Open Access Online Journal on Astronomy and Astrophysics
Acta Astrophysica Taurica
www.astrophysicataurica.org

Acta Astrophys. Tau. 2(1) 26–29 (2021) doi:10.31059/aat.vol2.iss1.pp26-29

Influence of the scattering particle shape on the SiO_2 silicate feature

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Submitted on November 7, 2020

ABSTRACT

Silicate dust particles are part of many astronomical objects such as comets and circumstellar disks. In a spectrum, silicates exhibit a number of characteristic silicate emission features. To study these features, Mie's theory is usually used. This theory assumes that the scattering object is an ideal sphere. In this work, we investigated the contribution of non-spherical quartz particles (SiO_2) to these features. We studied the influence of the deviation from sphericity on the 10-micron silicate feature of quartz. It is shown that the deviation from sphericity has a significant effect on both the scattered light intensity and the scattering factor Q_{sca}, and this effect increases with increasing scattering particle size. The main peculiarities of the 10-micron silicate feature have been studied for both prolate and oblate spheroids.

Key words: 10-μm silicate feature, circumstellar disks, comets, quartz, light scattering

1 Introduction

Silicate dust particles have been detected in circumstellar disks surrounding young stars (Waelkens et al., 1997; Malfait, 1998). The most wide-spread kinds of space dust are the compounds of silicon, iron, magnesium, oxygen, and carbon. The physical and chemical parameters of silicate dust particles such as size, shape, refraction index, and dimensional parameter are the result of a number of different chemical and physical processes of evolution. Silicate dust particles play an important role in understanding the evolution of circumstellar disks and processes of the formation of planet systems. There exist a number of observations directed to studying silicate dust characteristics (e.g., Weintraub, 1989; Strom et al., 1989; Beckwith et al., 1990; Skrutskie et al., 1990).

The matter of circumstellar disks arises from the interstellar medium, namely from the core of the host molecular cloud. The dust composition of the protoplanetary accretion disk is believed to approximately coincide with the initial dust composition of the protoplanetary accretion disk. A small difference in the composition can be explained by the evaporation of volatile molecular ice during the passage of the accretion shock wave front. Thus, oxygen could interact with silicon atoms forming SiO_2 (quartz). A more detailed discussion on the appearance of quartz particles in molecular clouds is described in the review of Dorschner and Henning (1995).

2 10-micron silicate feature

The presence of silicates in circumstellar disks is manifested as a silicate spectral feature. The most conspicuous spectral feature is observed in the vicinity of the 10 μm wavelength. Therefore, it is often called a 10-micron silicate feature (10-μm silicate feature) (Hanner et al., 1993). This feature is manifested in an increase of radiation intensity in a spectral range of 8 to 12 μm. The silicate particles can exhibit an emission feature at these wavelengths due to the presence of oscillating energy levels of Si – O bonds (Potter Jr. and Morgan, 1982; Hanner et al., 1997). Note that this silicate feature is revealed by only those particles whose temperature is more than 100 K (Lee et al., 2013). Furthermore, speaking of the silicate feature, we imply that the temperature of a scattering object is more than 100 K.

This emission feature is revealed in many astronomical objects. For instance, it was detected in radiation from quasars (Hao et al., 2005; Siebenmorgen et al., 2005). Many comets have the 10-micron silicate feature. For example, the comets Mueller (1994 I = C/1993 A1) (Hanner et al., 1994), Bradfield (1987 XXIX = C/1987 P1) (Hanner et al., 1990), Hyakutake (C/1996 B2), Hale–Bopp (C/1995 O1) (Hayward et al., 2000; Wooden et al., 1999), 1P/Halley (Bregman et al., 1987; Campins and Ryan, 1989), and Levy (1990 XX = C/1990 K1) (Lynch, 1992). However, it should be clarified that only small particles of comet dust up to 1 μm contribute to the formation of the 10-micron silicate feature. This is associated with thermodynamic properties of comet dust rather than optical – large-size particles just need more time to heat up enough to significantly contribute to this feature (Hanner and Bradley, 2004).

Moreover, two objects of Herbig Ae/Be, LkHα 208 and LkHα 198, have characteristics with a maximum of about 9 μm (Hanner and Brooke, 1998). In the infrared spectra of some T Tau stars derived with the infrared spectrograph *Spitzer Space Telescope*, Sargent et al. (2009) detected conspicuous narrow emission features at some wavelengths in a spectral range of 9 to 20 μm interpreting them as evidence for the presence of SiO_2.

It has long been established that the basic contribution to the formation of this feature is made by olivine that is thoroughly investigated (Hanner and Bradley, 2004). In particular, in the course of laboratory experiments using a mid-infrared spectrometer, the spectra of large (up to 0.5 mm) particles of olivine of irregular shape were studied searching for the 10-micron silicate feature. This feature was experimentally detected (Chornaya, 2020), although numerous attempts of computer modeling based on the assumption of the spherical shape of a scatterer showed that at such large sizes of particles the silicate feature should not exist (e.g., Hanner et al., 1987; Hage and Greenberg, 1990; Hanner et al., 1992). The only possible explanation is the influence of the nonspherical shape of a scatterer.

In addition to olivine, in the composition of celestial bodies there are other silicates capable of contributing noticeably to this feature. For instance, a study of the comet Wild 2 with the comet dust collector Stardust showed that the comet dust includes a significant number of SiO_2 particles in different samples of oxides (Kearsley et al., 2008). Therefore, consideration of the question concerning the contribution of quartz particles to the 10-micron silicate feature seems sufficiently important.

There are a small number of papers devoted to the 10-micron silicate feature of namely quartz. Henning and Meeus (2009) considered quartz particles whose size was only 0.1 μm, i.e., much smaller than the wavelength. Even small comet particles contributing to the emission feature can be substantially larger. Moreover, silicates involved in the composition of circumstellar disks can also be of much larger sizes.

Petrov et al. (2020) studied the basic properties of the 10-micron silicate feature of quartz for spherical particles that are comparable to and exceeding the wavelength. For calculations, the Mie theory was used (Mie, 1908), whose program realization is the fastest among all the analogous techniques for calculating characteristics of the scattered light. However, spherical particles are rather rare in nature. It is of interest to study the influence of deviations from sphericity on the 10-micron silicate feature. This paper is devoted to the study of this issue.

3 Method of calculating nonspherical particle scattering

To determine the scattering properties of nonspherical particles, a number of computer calculations were needed. Therefore, there was used the fastest program for calculating scattering properties of spheroids elaborated by Michail Mishchenko (Mishchenko, 1991, 1993; Mishchenko, Travis, 1994). The calculating method is based on the T-matrix method (Mishchenko et al., 1996) and optimized for particles having a rotation axis; this maximally simplifies and accelerates calculations (Wielaard et al., 1997). Moreover, the T-matrix method makes it possible to implement an analytical averaging of the scattered light characteristics based on orientations of a scattering particle (Petrov et al., 2006).

Spheroids (rotation ellipsoids) with the axis ratio a/b were used as a target. Here b is the particle size along the rotation axis, a is the size of the axis perpendicular to the rotation axis. Hence, at $a/b < 1$ there is a spheroid elongated along the rotation axis; at $a/b > 1$ there is a spheroid flattened along the rotation axis; at $a/b = 1$ there is a spherical particle. In this paper, we studied particles with the axis ratios $a/b = 0.5$, $a/b = 1.0$, and $a/b = 2.0$. The scattered light characteristics were averaged based on orientations of scattering particles. It is important to note that the position of the emission spectral feature is strongly dependent on the particle size R. In the case of a sphere, the particle size means the sphere radius, whereas in the case of prolate and oblate spheroids it means the radius of the sphere of equivalent volume.

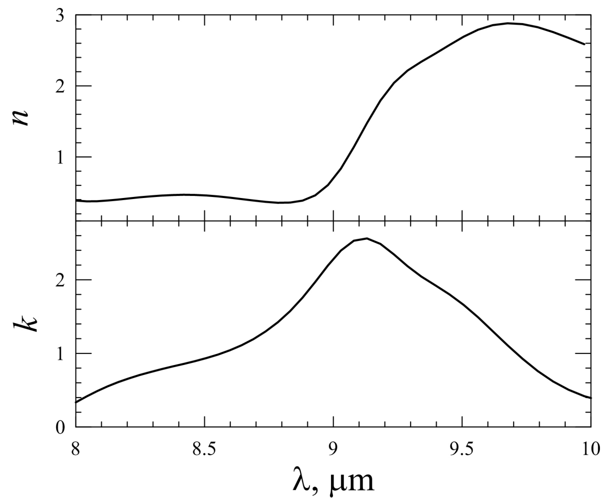

Fig. 1. Spectral dependence of the refraction index of SiO_2 (Popova et al., 1972). The top panel corresponds to the real part of the refraction index, the bottom panel – to the imaginary one

The basic parameter defining properties of the spectral emission feature is the complex refraction index $m = n + i \cdot k$. Spectral dependence of the real and imaginary parts of the refraction index of SiO_2 (see Fig. 1) was extracted from the paper of (Popova et al., 1972).

4 Results and discussion

We calculated the intensity of light scattered in quartz particles of different shape for different wavelengths and sizes of scattering particles. Since the particles of different size scatter light variously, the appropriate part of a spectrum was normalized for each size of the scattering particle – the maximum value of light intensity was taken equal to unity. Note that the calculations were carried out at a scattering angle of 0 degrees (scattering forward).

Figure 2 shows the dependence of the wavelength λ_{max} corresponding to the maximum of the 10-micron silicate feature on the scattering particle size. The black line corresponds to the spherical particle ($a/b = 1$), the blue line – to the oblate spheroid ($a/b = 2$), and the red line – to the prolate spheroid ($a/b = 0.5$). Lines break on the scattering particle size higher than which the program of Mishchenko is not capable of calculating scattering properties at a given relation of axes and refraction indices.

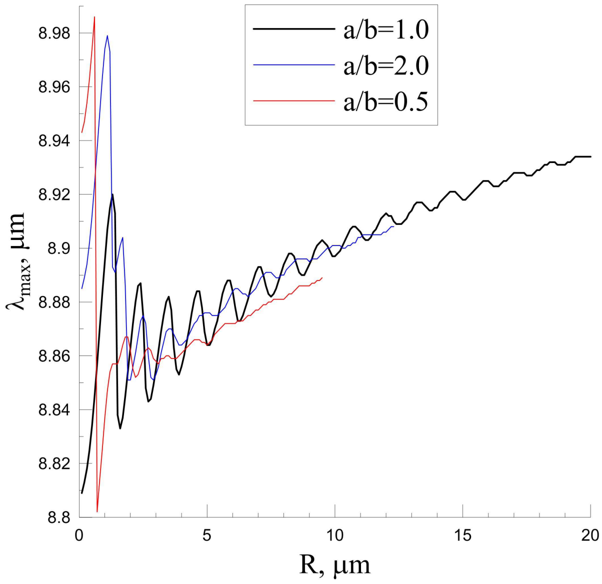

Fig. 2. Spectral position of maximum of the 10-micron silicate feature of quartz for spherical particles (black line), oblate spheroids (blue line), and prolate spheroids (red line) depending on the scattering particle size

However, even available data are sufficient for certain conclusions. Firstly, in the case of particles with a size of less than 1 μm contributing to 10-micron silicate features of comets, the position of maximum is shifted to the region of higher wavelengths. Moreover, the 10-micron silicate feature of the prolate spheroid differs strongly from the silicate feature of the spherical particle than in the case of the oblate spheroid. Furthermore, at larger sizes any nonsphericity causes a shift of the position of maximum of the silicate feature toward lower wavelengths.

The described program of Mishchenko allows one to calculate not only intensity of the scattered light but other characteristics of scattering. In particular, the product of the scatterring section C_{sca} by the value of the incident energy flow yields the total power extracted by an object from the incident field due to the rescattering of electromagnetic energy in all the directions (Mishchenko et al., 2000). All the optical sections are real and non-negative values and have the dimensionality of area. They depend on direction, polarization, and wavelength of incident radiation, as well as on the size, morphology, and orientation of a scattering object.

It is more illustrative to deal with not the scattering section but the scattering factor Q_{sca} defined as a ratio of the scattering section to the area of object's cross section (Farafonov et al., 2019):

$$Q_{sca} = \frac{C_{sca}}{\pi R^2}. \tag{1}$$

The scattering factor defines how effectively the area unit of a scattering object rescatters light. Spectral dependence of the scattering factor Q_{sca} is shown in Fig. 3 a–c. Similar to Fig. 2, the black line corresponds to the spherical particle (a/b = 1), the blue line – to the oblate spheroid (a/b = 2), and the red line – to the prolate spheroid (a/b = 0.5). Figure 3a corresponds to the scattering particle size R = 3 μm, Fig. 3b – R = 6 μm, and Fig. 3c – R = 9 μm.

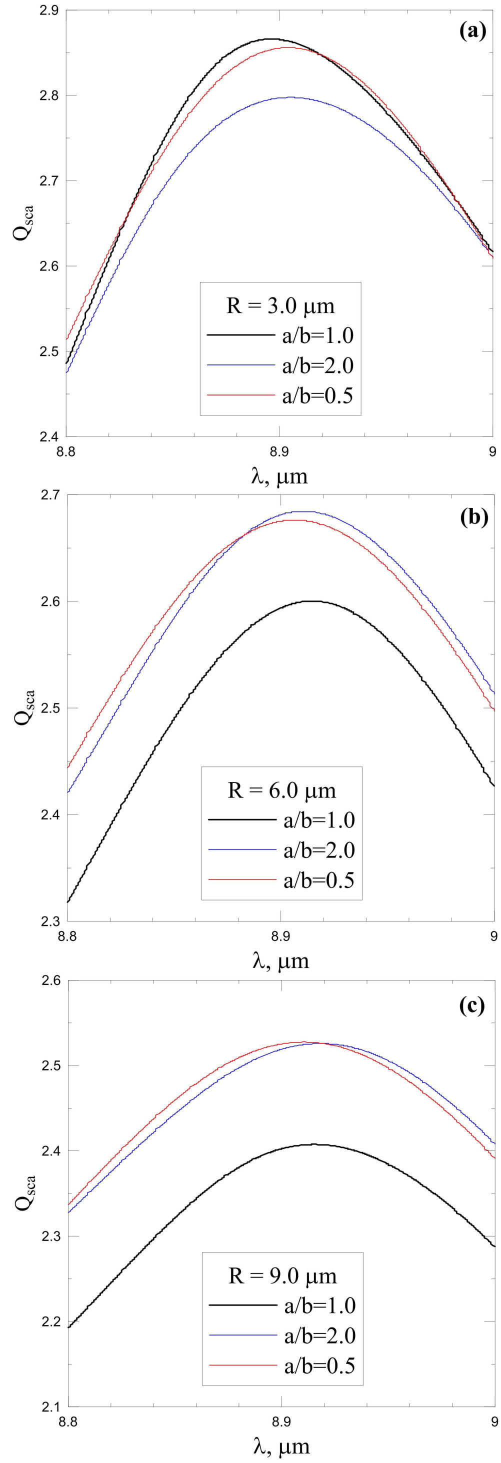

Fig. 3. Spectral dependence of the scattering factor Q_{sca} of the 10-micron silicate feature of quartz for spherical particles (black line), oblate spheroids (blue line), and prolate spheroids (red line) at different sizes of scattering particles: a) R = 3 μm; b) R = 6 μm; c) R = 9 μm

From the figure we can conclude that the scattering efficiency by the area unit of a scattering particle of quartz decreases with increasing size of the particle. In the case of very large particles (6 microns and more), the nonspherical particles of quartz in the region of the 10-micron silicate feature scatter light generally more effectively than the spherical ones. Furthermore, with increasing size the difference between nonspherical and spherical particles increases.

5 Conclusions

The basic conclusion of the current paper: the accounting of nonsphericity of particles is important for studying spectra of cosmic dust. The deviation from sphericity was shown to have an effect on the 10-micron silicate feature of quartz. For particles with a size of less than 1 μm generally contributing to the 10-micron silicate feature of comets the position of the spectral feature is shifted to the region of higher wavelengths. In the case of relatively large particles with a size that is comparable or exceeding the wavelength, the position of the spectral feature of prolate spheroid quartz particles is significantly shifted to the region of lower wavelengths; in the case of oblate spheroid particles this shift is practically absent. The deviation from sphericity was established to have a significant influence on the scattering factor Q_{sca}, whereas this influence increases with increasing size of a scattering particle.

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