Is the silicate emission feature only influenced by grain size?

N.V. Voshchinnikov\textsuperscript{1,2} and Th. Henning\textsuperscript{3}

\textsuperscript{1} Sobolev Astronomical Institute, St. Petersburg University, Universitetskii prosp. 28, St. Petersburg, 198504 Russia, e-mail: nvv@astro.spbu.ru
\textsuperscript{2} Isaac Newton Institute of Chile, St. Petersburg Branch
\textsuperscript{3} Max-Planck-Institut f"ur Astronomie, K"onigstuhl 17, D-69117 Heidelberg, Germany

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Abstract. The flattening of the 10 \( \mu \text{m} \) silicate emission feature observed in the spectra of T Tauri and Herbig Ae/Be stars is usually interpreted as an indicator of grain growth. We show in this paper that a similar behaviour of the feature shape occurs when the porosity of composite grains varies. We modelled the fluffy aggregates with inclusions of different sizes with multi-layered spheres consisting of amorphous carbon, amorphous silicate, and vacuum. We also found that the inclusion of crystalline silicates in composite porous particles can lead to a shift of the known resonances and production of new ones.

1. Introduction

The shape and strength of the silicate emission feature observed near 10 \( \mu \text{m} \) in the spectra of T Tauri and Herbig Ae/Be (HAeBe) stars is commonly used as a measure of grain growth in protoplanetary discs (see Natta et al. \textsuperscript{2007} for a review). It is well-known theoretically that with an increase of the grain size, the feature becomes wider and eventually fades away. In the case of compact spherical grains with a composition of astronomical silicate, the 10 \( \mu \text{m} \) feature disappears when the grain radius exceeds \( \sim 2 \mu \text{m} \) (see Fig. \textsuperscript{1}).

The standard approach to modelling the 10 \( \mu \text{m} \) feature includes calculations of light absorption by several populations of compact (and hollow) silicate spheres. We used amorphous and crystalline particles of small and large sizes to fit the observed emission profiles. The model was first suggested by Bouwman et al. \textsuperscript{2001} and then modified by van Boekel et al. \textsuperscript{2005}. It was used by Schegerer et al. \textsuperscript{2006}; Honda et al. \textsuperscript{2006}; Kessler-Silacci et al. \textsuperscript{2006}; Sargent et al. \textsuperscript{2006}; Sicilia-Aguilar et al. \textsuperscript{2007}; and Bouwman et al. \textsuperscript{2008} to fit the observational data. Further the authors searched for correlations between the estimated mass fractions of large and crystalline grains and different stellar and disc parameters like mass, luminosity, age, spectral type, etc. As a rule, the correlations are absent or rather weak (see Table 5, Sicilia-Aguilar et al. \textsuperscript{2007}).

In this Letter, we show that the shape, position, and strength of the 10 \( \mu \text{m} \) silicate feature is also influenced by variations of the properties of small mass composite aggregate grains. We modelled the fluffy aggregates by multi-layered spheres (see also Voshchinnikov et al. \textsuperscript{2006}). This particle model permits us to include an arbitrary fraction of materials, and computations do not require large resources.

2. Model of porous composite grains

Fluffy particles should appear as a result of grain coagulation in interstellar clouds and protoplanetary discs (e.g., Henning & Stognienko, \textsuperscript{1996} Dominik & Tielens, \textsuperscript{1997} Jones, \textsuperscript{2004} Ormel et al., \textsuperscript{2007}). It is expected that aggregates can consist of several silicate and carbon sub-particles of different sizes that can be treated as inclusions in a vacuum matrix.

We use the model of spherical multi-layered particles introduced by Voshchinnikov & Mathis \textsuperscript{1999}. Later, Voshchinnikov et al. \textsuperscript{2005} demonstrated that the optical properties of layered spheres resemble those of fluffy aggregates with inclusions of different sizes.

Our model parameters are: the refractive indices and volume fractions \( V_i/V_{\text{total}} \) of the materials and the radius of compact particles \( r_{\text{compact}} \). The amount of vacuum in the particle (the particle porosity \( \mathcal{P} \)), \( 0 \leq \mathcal{P} < 1 \) is

\begin{equation}
\mathcal{P} = V_{\text{vac}}/V_{\text{total}} = 1 - V_{\text{solid}}/V_{\text{total}},
\end{equation}

where \( V_{\text{solid}} \) is the sum of the volumes of all species excluding vacuum. The radius of porous particles is related to that of compact particles as

\begin{equation}
r_{\text{porous}} = r_{\text{compact}} (1 - \mathcal{P})^{1/3} = \frac{r_{\text{compact}}}{(V_{\text{solid}}/V_{\text{total}})^{1/3}}.
\end{equation}

The model of layered spheres combines all components, including vacuum in one particle (internal mixing) in contrast to the standard approach discussed above where “external mixing” (mixture of several individual populations of compact grains) is used.

For calculations, we use different kinds of carbon and silicates: amorphous carbon Be1 and AC1 (Rouleau & Martin, \textsuperscript{1991}), amorphous silicate with olivine composition (Dorschner et al. \textsuperscript{1995}), crystalline olivine (Fabian et al. \textsuperscript{2001}), and astronomical silicate (astrosil; Laor & Draine, \textsuperscript{1993}).
3. Analysis of silicate emission

The silicate feature in the \( N \) band was observed in spectra of a large variety of objects (see Henning [2008], for a recent review). We should caution the reader that we calculate absorption efficiencies, but measure the fluxes. A detailed analysis of disc spectra certainly requires radiative transfer calculations. Assuming that the silicate emission is optically thin, we can compare observed fluxes with theoretical profiles. The latter are proportional to the product of particle absorption cross section by the Planck function with the particle temperature \( \propto C_{\text{abs}}(\lambda) B_\nu(T_d) \). Radiative transfer calculations show that grains of different temperatures contribute to the silicate feature (see Fig. 1 in Schegerer et al., 2006). However, the dominant contribution for the 10 \( \mu m \) feature comes from particles with \( T_d = 200 \sim 400K \) for which the Planck function is approximately constant in \( N \) band. Therefore, we can adopt that the shape of the feature depends primarily on the emission properties of grains.\(^1\)

The profile of the feature can be described by the normalised absorption efficiency factor \( Q_{\text{abs}}(\lambda) / Q_{\text{abs}}(\lambda_0) - 1 \), where the flux at wavelength \( \lambda_0 \) characterises the continuum. As usual, the value of \( \lambda_0 = 8.2 \mu m \) is chosen (e.g., Schegerer et al., 2006).

Another representation of the optical behaviour is provided by the mass absorption coefficient, which is the ratio of absorption cross section \( C_{\text{abs}}(\lambda) \) to particle mass. In the case of a sphere of porosity \( \mathcal{P} \), it can be written as
\[
\kappa_{\text{abs}}(\lambda) = \frac{C_{\text{abs}}(\lambda)}{\rho_d V_{\text{total}}} = \frac{3}{4 \rho_d \text{ solid} r_s \text{ compact} (1 - \mathcal{P})^{2/3}},
\]
where \( \rho_d = \rho_d \text{ solid} (1 - \mathcal{P}) \) is the mean particle density. The value of \( \rho_d \text{ solid} \) is obtained by averaging the density of all species excluding vacuum. In our calculations, we assume that \( \rho_d \text{ Si} = 3.3 \text{ g/cm}^3 \) and \( \rho_d \text{ C} = 1.85 \text{ g/cm}^3 \) for silicate and carbon, respectively.

Figure 1 shows the wavelength dependence of the normalised absorption efficiency factors for compact silicate spheres of diverse sizes. With a growth of the particle size (and mass), the 10 \( \mu m \) silicate feature broadens, its height decreases and the position of maximum shifts to longer wavelengths.

In a similar manner, the silicate feature changes when the particle porosity grows (Fig. 2). However, in this case the particle size increases only moderately, while particle mass remains the same. With a growth of porosity, the peak strength decreases for normalised absorption (Fig. 2 upper panel) whereas the mass absorption coefficient becomes larger (Fig. 2 lower panel). The value of \( \kappa_{\text{abs}} \) almost doubles at the peak position when we replace the compact particle by porous particle.

It is well known that the shape and strength of the silicate feature depend on the type of the amorphous silicate, particle size, and fractal dimension (see, e.g., van Boekel et al., 2005; Schegerer et al., 2006; Min et al., 2006). Using the model of composite grains we can also investigate how carbon embedded in particles affects the characteristics of the silicate feature.

\(^1\) Note that our case differs from the case analysed by Li et al. (2004) where the cometary particles of different composition are located at the same distance from the Sun.

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\( Q_{\text{abs}}(\lambda) / Q_{\text{abs}}(8.2 \mu m) - 1 \) for compact spheres consisting of astrosil. The effect of variation of the silicate emission shape with the particle size is illustrated. The observational profile of the T Tauri star Tr 37 13-157 (Sicilia-Aguilar et al., 2009) is shown for comparison. Note that this profile is not continuum subtracted.

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Fig. 1. Wavelength dependence of the normalised absorption efficiency factor \( [Q_{\text{abs}}(\lambda)/Q_{\text{abs}}(8.2 \mu m)] - 1 \) for compact spheres consisting of astrosil. The effect of variation of the silicate emission shape with the particle size is illustrated. The observational profile of the T Tauri star Tr 37 13-157 (Sicilia-Aguilar et al., 2009) is shown for comparison. Note that this profile is not continuum subtracted.

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Fig. 2. Wavelength dependence of the normalised absorption efficiency factor (upper panel) and mass absorption coefficient (lower panel) for layered spheres with \( r_s \text{ compact} = 0.1 \mu m \). The particles consist of amorphous carbon (Be1), amorphous silicate with olivine composition (MgFeSiO\(_4\)), and vacuum. The volume fraction of components \( V_i/V_{\text{total}} \) is indicated. The particles are of the same mass \( (V_{\text{Be1}}/V_{\text{solid}} = V_{\text{Be1}}/(V_{\text{Be1}} + V_{\text{MgFeSiO}}) = 0.2) \), but of different porosity. The effect of variation of the silicate emission shape with the particle porosity is illustrated.
The estimated porosity and amount of carbon in grains producing the silicate emission feature in protoplanetary discs are collected in online Table 1. At this stage, the stars with very pronounced crystalline peaks were eliminated from consideration. Table 1 includes 47 stars (30 T Tau and 17 HAeBe stars). The obtained values of $P$, $V_{Be1}/V_{solid}$, the ratio of masses of carbon to silicate $M_{Be1}/M_{MgFeSiO_3}$, and stellar age (if known) are given. Note that the determination of the age is often quite uncertain for pre-mainsequence stars (see discussion in Blondel & Tjin A Djie, 2006). Therefore, we do not discuss possible correlations.

The grain porosity exceeds 0.5 and the average value of $P$ is equal to $\langle P \rangle = 0.64 \pm 0.15$. Such particles resemble aggregates obtained both experimentally (Kempf et al., 1999) and theoretically (Shen et al., 2008). The amount of carbon in grains is not very large (average volume fraction $V_{Be1}/V_{solid} = 0.24 \pm 0.10$ and average mass ratio $M_{Be1}/M_{MgFeSiO_3} = 0.19 \pm 0.12$). These values increase by a factor of 3 – 4, if we replace Be1 by the less absorbing amorphous carbon 3C. This fact is illustrated in Fig. 4 where the results are given for both particle materials. Note that the particles containing 3C are less porous.

The variation of grain porosity without significant change of grain mass may explain the behaviour of silicate emission. This explanation is an alternative to the commonly used idea of large grains in protoplanetary discs. We will be able to decide between the two hypotheses after conducting spectropolarimetry in the 10 $\mu$m feature because a noticeable albedo of large grains manifests itself in polarisation of the scattered light. In this case, we expect unusual behaviour of polarisation parameters (especially positional angle) within the feature profile in comparison with calculated profiles for dichroic extinction (see, e.g., Henning & Stognienko, 1993; Prokopjeva & Il'in, 2007).

4. Crystalline silicates in composite grains

Another interesting problem is the degree of crystallinity of dust in protoplanetary discs, which is related to the processes of partial grain evaporation and annealing (e.g., Gail, 2004). Due to the conversion of amorphous silicates to crystalline minerals, the particles may consist of different types of silicates. In order to show the effect of amorphous silicate matrix and vacuum on resonances produced by crystalline silicates, we calculated the feature profiles for composite particles containing Mg-rich crystalline olivine $Mg_{1.3}Fe_{0.7}SiO_3$ as a component. The results are plotted in Fig. 5 where the upper panel illustrates the influence of particle porosity on position and strength of emission peaks. It is seen that variations of spectra are significant: the shape of the feature changes (cf. Fig. 2), some peaks totally disappear and new peaks arise. A very pronounced peak with a maximum near $\lambda = 11.37$ $\mu$m is observed for very porous particles whereas compact and medium-porous particles have resonances near $\lambda = 10.89$ $\mu$m. The inclusion of crystalline silicates...
Fig. 5. Wavelength dependence of the mass absorption coefficient for compact and layered spheres with $r_{s,\text{compact}} = 0.1 \mu m$. The particles consist of crystalline olivine and vacuum (upper panel), amorphous silicate, crystalline olivine, and vacuum (middle panel) and amorphous carbon, amorphous silicate, crystalline olivine, and vacuum (lower panel). The volume fraction of crystalline olivine and BeI is indicated. The position of peaks is marked. The thick solid line at the lower panel shows the mass absorption coefficient for the mixture of compact grains (external mixing) with volume fractions of constituents corresponding to solid curve (internal mixing). The effect of variation of crystalline resonances with particle porosity and composition is illustrated.

in a composite particle containing amorphous silicate (middle panel) or amorphous silicate and carbon (lower panel) changes the picture. The resonance near $\lambda \approx 11.4 \mu m$ is clearly seen at the long-wavelength wing of the feature. Its position slightly shifts if the porosity changes. Fabian et al. (2001) found that such a peak appeared in the spectra of strongly-elongated particles. A double peaked structure around $\lambda = 10.25 \mu m$ arises as well. This structure was not noticed previously in spectra of crystalline olivines (H. Mutschke, priv. commun., 2007). Note that, as expected, the mixture of separate constituents (amorphous silicate, carbon and crystalline silicate, thick line in lower panel) do not lead to the shift of peaks. Further calculations with different materials for wider wavelength range and detailed comparison with Spitzer observations (see Watson et al., 2007) might help to resolve the problem of grain crystallisation in protoplanetary discs and to answer the question whether the crystals occur in “isolation” or as part of porous grains.

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### Table 1. Grain porosity and fractional amount of carbon in grains as derived from fitting the 10 µm silicate emission feature.

| Star Type | Type | \( P \) | \( \Phi_{\text{sil}} / \Phi_{\text{solid}} \) | \( M_{\text{sil}} / M_{\text{MgFeSiO}} \) | Age, Myr | Ref. | Comment |
|-----------|------|--------|-------------------------------|--------------------------|----------|-------|---------|
| Tr 37 73-758 | t | 0.784 | 0.259 | 0.196 | 1.8 | 1 |
| Tr 37 11-2146 | t | 0.705 | 0.217 | 0.156 | 0.9 | 1 |
| Tr 37 11-2037 | t | 0.615 | 0.232 | 0.170 | 2.5 | 1 |
| Tr 37 11-2031 | t | 0.542 | 0.167 | 0.113 | 2.5 | 1 |
| Tr 37 14-183 | t | 0.704 | 0.281 | 0.219 | 0.9 | 1 |
| Tr 37 82-272 | t | 0.726 | 0.188 | 0.130 | 10.5 | 1 |
| Tr 37 12-2113 | t | 0.650 | 0.186 | 0.128 | 1.1 | 1 |
| Tr 37 13-157 | t | 0.804 | 0.250 | 0.187 | 2.4 | 1 |
| Tr 37 91-155 | t | 0.976 | 0.320 | 0.264 | 1.7 | 1 |
| Tr 37 54-1547 | t | 0.556 | 0.132 | 0.085 | 5.7 | 1 |
| Tr 37 13-1250 | t | 0.649 | 0.124 | 0.079 | 3.3 | 1 |
| Tr 37 23-162 | t | 0.722 | 0.247 | 0.184 | 6.6 | 1 |
| Tr 37 01-580 | t | 0.604 | 0.167 | 0.112 | 8.7 | 1 |
| NGC 7160 DG-481 | h | 0.852 | 0.333 | 0.279 | 12.0 | 1 |
| SU Aur | t | 0.731 | 0.131 | 0.085 | 3.9 | 2 |
| GW Ori | t | 0.562 | 0.102 | 0.064 | 1.0 | 2 |
| CR Cha | t | 0.471 | 0.107 | 0.067 | 1.0 | 2 |
| Glass I | t | 0.671 | 0.208 | 0.147 | 1.0 | 2 |
| WW Cha | t | 0.539 | 0.194 | 0.135 | 0.3 | 2 |
| SZ 82 | t | 0.427 | 0.376 | 0.338 | 1.1 | 2 |
| AS 205S | t | 0.556 | 0.251 | 0.188 | 0.1 | 2 |
| Haro 1-16 | t | 0.425 | 0.141 | 0.092 | 0.5 | 2 |
| AK Sco | t | 0.519 | 0.116 | 0.073 | 7.6 | 2 |
| FM Tau | t | 0.598 | 0.256 | 0.193 | 2.8 | 3 |
| GG Tau A | t | 0.401 | 0.356 | 0.310 | 3.3 | 3 |
| GG Tau B | t | 0.841 | 0.342 | 0.292 | 1.6 | 3 |
| GM Aur | t | 0.700 | 0.162 | 0.109 | 7.4 | 3 |
| IP Tau | t | 0.493 | 0.213 | 0.152 | 4.3 | 3 |
| TW Hya | t | 0.756 | 0.158 | 0.105 | 10.0 | 3 |
| Hen 3-600 A | t | 0.860 | 0.239 | 0.176 | 3 |
| V410 Anon 13 | t | 0.651 | 0.398 | 0.370 | 3 |
| HD 104237 | h | 0.612 | 0.307 | 0.249 | 4.8 | 4 |
| HD 142527 | h | 0.673 | 0.301 | 0.242 | 1.0 | 4 |
| HD 142666 | h | 0.680 | 0.268 | 0.205 | 4.4 | 4 |
| HD 144432 | h | 0.440 | 0.123 | 0.078 | 6.65 | 4 |
| HD 144668 | h | 0.832 | 0.504 | 0.569 | 0.5 | 4 |
| HD 150193 | h | 0.398 | 0.180 | 0.124 | 2.6 | 4 |
| HD 163296 | h | 0.537 | 0.209 | 0.148 | 6.0 | 4 |
| HD 179218 | h | 0.948 | 0.292 | 0.231 | 1.3 | 4 |
| HD 245185 | h | 0.704 | 0.149 | 0.098 | 3.3 | 4 |
| HD 36112 | h | 0.431 | 0.122 | 0.078 | 4.4 | 4 |
| HD 37357 | h | 0.480 | 0.206 | 0.146 | 10.0 | 4 |
| HD 37806 | h | 0.732 | 0.405 | 0.382 | 0.8 | 4 |
| AB Aur | h | 0.714 | 0.187 | 0.129 | 4.8 | 4 |
| HK Ori | h | 0.551 | 0.400 | 0.374 | 5.8 | 4 |
| UX Ori | h | 0.392 | 0.160 | 0.107 | 2.8 | 4 |
| V380 Ori | h | 0.694 | 0.493 | 0.545 | 7.4 | 4 |

1Meaning of symbols: t = T Tau star, h = Herbig Ae/Be star.

3References for observational data: (1) Sicilia-Aguilar et al. (2007); (2) Schegerer et al. (2006); (3) Sargent et al. (2006); (4) van Boekel et al. (2005); (5) Blondel & Tjin A Djie (2006); (6) Güdel et al. (2007); (7) Bertout et al. (2007).