

MODELING THE ASTRONOMICAL SILICATE MINERALOGY: ON THE EFFECTS OF GRAIN TEMPERATURE

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ABSTRACT

The mineralogical composition of dust contains important information regarding the origin and processing of the dust and the physical, chemical, and evolutionary properties of the astrophysical environment where the dust is found. In the literature, the composition of cosmic dust is usually inferred by fitting the observed infrared (IR) emission spectrum with a sum of emission spectra calculated from various individual grain species of different sizes but *assuming a single, identical temperature* for them. However, we show in this work that these grains of different compositions and/or different sizes, while in thermal equilibrium with the radiation field to which the grains are exposed, achieve different temperatures. The effects of dust temperature on dust compositional studies are demonstrated by showing that the IR emission spectrum calculated from a mixture of grains emitting at different temperatures differs substantially from that of the same grain mixture but with a single, identical temperature. Therefore, the need for obtaining realistic temperatures from realistic cosmic dust analogs is a key to properly interpreting the observational IR emission spectra, e.g., the rich set of data that the *Spitzer Space Telescope* has been collecting.

Subject headings: comets: individual (C/2002 V1 (NEAT)) — dust, extinction — infrared: ISM — infrared: solar system — radiation mechanisms: thermal

1. INTRODUCTION

Astromineralogy, which deals with the science of gathering mineralogical information from the astronomical spectroscopy of small bodies in the solar system such as asteroids and comets and of dust in interstellar and circumstellar environments, has been developed unprecedentedly since the launch of the *Infrared Space Observatory (ISO)*; see Henning 2003). With considerable progress being made in the experimental characterization of cosmic dust analogs during the last decade (e.g., see Colangeli et al. 2002 and Henning et al. 2004), and with the rich set of high-quality spectroscopic data collected by *ISO* and the ongoing *Spitzer Space Telescope*, it is now possible to carry out detailed astromineralogical investigations of individual dust species under various astrophysical environments. By studying the mineralogical composition of dust, we can obtain important information regarding the origin and processing of the dust and the physical, chemical, and evolutionary properties of the astrophysical environment where the dust is found. This is clearly demonstrated in the mineralogical studies of cosmic silicate dust.

Silicates, which reveal their presence in astrophysical regions by their strong 9.7 and 18 μm absorption or emission features that are respectively ascribed to the Si-O stretching and O-Si-O bending modes, are ubiquitously seen in interstellar clouds, H II regions, circumstellar shells around evolved stars, circumstellar disks around young stellar objects (YSOs), main-sequence stars, and interplanetary and cometary dust (see § 1 of Li & Draine 2001 for a review). The shape of the interstellar silicate feature is broad and featureless, both of which suggest that the silicate

is amorphous. Li & Draine (2001) estimated that the abundances of $a < 1 \mu\text{m}$ crystalline silicate grains in the diffuse interstellar medium (ISM) is less than 5% of the solar Si abundance. Kemper et al. (2004) found that the crystalline fraction of the interstellar silicates along the sight line toward the Galactic center is $\sim 0.2\%$. Demyk et al. (1999) placed an upper limit of 1%–2% of the silicate mass being crystalline in two massive protostellar objects. Bowey & Adamson (2002) argued that a mixture of various crystalline silicate minerals with an appreciable mass fraction (up to $\sim 60\%$) could blend together to account for the observed smooth silicate absorption profile at 9.7 μm (but also see Draine 2003).

The originating source of the interstellar silicates is in the atmospheres of cool evolved stars of which the emission features often show a 9.7 μm feature consistent with amorphous silicates and sharper features arising from crystalline silicates (Waters et al. 1996). Crystalline silicates have also been seen in some comets (see Hanner 2004). How can interstellar crystalline silicate dust become amorphous? How can cometary amorphous silicate dust become crystallized? Note that comet nuclei are generally believed to be the most pristine bodies in the solar system and largely preserve the composition of the presolar molecular cloud (Greenberg 1982).⁵ Apparently, the precise mineralogical composition of silicate dust is a key to understanding the origin and energetic processing of grains in different environments and to understanding the evolutionary

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⁵ The upper limits placed on the interstellar crystalline silicate abundance are mainly inferred from the interstellar silicate *absorption* features (Li & Draine 2001; Kemper et al. 2004; Demyk et al. 1999), although attempts have also been made to compare the observed astronomical *emission* spectra with the IR emission spectra expected from stochastically heated ultrasmall (crystalline) silicate dust from a single energetic stellar photon (Désert et al. 1986; Li & Draine 2001). On the other hand, for cometary dust and dust around cool evolved stars, the mass fraction of crystalline silicate dust is derived from the observed *emission* spectra of these objects. For the latter, both the grain size and temperature effects are critical. But in the literature, one often encounters methods in which the grain temperature is taken as an independent parameter instead of derived physically (see Greenberg & Li 1999 for details).

connection among circumstellar, interstellar, protostellar, and cometary environments.

The analysis of astronomical silicate composition is commonly based on the direct comparison of astronomical absorption or emission features with laboratory data of terrestrial silicate candidates or with theoretical spectra calculated from the optical constants measured for silicate analogs. In a previous paper, we have discussed how critical it is to accurately remove the effects caused by the heterogeneous nature of the dust when interpreting the observed silicate *absorption* features (Li et al. 2002). In this work we will demonstrate how critical it is to properly take realistic dust temperatures into account when interpreting the observed silicate *emission* features.

Except for cool dust obscuring IR sources, in the literature, cosmic silicate mineralogy is often inferred by fitting the observed IR *emission* spectrum with a sum of emission spectra calculated from various individual grain species of different sizes but *assuming a single, identical temperature* for them (e.g., see Honda et al. 2004a, 2004b). However, we will show in this work that these grains of different compositions and/or different sizes, while in thermal equilibrium with the radiation field to which the grains are exposed, have different temperatures. Not unexpectedly, the IR emission spectrum calculated from a mixture of grains emitting at different temperatures therefore differs substantially from that of the same grain mixture but with a single, identical temperature. This demonstrates that the *single-temperature assumption* is inappropriate in modeling the observed silicate emission features as a mixture of grains of different compositions and/or sizes. We should stress that the purpose of this work is not to model any specific observations. For illustrative purpose, we will use the 8–13 μm emission spectrum of comet C/2002 V1 (NEAT) observed by Honda et al. (2004a) using the 8.2 m Subaru Telescope just as a basis for comparison.

2. THE “SINGLE-TEMPERATURE APPROACH”

The “single-temperature approach,” originally proposed by Hanner et al. (1994), has been widely used in modeling the 9.7 μm silicate emission spectra observed for comets and dust disks around Vega-type stars, Herbig Ae/Be stars, and T Tauri stars (e.g., see Bouwman et al. 2001, Meeus et al. 2003, and Honda et al. 2004a, 2004b). In this approach, the model spectrum consists of two components: the featureless gray-body continuum emission and optically thin emission of dust features (see Hanner et al. 1994, Colangeli et al. 1995, and Malfait et al. 1998). Both components are usually assumed to have the same source function (see Honda et al. 2004a, 2004b). For producing the dust features, four grain species are usually assumed: 0.1 and 2 μm glassy olivine, 0.1 μm glassy pyroxene, and 0.1 μm crystalline olivine (e.g., see Bouwman et al. 2001, Meeus et al. 2003, and Honda et al. 2004a, 2004b). Therefore, the model emission spectrum can be written as

$$F_{\lambda}^{\text{sta}} = (c_0 + c_1 \kappa_{\text{aolv}}^{0.1 \mu\text{m}} + c_2 \kappa_{\text{aolv}}^{2 \mu\text{m}} + c_3 \kappa_{\text{apyx}}^{0.1 \mu\text{m}} + c_4 \kappa_{\text{forst}}^{0.1 \mu\text{m}}) B_{\lambda}(T), \quad (1)$$

where $\kappa_{\text{aolv}}^{0.1 \mu\text{m}}$, $\kappa_{\text{aolv}}^{2 \mu\text{m}}$, $\kappa_{\text{apyx}}^{0.1 \mu\text{m}}$, and $\kappa_{\text{forst}}^{0.1 \mu\text{m}}$ are the mass absorption coefficients of 0.1 μm glassy olivine, 2 μm glassy olivine, 0.1 μm glassy pyroxene, and 0.1 μm crystalline forsterite grains, respectively; the six free parameters—five multiplication factors, c_0, c_1, c_2, c_3, c_4 , and the emitting dust temperature T —are determined by fitting the observed 9.7 μm silicate feature with a least-square minimization method (see Honda et al.

2004a for details).⁶ This single-temperature approach is very successful in closely reproducing the 9.7 μm silicate emission spectra of various objects (e.g., see Bouwman et al. 2001, Meeus et al. 2003, and Honda et al. 2004a, 2004b). However, this approach is not *physically* justified: *one should not expect the four grain species with different compositions and/or different sizes to emit at the same temperature in an optically thin environment!* If grains are mainly heated by starlight photons (which is the case for dust in interstellar, cometary, and dust disk environments), their temperatures depend on their optical properties and sizes (i.e., on the way they absorb and emit radiation) as well as on the illuminating starlight intensity. In § 3 we will use comet C/2002 V1 (NEAT) as an example to show that these four different grains, exposed to the solar radiation, will emit at very different temperatures and that therefore the emergent emission spectrum differs substantially from F_{λ}^{sta} given in equation (1).

3. COMET C/2002 V1 (NEAT): A TEST CASE

To test the validity of the single-temperature approach, we use the 8–13 μm mid-IR emission spectrum observed on 2003 January 10 for comet C/2002 V1 (NEAT) as a basis for comparison. This spectrum was obtained using the Cooled Mid-Infrared Camera and Spectrometer on the 8.2 m Subaru Telescope when comet NEAT was at a heliocentric distance of $r_h \approx 1.18$ AU and an Earth-to-comet distance of $\Delta \approx 0.84$ AU (Honda et al. 2004a).

Exposed to solar radiation, a cometary grain of spherical radius $a \gtrsim 100$ Å attains an equilibrium temperature \bar{T} from the energy balance between absorption at the ultraviolet (UV) and visible wavelength range and emission at longer wavelengths:

$$\left(\frac{R_{\odot}}{2r_h}\right)^2 \int_0^{\infty} 4\pi J_{\lambda}^{\odot} C_{\text{abs}}(a, \lambda) d\lambda = \int_0^{\infty} 4\pi B_{\lambda}(\bar{T}(a)) C_{\text{abs}}(a, \lambda) d\lambda, \quad (2)$$

where R_{\odot} is the solar radius, $C_{\text{abs}}(a, \lambda)$ is the absorption cross section for a spherical grain of radius a at wavelength λ , J_{λ}^{\odot} is the solar radiation intensity, and $B_{\lambda}(\bar{T}(a))$ is the Planck function at temperature \bar{T} . The absorption cross section $C_{\text{abs}}(a, \lambda)$ for spherical grains can be calculated from Mie theory (Bohren & Huffman 1983), if their complex refractive indices (“optical constants”) $m(\lambda) = m'(\lambda) + m''(\lambda)$ are known. In equation (2) we have neglected the heating of dust by the IR radiation from other grains. While this is valid for cometary dust in optically thin coma, it is certainly invalid for heavily obscured regions (e.g., dense molecular clouds) where the IR radiation from other grains may be an important or even dominant heating source.

Following Honda et al. (2004a), for amorphous olivine we take the optical constants of amorphous MgFeSiO_4 measured by Dorschner et al. (1995), but with the far-UV part constructed by Li & Greenberg (1997). For amorphous pyroxene $\text{Mg}_{0.5}\text{Fe}_{0.5}\text{SiO}_3$, we take the following “synthetic” procedure: for $0.1 \mu\text{m} < \lambda \leq 1 \mu\text{m}$, we take m'' of Pollack et al. (1994) for crystalline

⁶ We note that in this approach, the inclusion of the carbonaceous dust component, whose presence in cometary nuclei as “CHON” particles has been shown by the in situ measurements of comet Halley (Kissel et al. 1986), is not obvious. It is probable that the authors conceivably attributed the gray-body continuum emission to carbonaceous dust (both small and large) and large silicate dust.

TABLE 1
COMPOSITIONS, SIZES, AND BULK DENSITIES FOR THE FOUR GRAIN SPECIES^a

Species	Composition	Size (μm)	Density (g cm^{-3})	T (K)	$T(\text{Honda})$ (K)	$ T - T(\text{Honda}) $ (K)
Olivine	MgFeSiO_4	0.1	3.71	307.8	280	27.8
	MgFeSiO_4	2	3.71	259.4	280	20.6
Pyroxene	$\text{Mg}_{0.5}\text{Fe}_{0.5}\text{SiO}_3$	0.1	3.20	376.0	280	96
Forsterite	Mg_2SiO_4	0.1	3.33	334.8	280	54.8

^a These four grain species were used by Honda et al. (2004a) to fit the 8–13 μm mid-IR spectrum of comet C/2002 V1 (NEAT) at $r_h \approx 1.18$ AU. Also listed are the equilibrium temperatures that those grains achieve when heated by the Sun and the single-temperature $T = 280$ K of Honda et al. (2004a) assumed for all four grain species.

orthopyroxene MgFeSiO_3 ; for $1 \mu\text{m} < \lambda \leq 500 \mu\text{m}$, we take m'' of Dorschner et al. (1995) measured for amorphous $\text{Mg}_{0.5}\text{Fe}_{0.5}\text{SiO}_3$; and for $\lambda > 500 \mu\text{m}$, we assume $m''(\lambda) = m''(500 \mu\text{m})(500 \mu\text{m}/\lambda)$. After smoothly joining the adopted m'' , we calculate the real part m' from the imaginary part m'' using the Kramers-Kronig relation (Bohren & Huffman 1983). For crystalline forsterite Mg_2SiO_4 , we take the (m', m'') -data of Li & Draine (2001) since we could not get access to those of Koike et al. (2003) that were used by Honda et al. (2004a).

⁷ Very recently, Jäger et al. (2003) measured the optical constants of amorphous $\text{Mg}_{0.5}\text{Fe}_{0.5}\text{SiO}_3$ in the broad wavelength range 0.2–500 μm , with the sample prepared by the sol-gel process, a chemical technique based on the condensation of Mg- and Si-hydroxides in a liquid phase. The reason we chose to adopt the m'' of Dorschner et al. (1995) is that Honda et al. (2004a) used the Dorschner et al. (1995) data, and the purpose of this work is to illustrate the temperature effects by comparing our results with those of Honda et al. (2004a, 2004b) using the same sets of optical constants.

We then calculate the absorption cross sections $C_{\text{abs}}(a, \lambda)$ and equilibrium temperatures of glassy olivine of spherical radius $a = 0.1 \mu\text{m}$ ($\bar{T}_{\text{aolv}}^{0.1 \mu\text{m}}$), glassy olivine of spherical radius $a = 2 \mu\text{m}$ ($\bar{T}_{\text{aolv}}^{2 \mu\text{m}}$), glassy pyroxene of spherical radius $a = 0.1 \mu\text{m}$ ($\bar{T}_{\text{apx}}^{0.1 \mu\text{m}}$), and crystalline forsterite of spherical radius $a = 0.1 \mu\text{m}$ ($\bar{T}_{\text{forst}}^{0.1 \mu\text{m}}$). At a heliocentric distance of $r_h \approx 1.18$ AU, we find $\bar{T}_{\text{aolv}}^{0.1 \mu\text{m}} \approx 307.8$ K, $\bar{T}_{\text{aolv}}^{2 \mu\text{m}} \approx 259.4$ K, $\bar{T}_{\text{apx}}^{0.1 \mu\text{m}} \approx 376.0$ K, and $\bar{T}_{\text{forst}}^{0.1 \mu\text{m}} \approx 334.8$ K (see Table 1, significantly differing from $T \approx 280$ K, the “best-fit dust temperature” derived by Honda et al. (2004a). If we adopt the five multiplication factors c_0, c_1, c_2, c_3 , and c_4 determined by Honda et al. (2004a; see their Table 3) and take the physical temperatures $\bar{T}_{\text{aolv}}^{0.1 \mu\text{m}}, \bar{T}_{\text{aolv}}^{2 \mu\text{m}}, \bar{T}_{\text{apx}}^{0.1 \mu\text{m}}$, and $\bar{T}_{\text{forst}}^{0.1 \mu\text{m}}$ calculated from equation (2), the actual emission spectrum would be

$$\begin{aligned}
 F_{\lambda}^{\text{phy}} = & c_0 B_{\lambda}(T = 280 \text{ K}) + c_1 \kappa_{\text{aolv}}^{0.1 \mu\text{m}} B_{\lambda}(\bar{T}_{\text{aolv}}^{0.1 \mu\text{m}}) \\
 & + c_2 \kappa_{\text{aolv}}^{2 \mu\text{m}} B_{\lambda}(\bar{T}_{\text{aolv}}^{2 \mu\text{m}}) + c_3 \kappa_{\text{apx}}^{0.1 \mu\text{m}} B_{\lambda}(\bar{T}_{\text{apx}}^{0.1 \mu\text{m}}) \\
 & + c_4 \kappa_{\text{forst}}^{0.1 \mu\text{m}} B_{\lambda}(\bar{T}_{\text{forst}}^{0.1 \mu\text{m}}).
 \end{aligned} \quad (3)$$

In Figure 1a we plot the model spectra calculated from the single-temperature approach of equation (1) and from the same approach but using physical dust temperatures (see eq. [3]) derived from the energy balance between absorption and emission (see eq. [2]). For illustration, we show in Figure 1b the error $\chi \equiv |F_{\lambda}^{\text{phys}} - F_{\lambda}^{\text{sta}}|/F_{\lambda}^{\text{sta}}$. As can be seen in Figures 1a and 1b, the emission spectrum calculated using physical temperatures deviates significantly from that of the single-temperature approach in the wavelength range of 8–12 μm . Most noticeable are the two distinct peaks at 9.96 and 10.9 μm that differ by $\sim 20\%$ and 11%, respectively. In addition, there is a shoulder at the blue wing in the physical model spectrum, which is not seen in the single-temperature approach spectrum of Honda et al. (2004a).

Since the 8–12 μm wavelength range is critical for silicate mineralogical analysis, it is clear that the grain temperature effect will affect the mineralogical composition determination dramatically. Although the single-temperature approach spectrum of Honda et al. (2004a) can give an excellent fit to the observed data (see their Fig. 1), it does not provide meaningful insight into the silicate composition because the assumption of a single temperature $T = 280$ K is unphysical! The pronounced differences at 9.0, 10.0, and 10.9 μm could mislead us in considering the presence or absence of certain silicate minerals. In comparison, for comet Hale-Bopp (C/1995 O1), the strongest IR features occur at 9.2, 10.0, and 11.2 μm , which are attributed to glassy pyroxene, amorphous silicate, and crystalline olivine, respectively (Wooden et al. 1999). Therefore, of course, the abundance

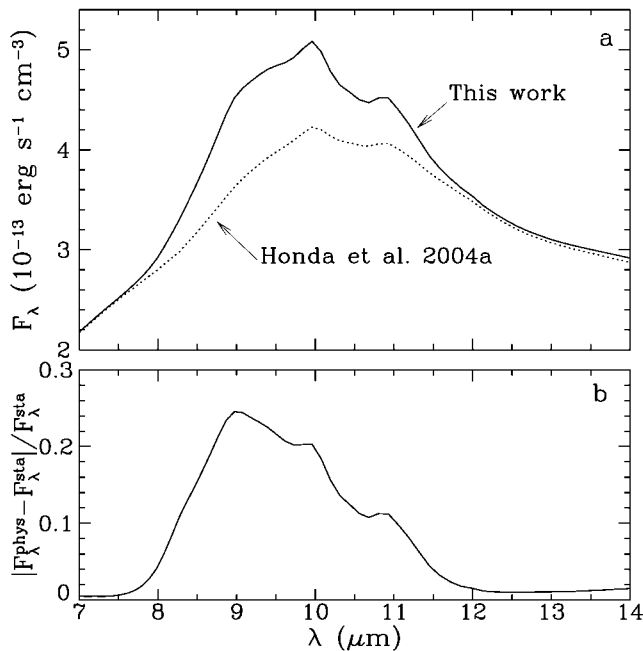


FIG. 1.—(a) The 9.7 μm silicate spectra of comet C/2002 V1 (NEAT) at $r_h \approx 1.18$ AU calculated from the single-temperature approach (dotted line) and from the same approach but using physical dust temperatures derived from the energy balance between absorption and emission (solid line). The single-temperature approach spectrum (dotted line) is identical to the best-fit model spectrum of Honda et al. (2004a; see their Fig. 1), who took all four grain species (0.1 and 2 μm glassy olivine, 0.1 μm glassy pyroxene, and 0.1 μm crystalline forsterite) to obtain a single temperature of $T \approx 280$ K. (b) Contrast between the single-temperature approach spectrum of Honda et al. (2004a; see our eq. [1]) and the physical model spectrum of eq. (3). All parameters are tabulated in Table 1 of this Letter and in Table 3 of Honda et al. (2004a).

of different dust species derived from the single-temperature approach is not reliable, and the conclusion about grain processing (in particular, the degrees of processing and crystallinity) in the early solar system, in protostellar disks, or in the ISM should be taken with caution. As summarized in § 1, the presence and quantity of crystalline silicate dust in astrophysical environments are of considerable astrophysical significance (see Wooden 2002). The single-temperature approach can at most serve as an initial guess in order to gain some very rough qualitative feeling about grain composition. More detailed modeling of the heating and cooling processes of various different dust components in a range of sizes will be needed in order to place firm constraints on their size and abundance and to obtain information regarding their origin and processing history (e.g., see Li & Greenberg 1998, Wooden et al. 1999, and Harker et al. 2002).⁸ We emphasize that we do not consider equation (3) as a physical approach for modeling the cosmic silicate mineralogy. A real physical approach should start with an initial guess as to the presence of certain grain species together with astrophysical considerations (e.g., in cometary comae and the ISM there exist both silicate dust and carbonaceous dust) and then a calculation of their equilibrium temperatures as a function of size, shape, and morphology (and as a function of radial distance from the central heating source if the emitting dust is spatially distributed) using the optical constants measured for realistic cosmic dust analogs for these grain species. For optically thick objects (e.g.,

⁸ This will provide a direct test on the suggestion of Bowey & Adamson (2002), who argued that the diffuse ISM may have a large amount of crystalline silicates (of different kinds; up to a mass fraction of 60%). As pointed out in Draine (2003), although such a mixture of crystalline grains gives a smooth absorption profile, it will not give a smooth emission profile since the different crystalline materials are expected to be heated to different temperatures (e.g., iron-rich silicates of the same size will be heated to higher temperatures than iron-poor silicates since the former have higher UV/optical absorptivity [see Fig. 4 of Dorschner et al. 1995]). Note that the 9.7 μm silicate emission band of the Trapezium region is almost identical to the 9.7 μm silicate absorption band of dark clouds (see Gillett et al. 1975).

quiescent dark molecular clouds externally heated by the ambient interstellar radiation field, deeply embedded YSOs heated by the central hot young star[s], envelopes around post-asymptotic giant branch stars, and dusty tori around active galactic nuclei), a detailed radiative transfer involving various grain species of a range of sizes (often taken to have a power-law size distribution functional form) is required (e.g., see Pascucci et al. 2004 and references therein).

4. CONCLUDING REMARKS

We have examined the single-temperature approach, a method widely used to model the astronomical IR emission spectrum using a mixture of grains of different compositions and different sizes. This approach assumes that all grains emit at the same temperature, despite the fact they have different optical properties and sizes and thus absorb and emit differently. We demonstrate the invalidity of this approach by showing that the IR emission spectrum calculated from a mixture of grains emitting at their physical temperatures in thermal equilibrium with the illuminating radiation field differs substantially from that of the same grain mixture but with a single, identical temperature. We conclude that in order to correctly infer the dust mineralogical composition, care should be taken to properly calculate the dust physical temperature. This is particularly important in view of the successful operation of the *Spitzer Space Telescope*, which is tirelessly collecting a rich set of high-quality spectroscopic data that awaits our interpretation!

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