ds} = s_x \frac{\partial I_\nu(r,\hat{s})}{\partial x} + s_y \frac{\partial I_\nu(r,\hat{s})}{\partial y} = -\chi_\nu(r) [I_\nu(r,\hat{s}) - S_\nu(r)],
\]

(2.16)

where \( \mathbf{s} = (s_x, s_y) \) and \( \mathbf{r} = (x, y) \). This equation can be solved by constructing sets of rays, covering all directions, along which formal solutions (i.e. with given source function) are performed that end in all points \( \mathbf{r}_e = (x_r, y_r) \) defined within the Cartesian system, for which the specific intensity is wanted. If the grid points \( \mathbf{r}_e \) are chosen sensibly and if averaging procedures are employed, one needs only to solve for transfer along portions of these long rays as one ‘sweeps’ through the grid. The method of solving the integral only along small portions of the ray is generally referred to as Short Characteristics. In Chapter 7, we will use a radiative transfer model based on a Short Characteristics method defined in spherical coordinates (Dullemond and Turolla 2000), to study the disks of HAEBE systems.

What to expect for the temperature structure of dust distributed in a disk? To give an impression, let us assume a disk which is optically thick to the stellar radiation (i.e. at UV and visible wavelengths), and geometrically flat. In this case, unattenuated stellar light striking the disk at an angle \( \Theta \) is fully absorbed by the dust. Because of this angle, the absorbed energy at \( r \) is only \( \sin \Theta \) times the energy absorbed in an optically thin medium. For sufficiently large distances from the central star, it holds that \( \sin \Theta \approx \frac{R_*}{r} \). In a derivation very similar to the one discussed in section 2.1.1, we find for the temperature distribution

\[
T(r) \approx \frac{R_*}{r^{3/4}} \left( \frac{R_*}{r} \right)^{3/4(p+1)}
\]

(2.17)

which is simply the optically thin result, multiplied by a factor \( \frac{R_*}{r} \). In case \( p = 1 \), this reduces to \( T(r) \approx T^{-0.6} \). This implies that in an optically thick and geometrically thin disk, the temperature shows a faster decline with radial distance than in an optically thin medium. The flat disk assumption is an oversimplification for the actual disk structure of HAEBE systems. More complicated disk geometries, based on hydrostatic and radiative equilibrium, show that the disks are expected to be flared, i.e. that the angle \( \Theta \) increases with increasing distance from the central star (Chiang & Goldreich 1997; Dullemond, Dominik & Natta 2001). A simplified treatment of radiative transfer in these disks defines two regimes: first, an optically thin surface layer where dust is irradiated by direct stellar light; and second, an optically thick interior in which dust only receives processed photons emitted from the surface layer. Because of the flaring of the disk, the dust temperature profile in the surface layer is in between that of an optically thin medium and an optically thick flat disk. Still, the dust in the surface layer is heated to higher temperatures relative to dust in the interior.

In Chapter 5 we will show that if we assume the dust medium to be optically thin, one typically finds that two geometrically separated dust regimes are needed to explain the spectral energy distribution. An inner regime containing relatively hot grains, and a more distant regime containing relatively cool grains. One cannot exclude on the basis
of SED fitting alone that such a bi-modal temperature distribution is the result of a physical gap in the disk of HAEBE systems due to the clearing out of dust by a protoplanet. However, in view of the discussion above, it may be more likely that it results from the presence of a hot surface layer and a cool disk interior occupying essentially the same radial zone.

2.2 Chemical composition and grain structure of circumstellar dust

As briefly mentioned in Chapter 1, dust grains are formed in the stellar winds of stars in the late phases of stellar evolution. Depending on the atomic C/O ratio, either oxygen rich dust species like silicates, both crystalline and amorphous, are formed (e.g. OH/IR stars Sylvester et al. 1999), or dust species typical for a carbon rich environment, such as amorphous carbon or graphite, or magnesium sulfides (e.g. carbon rich AGB stars Begemann et al. 1994). The dust species formed in the stellar wind will be injected into the interstellar medium (ISM), where they will mix with dust grains already present. Within the ISM substantial processing takes place (e.g. Henning 1999; Tielens 1998). This processing leads to the formation of dust grains of a mixed carbon and oxygen chemistry. Since no crystalline silicates are observed in the ISM, the processing must also lead to the amorphisation of the crystalline silicates initially formed in outflows. It is this dust composition that is present at the onset of star formation. At later phases, substantial dust processing takes place in the disks surrounding the protostars. Using the spectrographs onboard the Infrared Space Observatory (ISO; Kessler et al. 1996) satellite, enormous progress has been made in determining both the dust composition as well as the processes that govern this composition in pre-main-sequence systems. By comparing the ISO spectra with laboratory spectra of dust material (e.g. see Fig. 1.3), the individual dust species contributing to the ISO spectra can be identified. Dust species such as silicates, both crystalline as well as amorphous, metallic iron, iron oxide, carbonaceous grains and water ice, have been identified in the ISO spectra of Herbig Ae/Be (HAEBE) systems (e.g. van den Ancker et al. 2000; Bouwman et al. 2000a; Malfait et al. 1999, 1998b). In the following we will discuss the properties and chemistry of the species present in the protoplanetary disks around HAEBE stars.

2.2.1 Silicates

The most abundant rock forming dust species are silicates, a class of materials also commonly found on Earth (i.e. 90% of the Earth's crust consists of silicates). The fundamental unit on which the structure of all silicates is based consists of four O\(^{2-}\) ions forming a regular tetrahedron, with at its center one Si\(^{4+}\) ion. The bond between the oxygen and silicon ions is about 50% ionic and 50% covalent. So, although the bond arises in part from the attraction of oppositely charged ions, it also involves sharing of electrons and inter-penetration of the electronic clouds of the ions involved. Each O\(^{2-}\) ion can potentially bond to another silicon ion and enter into another tetrahedral grouping. In this
way oxygen is used to bridge different tetrahedral groups. The silicates can be divided into several families based on their chemical composition and structure. We will discuss the most important silicates, which are the ones used in the modeling presented in this thesis.

**Olivine**

If no oxygen ions are shared, implying that the silicate is made up of independent $\text{(SiO}_4)^{4-}$ groups, the silicate is called a nesosilicate. A schematic representation of this structure is shown in Fig. 2.1. A member of this class of silicates is olivine. The tetrahedral units in olivine are bound to each other only by ionic bonds from interstitial (i.e. in the spaces between the tetrahedral units) cations (Fe$^{2+}$ and Mg$^{2+}$), forming an orthorhombic crystal. The chemical composition of olivine is given by $\text{Mg}_{2x}\text{Fe}_{2-2x}\text{SiO}_4$, where $x$ is between 1 and 0. Olivine forms a complete solid solution series from forsterite ($\text{Mg}_2\text{SiO}_4$) to fayalite ($\text{Fe}_2\text{SiO}_4$).
Pyroxene

If two of the four oxygen ions in the SiO$_4$ tetrahedron are shared, the silicate is called an inosilicate. The tetrahedral units in such a silicate form a chain, resulting in a bulk atomic ratio Si:O of 1:3. This structure is also plotted in Fig. 2.1. A member of this class of silicates is pyroxene. The chemical composition of pyroxene is given by $\text{Mg}_2\text{Fe}_2-x\text{Si}_x\text{O}_6$, where $x$ is between 1 and 0. Pyroxene forms a solid solution series from enstatite $\text{Mg}_2\text{Si}_2\text{O}_6$ to ferrosilite $\text{Fe}_2\text{Si}_3\text{O}_6$. The crystal structure of these silicates is orthorhombic. The iron and magnesium cations can be substituted by other ions like Ca$^{2+}$, forming a mineral like diopside ($\text{CaMgSi}_2\text{O}_6$), which has a monoclinic lattice structure.

Silica

Another important class of silicates, which for instance make up for about 64% of the Earth's rocky crust, are minerals built about a three dimensional framework of linked SiO$_4$ tetrahedra. These minerals belong to the tectosilicate class in which all the oxygen ions in each tetrahedron are shared with neighboring tetrahedra. This results in a bulk Si:O atomic ratio of 1:2. A schematic representation of this structure can be seen in Fig. 2.1. A member of the tectosilicate class is silica, consisting only of SiO$_4$ tetrahedra, with the bulk chemical composition given by SiO$_2$. Silica has nine polymorphs among which are quartz, tridimite and cristobalite, differing in crystal structure. While all these silicates quartz is the most common form found on Earth, the common form found in interplanetary dust particles (IDPs) is tridimite (Rietmeijer 1988).

Amorphous silicate

The minerals discussed above were ordered by their lattice structure. However, apart from forming crystals, silicates can also be amorphous, i.e. have neither lattice order nor orientational order. Such materials are glasses or smokes. As will be discussed in the following chapters in this thesis, the bulk of the silicate dust seen in space is in this form. In an amorphous silicate, such as a glass, the basic unit is still the SiO$_4$ tetrahedron, but each such tetrahedron has a different number of bridging oxygen ions randomly linked to other tetrahedra. The resulting distribution of bridging oxygen ions per tetrahedral unit is peaked around the average bulk crystalline value (Farnan et al. 1992).

2.2.2 Other dust species

Though the silicates make up for most of the dust mass in HAEBE systems, several other dust species have been identified, and they can dominate the ISO spectra within specific frequency intervals.
Carbonaceous grains

As mentioned previously, the dust seen in HAEBE systems is a mixture of oxygen rich and carbon rich materials. The ISO spectra show emission bands which can be attributed to polycyclic aromatic hydrocarbons (PAHs; see for instance Chapter 3). These are large molecules with an aromatic structure transiently heated by the central star. As will be discussed in Chapter 4, evidence for the presence of aliphatic hydrocarbons can also be found. These molecules are, contrary to the PAHs, most likely incorporated in carbonaceous grains. Modeling of these molecules is beyond the scope of this thesis. We will, however, include carbonaceous grains in the dust mixture used in our models. A form of carbonaceous material is graphite. In this material the carbon atoms are arranged in layers with a covalent bonding, while the layers themselves are held together by van der Waals bonds. This type of material is a high temperature condensate. If carbonaceous material has been formed within the cold ISM or at lower temperatures in outflows, the carbonaceous material will be amorphous in nature, i.e. will not have such layered structure.

Iron

Another spectroscopically important dust species is iron or iron containing material. As we will see in following chapters, these dust grains can dominate the near-IR emission seen in HAEBE systems. Apart from being incorporated in silicates, iron can also be in the form of metallic iron, iron oxide, or iron sulfide. Both iron oxide and iron sulfide have been used to identify an emission band around $\sim$23 $\mu$m. In this thesis we will use FeO to explain this band. However, the possibility that this emission is due to iron sulfide cannot be ruled out.

Water ice

At temperatures below 150 K, water will be in the form of ice. The water molecules in the ice are bonded to each other by hydrogen bonds. In total nine polymorphs of ice are known. Water ice can be both crystalline as well as amorphous. The ice crystals can be cubic or hexagonal. Spectroscopically, however, there is little difference between the different crystalline forms.

2.2.3 Dust chemistry

The grain species discussed in the previous section do not exist independently but are part of a complex chemical network, in which dust species are transformed into one another. The reactions depend on temperature and to a lesser extent on pressure. Though we do not include a detailed chemical network in our models we do include a temperature dependency of the dust composition. Important processes that are determined by the dust temperature are crystallisation and grain evaporation by either heating the grain above the the thermal stability limit or by chemical sputtering. Crystallisation occurs at
sufficiently high temperatures, when the atoms in the amorphous material start to re-arrange themselves into energetically more favorable positions and orientations within the lattice structure. Silicate dust grains will crystallise at temperatures above 1100 K at timescales much shorter than any dynamical timescale (e.g. Hallenbeck et al. 2000; Gail 1998). In our calculations we will therefore adopt this temperature as the maximum temperature of the amorphous silicate dust. The evaporation temperature of the crystalline silicates is higher than the crystallisation temperature, and depends on chemical composition and lattice structure. The most stable silicates, the pure magnesium end members of the olivine and pyroxene silicate family, forsterite and enstatite respectively, will evaporate at temperatures of \( \sim 1400 \) K. We will adopt this temperature as the maximum grain temperature of the silicates.

As we will see in Chapter 4, when we discuss the crystallisation process of the silicate forsterite, if the bulk composition of the amorphous silicate differs from the crystalline silicate, also silica will be formed. Assuming an amorphous silicate with a serpentine composition (Mg\(_3\)Si\(_2\)O\(_7\)) forsterite and silica will be formed by the reaction

\[
2\text{Mg}_3\text{Si}_2\text{O}_7 \rightarrow 3\text{Mg}_2\text{SiO}_4 + \text{SiO}_2. \tag{2.18}
\]

Forsterite and silica form a meta-stable system. Depending on the amount of reaction surface between both minerals, they will form enstatite by the reaction

\[
\text{Mg}_2\text{SiO}_4 + \text{SiO}_2 \rightarrow \text{MgSiO}_3. \tag{2.19}
\]

Olivine and pyroxene can incorporate iron in their lattice structure. However, at high temperatures of \( \sim 800 \) K in a reducing environment (i.e. low oxygen pressure), iron will be removed from the lattice. For olivine dust grains this reaction is

\[
2\text{MgFeSiO}_4 + 2\text{H}_2 \rightarrow \text{Mg}_2\text{SiO}_4 + 2\text{Fe} + \text{SiO}_2 + 2\text{H}_2\text{O}. \tag{2.20}
\]

This process will form the pure magnesium end member forsterite as well as silica and metallic iron grains (e.g. Allen et al. 1993). The evaporation temperature of metallic iron is comparable with that of the silicate dust. We have adopted in our models a maximum grain temperature for the metallic iron grains of 1500 K. At temperatures below 720 K metallic iron can react with sulphur containing molecules to form iron sulfide

\[
\text{Fe} + \text{H}_2\text{S} \rightleftharpoons \text{FeS} + \text{H}_2, \tag{2.21}
\]

or oxidize below 400 K to form iron oxide.

\[
\text{Fe} + \text{H}_2\text{O} \rightleftharpoons \text{FeO} + \text{H}_2. \tag{2.22}
\]

In principle, carbonaceous grains may be heated to \( \sim 1500 \) K before they will thermally decompose. However, Finocchi et al. (1997) point out that at temperatures above 1000 K the carbonaceous grains will be destroyed by chemical surface reactions. This
would also imply that amorphous carbon grains will not reach sufficiently high temperatures to form graphite, but will be destroyed before that can happen. We will therefore adopt 1000 K as the maximum grain temperature for the carbonaceous grains.

Given the gas pressure conditions in the circumstellar disks surrounding the HAEBE stars, water ice will vaporize at temperatures in excess of 150 K. The water ice will be crystalline if formed at temperatures above \( \sim 120 \) K. If formed below this temperature, it will be amorphous.

### 2.2.4 The grain structure

Apart from dust processes discussed above, the dust grains in the protoplanetary disks are also subject to coagulation and shattering by grain-grain collisions (e.g. Weidenschilling 1997). Grain growth can proceed either directly from the gas phase or by aggregation of smaller grains. This latter process will lead to “fluffy” chemical inhomogeneous grains resembling IDPs. Also the processes described in the previous section can lead to chemically inhomogeneous grains. Incomplete crystallisation of an amorphous grain will obviously lead to a grain that is partially crystalline and partially amorphous. Crystallisation reactions such as \( \text{Eq. (2.18)} \) will also lead to inhomogeneous grains. Furthermore, water will most likely freeze out onto the grain surface at temperatures below 150 K, leading to a core-mantle structure.

It is, however, debatable whether inhomogeneities in grain structure can be identified spectroscopically. If for instance the dust grains in the protoplanetary disks around HAEBE stars bear resemblance to cometary grains this could well be the case. Theoretical considerations suggest cometary grains to be extremely fluffy, implying that the spectroscopic properties of the grains will be dominated by the smaller compact units making up the porous aggregate (Greenberg and Hage 1990; Brucato et al. 1999). The larger aggregate would spectroscopically behave as a cloud of smaller compact grains. Also, if the timescales on which crystallisation proceeds are sufficiently short, any phase in which the grain is inhomogeneous and unequilibrated might not be observable. Similarly, if ice condensation is an efficient process, leading to an ice mantel much larger than the core, it could effectively shield the core and consequently the particle will behave spectroscopically as a homogeneous grain.

In our modeling we will therefore treat the dust grains in a first order approximation as single, chemically homogeneous and compact. The effect of grain coagulation and/or shattering is incorporated in the models by assuming a power-law grain size distribution. The number density of grains with (volume equivalent) radii between \( a \) and \( a + da \) is given by

\[
n(a)da = A \left( \frac{a}{a_{\text{min}}} \right)^m da,
\]

where the grain radius \( a \) is limited between a minimum and maximum value, \( a_{\text{min}} \) and \( a_{\text{max}} \), respectively. The normalisation constant \( A \) is determined by

\[
\rho = \int_{a_{\text{min}}}^{a_{\text{max}}} \frac{4}{3} \pi a^3 \rho_{\text{gr}} n(a)da
\]

23
where \( \rho \) is the density of the medium due to the dust species and \( \rho_d \) is the bulk density of the dust grains.

### 2.3 The optical properties of dust grains

The absorption, scattering, and thermal emission properties of a dust grain are determined by its chemical composition, lattice structure, shape and size. Once these grain properties are known, it is in principle possible to calculate the interaction of an incoming electromagnetic wave with the grain. Depending on its wavelength, radiation will be able to interact with the electrons, or it will excite vibrations in the material. Electronic transitions are mostly found at ultraviolet and optical wavelengths; conductors and isolators show different behaviour depending on the availability of free electrons.

Vibrational modes are found in the mid- and far-infrared. This wavelength range is particularly rich in strong vibrational resonances of abundant molecular bonds in solids, such as the Si-O fundamental vibrational band at about 10 \( \mu \)m, seen in amorphous silicates. The lattice structure strongly influences the vibrational resonances that can be distinguished observationally. For instance, in crystalline silicates the ordered lattice structure causes well-defined wavelengths of resonances and thus a multitude of sharp bands, while in amorphous silicates many of these bands merge into two broad resonances at \( \sim 10 \) and \( \sim 18 \) \( \mu \)m, while other bands disappear all together.

Whether these resonances actually show up in the infrared spectrum (either as emission or absorption bands), depends on the grain size: if the grain dimensions are large compared to the wavelength of the resonance, phonons generated in the solid will be scattered inside the particle, resulting in black body emission of the grain. This implies that we cannot determine the chemical composition of large (typically \( > 10 \mu \)m) grains. In our analyses, we have assumed that the grain composition of large grains is similar to that found for the small grain population.

In addition, the wavelength of some resonances in materials such as FeO and MgO, are very sensitive to grain shape. This occurs because of the generation of surface phonon modes whose wavelength depends on grain shape. The fact that bands shift due to grain shape effects complicates the identification of these materials in astronomical spectra. Therefore, it is important to characterize the grain population not only in terms of composition and lattice structure, but also in terms of grain size and shape (see also Sect. 2.2.4 for the effects of grain aggregates on optical properties).

#### 2.3.1 The refractive index

The optical properties of a material can be characterized by the complex refractive index

\[
N_k = n'_k + in''_k \tag{2.25}
\]

where \( n' \) and \( n'' \) are the real and imaginary part respectively, also referred to as the optical constants, and \( k \) is the wavelength. A plane wave traveling in a direction \( \vec{z} \) through a
medium which has a refractive index \( N \), has the form

\[
E = E_0 \exp \left( -\frac{2\pi n'' z}{\lambda} \right) \exp \left( -\frac{i2\pi n' z}{\lambda} - i\omega t \right),
\]

(2.26)

where \( \omega \) is the angular frequency. As one can immediately see from Eq. (2.26), the imaginary part of the refractive index, \( n'' \), determines the exponential decay of the wave as it moves through the medium. This directly links \( n'' \) to the absorption coefficient of the material. The real part of the refractive index, \( n' \), determines the phase velocity \( v = c/n' \), where \( c \) is the speed of light.

The refractive index can be linked to the microscopic properties of a material by treating the ions, electrons and lattice as simple harmonic oscillators (e.g. see Chapter 9 of Bohren and Huffman 1983). From laboratory measurements of the refractive index for a specific material, the extinction behaviour of dust grains can, in principle, be calculated.

### 2.3.2 Basic scattering theory

In this section we will discuss some basic concepts of light scattering. For details we refer to van de Hulst (1957) and Bohren and Huffman (1983). Consider a single particle of arbitrary size and shape, illuminated by a plane harmonic wave traveling in a direction \( z \).

A schematic representation of the situation is given in Fig. 2.2. The incident plane wave can be written as

\[
E_i = \left( E_{0||} \hat{e}_{||} + E_{0\perp} \hat{e}_{\perp} \right) e^{i(kz-\omega t)};
\]

(2.27)

where \( k \) is the wave number in the medium surrounding the particle, and \( \hat{e}_{||} \) and \( \hat{e}_{\perp} \) are basis vectors parallel and perpendicular to the scattering plane, i.e. the plane containing the directions of the incident light and the light scattered in a particular direction. First we assume that the particle is spherical, i.e. a homogeneous isotropic sphere. The scattered field at a distance \( r \) of the particle in a direction making an angle \( \theta \) with the
direction of the incident light can be represented by

\[ \mathbf{E}_i = \mathbf{S}(\vartheta) \frac{e^{ikr-W}}{-ikr}. \]  

(2.28)

Here \( \mathbf{S}(\vartheta) \) is a \( 2 \times 2 \) complex matrix, called the amplitude scattering matrix, which depends on the scattering angle \( \vartheta \), and on the size as well as the refractive index of the spherical particle. Eqs. (2.27) and (2.28) can be combined to give the relation between the incident and scattered fields. The result is

\[
\begin{pmatrix}
E_{\parallel} \\
E_{\perp}\end{pmatrix} = e^{ik(W-\vartheta)} 
\begin{pmatrix}
S_2(\vartheta) & 0 \\
0 & S_1(\vartheta)\end{pmatrix} 
\begin{pmatrix}
E_{\parallel} \\
E_{\perp}\end{pmatrix},
\]

(2.29)

where \( S_i \) are the elements of the amplitude scattering matrix. For the forward direction \( (\vartheta = 0) \) we have \( S_1(0) = S_2(0) \).

The extinction cross section of the particle is given by

\[ C_{\text{ext}} = \frac{4\pi}{k^2} \text{Re}\{S_1(0)\} \]

(2.30)

and its scattering cross section by

\[ C_{\text{sca}} = \frac{\pi}{k^2} \int_0^{\pi} \left\{ |S_1(\vartheta)|^2 + |S_2(\vartheta)|^2 \right\} \sin \vartheta d\vartheta. \]

(2.31)

The absorption cross section can be calculated from

\[ C_{\text{abs}} = C_{\text{ext}} - C_{\text{sca}}. \]

(2.32)

The extinction efficiency factor is defined as

\[ Q_{\text{ext}} = \frac{C_{\text{ext}}}{\pi a^2}, \]

(2.33)

where \( a \) is the radius of the spherical particle. The scattering efficiency factor \( Q_{\text{sca}} \) and absorption efficiency factor \( Q_{\text{abs}} \), are defined analogously. For scattering by a collection of spherical particles one can add the cross sections of the individual spheres.

The exact solution of Maxwell's equations for homogeneous isotropic spheres is referred to as Mie theory after Gustav Mie (1908). Using this theory we can compute the scattering and absorption properties of spherical particles for all values of refractive index, size and wavelength needed for the studies described in this thesis.

Computations and experiments to obtain the scattering and absorption properties of non-spherical particles are, in general, much more difficult than for spherical particles (e.g. Mishchenko et al. 2000). A notable exception is, however, Rayleigh scattering, which is a good approximation for particles whose size is small compared to the wavelength inside and outside the particle. To estimate the effects of non-spherical grain
shapes on the absorption cross section we will use a statistical approximation in the Rayleigh domain. This is based on the assumption that cross sections of collections of randomly oriented irregular particles can be approximately calculated by averaging over a uniform distribution of ellipsoidal shapes of a collection of ellipsoids with random orientation. This method is usually referred to as continuous distribution of ellipsoids (CDE). If the ellipsoids have the same volume and $a$ is the radius of an equal-volume sphere, we find for the absorption cross section in the Rayleigh domain (see Bohren and Huffman 1983, Section 12.2)

$$C_{\text{abs}} = \frac{8\pi^2 a^4}{3\lambda} \ln\{\alpha\} \quad (2.34)$$

where

$$\alpha = 2 \frac{N^2}{N^2 - 1} \log N^2 - 2 \quad (2.35)$$

is the polarizability per unit particle volume, in which $\log N^2$ denotes the principal value of the natural logarithm of the complex number $N^2$.

### 2.3.3 Extrapolation of the refractive index to short and long wavelengths

Ideally one would like to have the measured values of the refractive index for the entire wavelength range, i.e. from UV to far-IR, required for radiative transfer calculations. However, often the laboratory measurements do not cover this entire wavelength interval. By using the results from the oscillator model for the refractive index outside of the measured wavelength ranges we can make the following extrapolations. At wavelengths shorter than those at which the electronic transitions occur, i.e. in the far-UV, the refractive index given by Eq. (2.25) can be extrapolated far from resonances by using

$$n' \simeq 1 - \frac{\omega_p^2}{2\omega^2} \quad (2.36)$$

$$n'' \simeq \frac{\gamma \omega_p^2}{2\omega^3} \quad (2.37)$$

with $\omega$ the angular frequency, $\omega_p$ the plasma frequency, and $\gamma$ a damping factor of the electromagnetic wave (see e.g. Bohren and Huffman 1983, Sect. 9.1.2). Both insulators and metals show the same behaviour at these wavelengths. These extrapolations are reasonable for wavelengths shorter than $\sim 0.2 \mu m$ and can thus be used to compute the cross sections. At long wavelengths (sub-millimetre and millimetre) there is a marked difference in optical properties between grains of different solid-state structure, composition and shape. In this regime, we extrapolate the cross section (see also Sect. 2.3.2),

$$C_{\text{ext},\lambda} \approx \frac{1}{\lambda^w} \quad (2.38)$$

where $w$ is between 1 and 2 for small grains, depending on lattice structure and grain shape.
2.4 The spatial distribution of the dust

The exact geometry of the circumstellar dust in HAEBE systems is still a matter of controversy. The emission features seen in the ISO spectra, however, suggest that a substantial optically thin medium must be present. As discussed in previous sections, this prompted us to use an optically thin, spherically symmetric model. The dust grains are distributed in a single shell or in multiple shells. The density structure within each shell is given by

$$\rho(r) = \rho_0 \left( \frac{r}{R_{in}} \right)^n,$$  \hspace{1cm} (2.39)

where $r$ is the radial coordinate measured from the central star and limited between the inner radius $R_{in}$ and outer radius $R_{out}$ of the dust shell, and $\rho_0$ the density at the inner radius.

If the medium is optically thin, both disk as well as spherical geometries, provided they have the same radial density distribution, will produce identical thermal emission spectra. As discussed in Sect. 2.1.1, a more useful diagnostic than the actual spatial distribution is therefore the mass-temperature distribution, $M_{dust}(T)$, which determines the resulting dust emission. The derived $M_{dust}(T)$ is actually a quite robust result that is expected to reproduce well the actual mass over temperature distribution in disks that are optically thick in radial directions through the disk. When seen at an inclination for which along the line-of-sight the medium is optically thin, the derived $M_{dust}(T)$ still provides the correct result. In a detailed study of HD104237 (Chapter 7) we indeed found that at almost all wavelengths the disk is indeed optically thin for the inclination at which the system is observed. However, even if $M_{dust}(T)$ is identical, the actual spatial mass distribution, $M_{dust}(r)$, of a radial optically thick disk can deviate significantly from the optically thin model. To investigate the effect of a disk like geometry on the modeling results compared to spherical models, we will use a simple parameterised disk model. In this model the density in polar coordinates is defined as follows:

$$\rho(r, \theta) = \rho(r)\rho(\theta)$$  \hspace{1cm} (2.40)

where the functions $\rho(r)$ and $\rho(\theta)$ are defined by

$$\rho(r) = \rho_n \left( \frac{r}{R_n} \right)^n,$$  \hspace{1cm} (2.41)

$$\rho(\theta) = x + (1-x)\cos^2(\theta).$$  \hspace{1cm} (2.42)

Here $\theta$ is the angle between $r$ and the mid-plane, $x = \rho_p/\rho_n$ is the ratio of the density at the poles, $\rho_p$, and the density in the mid-plane, $\rho_n$, and $\rho_n = \rho(R_{in}, 0)$ is the mid-plane density at the inner radius of the disk. An example of this density structure is plotted in Fig. 7.1.
2.5 The strategy of modeling

The goal of modeling HAEBE systems is to recover the properties of the circumstellar dust. The main diagnostics that one has available, at least in principle, are the infrared spectral energy distribution as well as ground-based near- & mid-IR and millimetre imaging. The HAEBE systems studied in this thesis are relatively near-by and have been well studied from the ground as well as with the ISO satellite. For a sample of fourteen HAEBE stars we have obtained IR-spectra in the range from 2-200 µm using the Short Wavelength Spectrometer (SWS; de Graauw et al. 1996) and Long Wavelength Spectrometer (LWS; Clegg et al. 1996) instruments onboard the ISO satellite. Several attempts have been made to image the HAEBE stars in the near-IR. However, these data are of limited use as the characteristic emitting region of the hot dust responsible for the near-IR flux is limited to a few AU from the central star. Given a typical distance of 150 pc for our set of HAEBE stars, this implies that the near-IR radiation originates from within the order of a few 0.01 arcsec from the central star, which is below the angular resolution limit of direct imaging of ∼0.5 arcsec. At this time, the only way to resolve the inner disk structure, where the hot dust is located, is using interferometric instruments. However, near-IR observations of this type only use a very small number of baselines (two) and provide no phase information, which does not allow to reconstruct a detailed image. Still, these observations are useful as they provide constraints on the location of the inner edge of the circumstellar dust disk by using the visibility data (Millan-Gabet et al. 2001).

Imaging at longer wavelengths, i.e. in the far-IR, millimetre and radio regime suffers less from the angular resolution problems that exist in the near-IR. First, this is because the flux at these wavelengths is emitted by cold dust located at relatively large distances from the star, i.e. up to order 100 AU. Second, the interferometric instruments operating at these wavelengths have a larger number of independent baselines and provide phase information which makes the reconstruction of an image possible. These two properties combined allow, at least in principle, to image the spatial distribution of the cold dust. Indeed, several of the sources studied in this thesis have been resolved at millimeter wavelengths (e.g. Mannings and Sargent 1997).

The above discussion shows that at least the modeling of the inner disk relies almost solely on spectral fitting. The great challenge is to constrain as many dust properties as possible from this fitting. These include the chemical composition and lattice structure of the grain material, the size and shape of the particles, and their spatial distribution. Because of the many ways in which these dust properties can affect the infrared energy distribution, it is found that the geometry and properties of the material cannot be determined uniquely, if only the spectrum is available.

To some extent this problem is independent of the optical thickness of the material. Here, we will illustrate this ambiguity using predictions based on the assumption of an optically thin medium. Four types of degeneracies may readily be identified. The first three relate to the degeneracy in the mass-temperature distribution (cf. Sect. 2.1.1). More specific, for a fixed grain composition, the shape and strength of the SED is determined by an average mass-temperature profile. The grain temperature depends on the radial distance to the star and on grain size, where the smallest grains have the high-
Figure 2.3: Model spectra of amorphous olivine (Dorschner et al. 1995). The solid line in both panels indicates a model with a power-law grain size distribution with power $m = -2.8$ (see Eq. 2.23) and spherical grains with radii between 0.01 and 5.0 $\mu$m. The density distribution is proportional to $r^{-1}$ and an inner and outer bound of 160 and 1000 stellar radii, respectively, has been adopted. Panel a: Variations of the grain-size distribution. Panel b: Variation of the inner-and outer boundary of the dust region.

...temperatures. This implies that the mass-temperature profile will be determined by average grain size and spatial distributions.

i) Different grain size distributions with the same average temperature will produce identical spectra if the density ($g$ cm$^{-3}$) is appropriately scaled. Fig. 2.3a shows this degeneracy, using a power-law grain size distribution for the emission of amorphous spherical olivine grains. The test indicates that in this way minimum and maximum grain sizes may be varied by about an order of magnitude!

ii) One may also play this game using the inner- and outer boundary of the dust region. Fig. 2.3b shows an example in which the size distribution is kept invariant, but where the geometrical extent of the dust region is modified. This shows it is also possible to change the dimension of the dust region by almost an order of magnitude without modifying the flux distribution.

iii) Similar average mass over temperature profiles may also be reached by placing small grains further out or large grains closer to the central star. This ambiguity, however, only plays a rôle in certain regimes of the grain size. For instance, in the case of metallic iron (Fig. 2.4a) a change in grain size of over two orders of magnitude is possible.
without significantly changing the emergent NIR flux distribution. For a large part this same result can be obtained for amorphous olivine grains (Fig. 2.4b), although when a certain maximum grain size is reached ($\sim 1\mu m$) the feature amplitude suddenly changes dramatically even after tuning of the extent of the dust region.

iv) A further problem arises when no clear spectral signature, such as the 9.7 $\mu m$ silicate feature, is present but only a broad continuum. The possibility of confusion of the relative contribution of the individual dust species then exists. Fig. 2.5 shows the continuum dust emission from dust species other than silicates for three different models. The predicted NIR fluxes are almost indistinguishable, although the adopted chemical compositions vary significantly.

It may seem that the above test results sketch a somewhat gloomy picture for our chances of improving our insight in the properties of the ambient medium of HAEBE stars if only spectra are available. Fortunately, the situation is not as bad as it may seem.

Some degeneracies in the modeling may be resolved using physical constraints such as dust destruction temperatures. For example, the test case shown in Fig. 2.5 in which an identical near-IR flux is produced by three distinctly different chemical compositions may be resolved using $T_{\text{evap}}$ (see also Sect. 2.2.3). The temperatures required to emit efficiently in the 1 to 4 $\mu m$ region are of the order of 1500 K. As argued in Sect. 2.2.3,
Figure 2.5: Continuum dust emission from dust species contributing to the NIR between 1 and 9 \( \mu \text{m} \) for three different models. The solid line indicates a model consisting of amorphous carbon (Preibisch et al. 1993), metallic iron and iron oxide, with mass fractions of 0.55, 0.2 and 0.25 respectively. The dashed line indicates a model with only amorphous carbon and metallic iron with mass fractions of 0.53 and 0.47. The dotted line indicates a model where the entire NIR emission is due to graphite (Laor et al. 1993).

Chemical processes may also be used to constrain the dust formation history. An example is the expected coexistence of forsterite and silica as a consequence of the crystallisation process at high temperatures (see Eq. 2.18). This thermal annealing argument is used in Chapters 4 and 6 to establish or exclude high temperature crystallisation as the formation mechanism of forsterite.

In this thesis we will demonstrate that imposing physical constraints on spectral analysis results – even in the absence of imaging data – provides a powerful tool to learn more about the properties and processing of dust around HAEBE stars.