

Optical Properties of Core Mantle Grains with Ices as Mantle

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Abstract: We calculate the absorption cross sections of core mantle grains in the spectral range between 8.0 - 25 μ m. The core-mantle grains consist of spherical silicate core and H₂O ice mantles. We study the variation in the absorption profiles of the silicate grain with the mantle thickness of ices. In particular, we study the variation in the peak absorption wavelength with the mantle thickness of H₂O ice. We find that the absorption profiles of silicate grains are modified considerably with the ice-mantles, and the absorption peaks also vary with the mantle thickness. These results on the core-mantle grain models with ices as mantles would help to get the composition of the interstellar dust, circumstellar dust and the dust in the solar system objects, better. We present the core-mantle grain model and discuss the results.

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I. Introduction

Cosmic dust grains are evolved either by coagulation of Silicates and Carbonaceous material (e.g. Amorphous Carbon, Graphite, PAHS) (Mathis et al, 1977) or by accretion of two materials, in the form of a core-mantle structure (i.e. accretion of some material as a mantle on a core, e.g. Silicate as a core material with ices as mantle) with a particular emphasis on changes in size and chemical and morphological structure (See E.G. Anheuser 1975, J.M. Greenberg and Li, 1993 Williams DA, 1989). In the dense star forming regions of molecular clouds the formation of mantles of “ice” by the accretion of gas molecules onto cool grains is expected theoretically and established observationally (Drain, 1985). Condensation process of the gas phase over cold dust particles lead to the formation of ices over the grain was realized by Van de Hulst (1946) in the studies of elemental abundances.

Ices in interstellar environment are traced by their molecular vibrational transitions in the near to far infrared. In general, combination of overtone modes are contained in the 1-3 micron wavelength range, the stretching is in 3-6 micron region, band and liberation vibrations are in 6-30 micron region and torsional and intermolecular modes are in 25 to 300 micron portion. A vast majority of interstellar and circumstellar ice studies is in the 3-16 micron range. This is because, below 3 micron, the signals are weak because of dust continuum extinction and above 30 micron, there is limitation in the availability and capability of the instrument.

Most ice features discovered show complex profiles as a result of the ice composition, structure, grain shape and size in extremely impressive manner. The peak position, widths and shapes of the observed ice bands are influenced by the composition and structure of ices as a result of the attractive and repulsive dipole interactions between neighboring molecules and are also influenced by relative mantle and core volumes of the dust grains.

II. Core mantle Model

Basically there are three types of dust models on the basis of three distinctly different grain morphologies. (1) In silicate-graphite model and their updated versions. In this model, bare silicate and graphite grains are treated physically separate from each other (Duley and Williams, 1986, Drain and Lee, 1984, Seibenmorgen and Krugel, 1992, Dwek et al. 1997, Lee and Drain, 2001, Weingartner and Drain, 2001) (2) In a core mantle model, silicate is treated as a core and it is coated with carbonaceous mantle or mantle of hydrogenated amorphous carbon (Greenberg, 1989, Desert et al., 1990, Lee and Greenberg, 1997, Duley et al., 1989, Jones et al., 1990) and (3) Composite dust model in which, interstellar grains are taken to be fluffy aggregates of small silicates, vacuum and carbon of various kinds (Mathis and Whiffen, 1989, Mathis, 1996, Vaidya and Gupta, 1997, 1999, 2009, 2010, 2011, 2013, Vaidya et al. 2001, 2007, Gupta et al. 2016).

Spectropolarimetry of water ice features is correctly interpreted by core-mantle model (Hough et al.). All dust models are reasonably successful in reproducing the observed interstellar extinction and polarization, silicate absorption and polarization features and the dust thermal emission from the near IR to submillimeter (Duley and Williams, 1986, Drain and Lee, 1984, Dwek et al., 1997, Lee and Drain, 2001, Weingartner and Drain, 2001, Desert et al., 1990, Lee and Greenberg, 1997, Mathis and Whiffen, 1989, Mathis, 1996, Mathis, 1986, Greenberg and Lee, 1996, Mathis, 1998). Maldoni et al. (2003) has presented the extinction cross section profile for bare silicate grains and silicate grains coated with water-ice. Robinson and Maldoni (2010) have

calculated Q_{abs} for spherical core mantle grains using Mie theory for both alumina and Olivine bare cores of fixed radii coated with different water ice mantle thicknesses. The infrared observations have revealed that H_2O based ices trace dense clouds and these are mixed ices containing $\text{CO}_2, \text{NH}_3, \text{CH}_4$ and most ice features are consistence with molecule formation on cold grain surfaces (Boogert, 2015).

In this paper , we present a core-mantle grain model , with Silicate core and H_2O ice as mantle and calculated the absorption cross sections for silicate core envelopes with different thickness of coated ice. Silicates possess a characteristic absorption feature in the 8-12 μ waveband. We studied absorption features of all the ices accompanying the 10 micron silicate feature for mantle to core volume ratios from 0.01 to 0.04 in mid-infrared regions (5-30 μm region) in our core-mantle models .A mantle may be expected to broaden and slightly shift any absorption feature due to the core.

Here, Q_{abs} are calculated for spherical homogeneous or homogeneously coated particles when complex refractive indices of the involved materials are known as a function of wavelength (Bohren,1983). The optical constant data for silicate are taken from Drain(2003) and H_2O ice data are from Hudings et al. (1993). We have chosen a single grain size of 0.1 micron in our computational work as it is assumed to represent the size distribution of grains in the interstellar medium(Taylorand Robbin ,2016). For spherical noncomposite particles , the absorption efficiencies are calculated according to the well known Mie formula. For spherical core mantle particles , the Guttler formula is used (Wickramasinghe,1967).

The core-mantle grains model consist of spherical silicate core and ice mantles is proposed in the spectral range between 8.0 – 25 μ . In the study of variation in the absorption profiles of the silicate grain with the mantle thickness of ices , particular attention is given to the variation in the peak absorption wavelength with the mantle thickness.

III. Result and Discussion

Using Mie theory , the wavelength dependent cross-sections for Basic absorption band profiles for silicate is as shown in figure 1 .

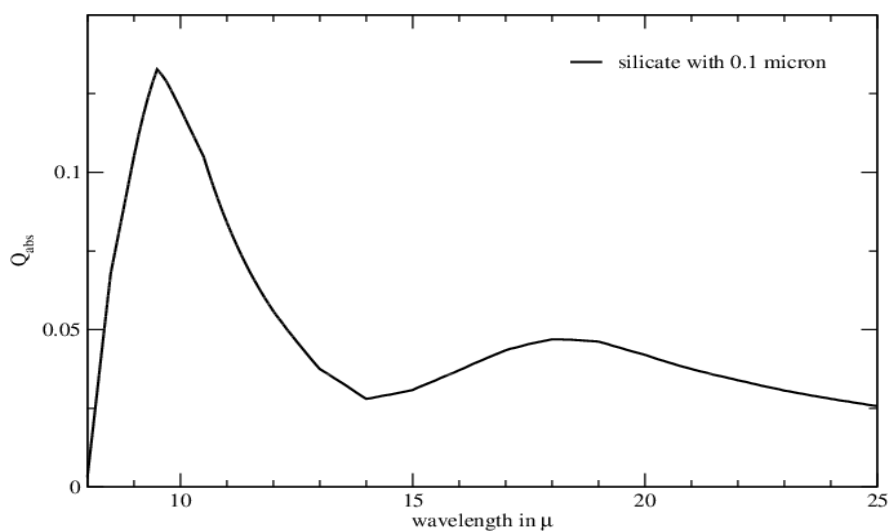


Fig.1 : Silicate absorption band profile.

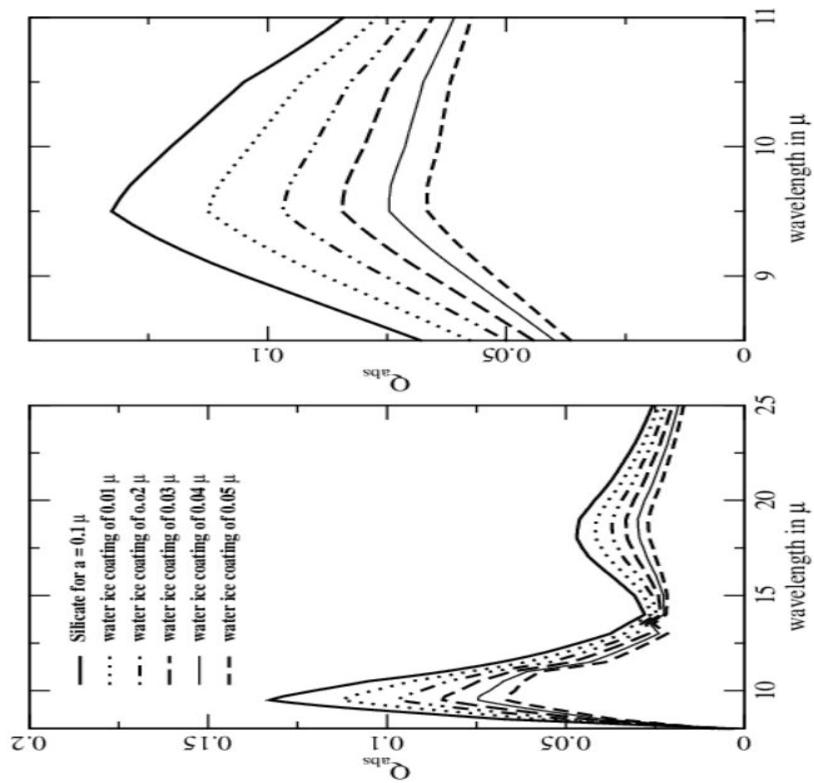


Figure 2. Q_{abs} versus wave length for ice coating of different thickness over silicate core.

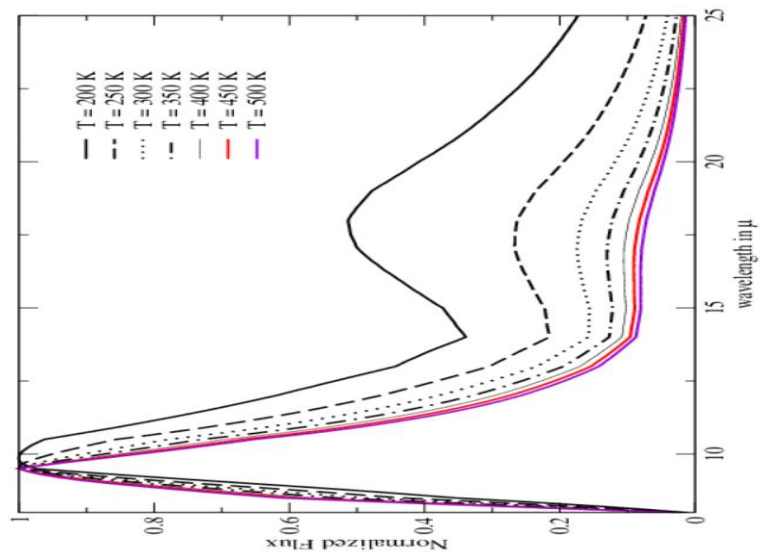


Figure 3. Flux calculated for silicate at different temperatures .

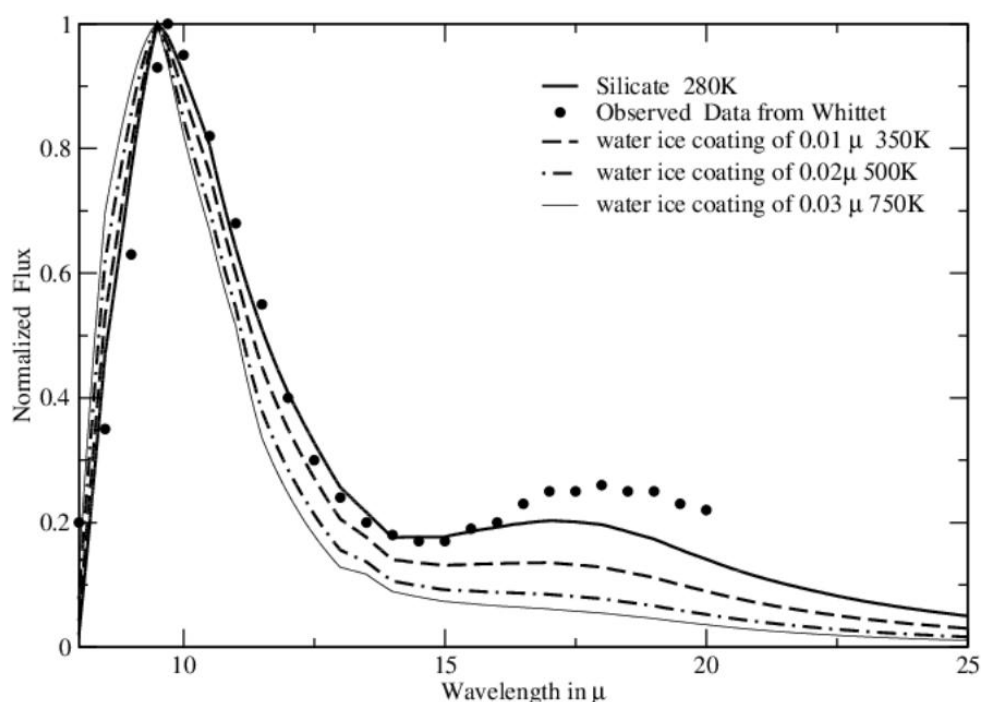


Figure 4. Flux for ice coating of different thickness over silicate core .

Effect of ice coating on 10 micron band region over flux for different coating thickness is displayed in figure 2. The figure shows that by increasing coating thickness , the peak wavelength is shifted towards lower wavelength .The Q_{abs} value decreases by increasing coating thickness and it seems to shift over higher wavelength . FWHM increases with ice coating .All these results are summarized in following tables.

Table 1 : Comparison 10 micron profile of silicate with observed data of Whittet.

| Thickness of ice coating over silicate core (in micron). | Temperature in kelvine |
|---|------------------------|
| Without coating | 280 |
| 0.01 | 350 |
| 0.02 | 500 |
| 0.03 | 750 |

In our this model , we studied absorption bands in 8-25 micron range for silicate core H₂O mantle . We studied the effect of coating thickness over the peak wavelength at 10 micron and it is observed that the peak wavelength is shifted to lower wavelength side as shown in the figure 2. We also compared our results with the observed data from Whittet.(44) as shown in the figure 3. Here the peak wavelengths shift to higher wavelength side and the Q_{abs} peak decreases in 8-25 micron band by increasing coating thickness. Similarly , FWHM shows steadily increases in 8-25 micron band by increasing the coating thickness. By increasing the coating thickness , the observed data shows matching at higher temperature as shown in table 2.

IV. Conclusion

We have presented calculations here which show the mutual influence between ice mantles and silicate cores in composite grains .This study has been done by varying the radius of coating layer of the ice with reasonable values and leaving the radius of silicate core as a free parameter. All cases have presented the same trend :

- The intensity of silicate absorptions are affected by the ice absorption even for very small coating thickness.
- FWHM has increasing trend by increasing coating thickness.
- Silicate core and H₂O molecules as outer mantle are directly observed in interstellar grains (Greenberg JM , 1989) , present calculations can be used for comparison.
- Calculations for nonspherical composite particles by T-matrix (
- http://www.giss.nasa.gov/staff/mmishchenko/t_matrix.html, Mishchenko ,1991, Mackowski and Mishchenko , 1996) is under progress.

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