Extinction Efficiency of Astrophysical Solid Materials

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1 Introduction

The radiation is not able to reach us without any interruption. Due to very efficient absorption and scattering, it is possible to recognize the existence of interstellar grains and molecules. All regions of the spectrum are determined by the direct interaction of such particles with the radiation fields of stars. The extinction efficiency of the material Q_{ext} is the important physical parameter, which determines the wavelength dependent interaction of matter with radiation. A theoretical approach to obtain the extinction efficiency is very important to study the formation and evolution of low mass stars and large planets, including Jupiter and Saturn in our solar system, the formation and structure of stellar winds, and the properties of the interstellar medium. Moreover, it does not only provide weighty information about the composition of interstellar grains, but also essential clues to the understanding of astrophysical phenomena.
We focused on low temperature ($T_{\rm eff} \approx 2000\,K$) extinction efficiency calculations of grains. Based upon our analysis of the most important condensed absorbers over a wide range of temperatures, we searched the literature to obtain optical constants for as many materials as possible. With the obtained data, we compute extinction efficiency of 23 different kinds of species with 29 different data sets.

2 Optical Constants and Method of Extrapolation

A solid particle obstructs the continuity of a light wave since the refractive index of the particle is greater than that of the surrounding medium. The refractive index is the ratio of the index of one medium to that of another, and is not an absolute value. When absorption is not significant, the refractive index of the material must be represented by a complex number. If one analyzes exactly the same species in a parallel or perpendicular measurement, one gets slightly different results leading to different real and imaginary parts of the optical constants. The refractive index is very important for our extinction efficiency calculations, in which we calculated 23 different kinds of species with 29 different data sets, including parallel and perpendicular sets (Tab. 1).

Tab. 1: Summary of extrapolation

Species	Ref.	Data Set [μm]	Extrapolation [μm]	Method
Silicate	[13]	0.4-500	0.1-0.4	H
α-SiC	[16]	0.1-243.67	243.67-500	F
$MgSiO_3$	[4]	0.32-500	0.1-0.32	H
$MgFeSiO_4$	[4]	0.2-500	0.1-0.2	F
Amorphous C	[19]	0.139-300.42	0.1-0.139, 300.42-500	H n:F k:H
FeS	[6], [17], [3]			
Fe	[10]	0.667-285.71	0.1-0.667 285.71-500	H n:F k:H
Cu	[12]	0.517-55.6	0.1-0.517 55.6-500	H n:F k:H
Ni	[11]	0.667-285.714	0.1-0.667 285.714-500	H n:F k:H
Nb	[14]	0.1016-10.33	0.1-0.1016 10.33-500	C n:F k:H
Ti	[10]	0.667-200	0.1-0.667 200-500	H n:F k:H
γ-Al_2O_3	[8], [2]	0.2-200	0.1-0.2 200-500	n:C k:F n:C k:F
α-Al_2O_3 (//)	[18]	0.29-55.556	0.1-0.29 55.556-500	n:C k:C n:C k:C
α-Al_2O_3 (+)	[18]	0.29-55.556	0.1-0.29 55.556-500	n:C k:C n:C k:C
Fe_2O_3(//)	[18]	0.21-55.556	0.1-0.21 55.556-500	H n:C k:F
Fe_2O_3(+)	[18]	0.21-45.455	0.1-0.21 45.455-500	H n:C k:F
Fe_3O_4	[18]	0.21-55.556	0.1-0.21 55.556-500	n:C k:F n:C k:C
H_2O (ice)	[17], [7]	0.092-666.7		
H_2O (liquid)	[14]	0.097943-230.15	230.15-500	n:C k:C
ZrO_2	[5]	4.545-100	0.1-4.545 100-500	n:C k:F n:C k:F
$MgAl_2O_4$	[14]	2.0-500	0.1-2.0	n:C k:F
$BaTiO_3$(o)	[14]	0.03668-1000	0.3548-0.422 7.5-10.31 0.69-2.5 7.5-10.31	n:H k:H n:H k:H n:H k:H
$BaTiO_3$(e)	[14]	0.03668-1000	0.342-0.422 7.5-10.31 2.309-2.5 7.69-8.33	n:H k:H n:H k:H n:H k:H
$SrTiO_3$	[14]	0.04133-1000	0.62-1.389 0.496-10	n:H k:H n:H k:H
α-SiO_2(Cry)(//)	[15]	n:0.9998-500 k:0.9998-250	0.1476-6.0 250-500	k:H k:C
α-SiO_2(Cry)(+)	[15]	n:0.2001-333.3 k:6.0-333.3	0.0998-6.0 333.3-500	n,k:S n,k:C
TiO_2(//)	[14]	n,k:0.1030-36.4	k:0.4410-11.2 n,k:36.4-500	k:H n,k:H
TiO_2(+)	[14]	n,k:0.1030-36.4	k:0.4410-11.2 n,k:36.4-500	k:H n,k:H
$Ca_2Al_2SiO_7$	[9]	6.6895-852.917	0.1-6.6895	n:H k:H

F: calculated via formula, H: extrapolated by hand, C: assuming a constant value, S: using SiO_2(//)data

In order to calculate the extinction efficiency, it was necessary to extrapolate most of the optical constant data sets since we wanted to obtain optical constants with wavelengths between 0.1 μm to 500 μm. The data sets for most species did not cover this entire wavelength range; therefore, we extrapolated short wavelength, long wavelength or both by using a formula, by hand, or by assuming a constant value. Tab. 1 presents the summary of the extrapolation for all data sets, which we used for our calculation.
We could not succeed to find the optical constants of $CaTiO_3$ and $MgTiO_3$, which are important species for the extinction efficiency calculation. Since Ca, Mg, Ba, and Sr belong to alkaline earth metals (group IIA) and their crystal structure are perovskite, we decided to use them as $CaTiO_3$ and $MgTiO_3$ for our calculations (Tab. 1).

3 Extinction Efficiency of Grain Species

The extinction efficiency of grain species Q_{ext} is shown as a function of wavelength (Fig. 1-5). The extinction efficiency is defined as the cross section, including both absorption and scattering, divided by πa^2, where a is the grain radius. We computed the extinction efficiency using the Mie theory, which represents the formal solution of the problem of light scattering by homogeneous spheres of arbitrary radius. This is an exact solution for grains that ranged in size from 0.000625 μm to 0.24027 μm, with an α=-3.5 power law distribution of grain sizes. The 19 grain species are divided into 5 groups where we obmitted metals. In case, Q_{ext}>1, the grain absorbs light more effectively than an inert, perfectly black sphere. On the other hand, if Q_{ext}<1, the grain is somewhat transparent.

• **High T Condensation (T~2000K)**
The high temperature condensation species presented in Fig. 1 are α-Al_2O_3(//), α-Al_2O_3(+), γ-Al_2O_3, $CaTiO_3$(//), $CaTiO_3$(+), $MgTiO_3$, ZrO_2, $MgAl_2O_4$, TiO_2(//), and TiO_2(+). ZrO_2 and γ-Al_2O_3 do not have a spike whereas other species have very sharp spikes. Absorption peaks of the depicted 10 species occur at wavelengths between 10 μm and 27 μm. γ-Al_2O_3 and TiO_2(//) have a single peak. However, α-Al_2O_3, ZrO_2, $MgAl_2O_4$, $CaTiO_3$ and $MgTiO_3$ have twin peaks whereas TiO_2(+) has triple peaks.

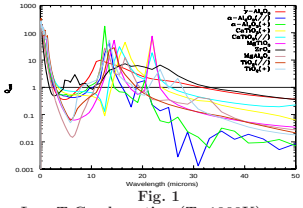

Fig. 1

• **Low T Condensation (T~1000K)**
The low temperature condensation species are FeS, Fe_2O_3(//), Fe_2O_3(+), and Fe_3O_4 (Fig. 2). Absorption peaks of these species occur at wavelength between about 15 μm and 30 μm, except for FeS which has a single absorption peak at approximately 4 μm. Although Fe_2O_3(//) has twin peaks and Fe_2O_3(+) has triple peaks, Fe_3O_4 does not have an absorption peak.

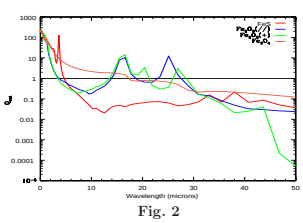

Fig. 2

• **Super Low T Condensation (T<500K)**
The super low temperature condensation species are H_2O (ice) and H_2O (liquid). Both have very similar absorption peaks: the first peak is at approximately 3.5 μm whereas the second one is at about 13 μm. Likewise, H_2O (ice) is an exception, because it is the only species which absorbs light again at a longer wavelength range (see small spike at about 40 μm in Fig. 3).

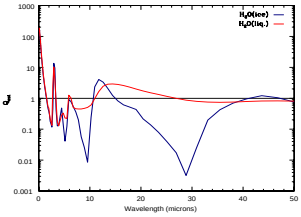

Fig. 3

• **Silicon Compounds**
The silicon compounds are silicate, $MgSiO_3$, $MgFeSiO_4$, α-SiO_2 (o), α-SiO_2 (e), and $Ca_2Al_2SiO_7$ (Fig. 4). Absorption peaks of the dipicted six species occur at wavelengths between about 7 μm and 22 μm. Silicate, $MgSiO_3$, $MgFeSiO_4$, and $Ca_2Al_2SiO_7$ do not show a big spike like α-SiO_2, instead, they have two very smooth absorption peaks. Conversely, both α-SiO_2(//) and α-SiO_2(+) have four spikes.

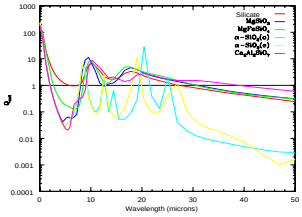

Fig. 4

• **Carbon Compounds**
Carbon compounds calculated in our studies are amorphous carbon and SiC. Amorphous carbon does not show any absorption peak (analog to other metal species not included in Fig. 5). Contrary to the previously named species SiC shows a single peak approximately at 12 μm.

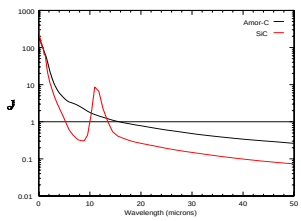

Fig. 5

4 Conclusion

Through an extended literature search we obtained optical constants for low temperature condensates. With this data we were able to calculate the extinction efficency of the high, low and super low condensation species as well as the silicon and carbon compounds. In the following we summarize our results:

• **In general:**
– Not all of the species do absorb light effectively at long wavelength.
– Resulting absorption peaks of all species are at less than 30 μm in wavelength (for exact wavelengths of the peaks see Tab. 2).

• **Extinction efficiency of grains:**
– The high temperature condensation species absorb light more effectively than the low temperature ones.
– All silicon compounds show a very similar behavior, except for α-SiO_2 which shows much more pronounced absorption peaks.

Tab. 2: Wavelength of the major absorption peaks

Species	Absorption Peak Wavelength [μm] †
High Temperature Condensation Species	
γ-Al_2O_3	11.749
α-Al_2O_3 (//)	13.490 20.417
α-Al_2O_3 (+)	12.589 20.417
$CaTiO_3$(+)	21.878 16.596
$CaTiO_3$(//)	15.488 21.878
$MgTiO_3$	21.878 14.454
ZrO_2	16.596 23.442
$MgAl_2O_4$	12.589 16.596
TiO_2(//)	14.454
TiO_2(+)	13.490 23.442 26.915
Low Temperature Condensation Species	
FeS	3.6308
Fe_2O_3(//)	25.119 16.596
Fe_2O_3(+)	16.596 20.417 26.915
Fe_3O_4	none
Super Low Temperature Condensation Species	
H_2O(ice)	3.1623 11.749
H_2O(liq.)	3.1623 14.454
Silicon Compounds	
Silicate	10.233 17.783
$MgSiO_3$	9.5499 17.783
$MgFeSiO_4$	9.5499 17.783
α-SiO_2(o)	20.417 8.3176 25.119 12.589
α-SiO_2(e)	19.055 8.3176 12.589 26.915
$Ca_2Al_2SiO_7$	10.233 20.417
Carbon Compounds	
Amorphous C	none
SiC	10.965

† Most dominant peak given first followed by peaks in decreasing order of dominance.

5 Outlook

Our future work will concentrate on further efforts to obtain more optical constants. Especially, species that condense at higher temperature, such as calcium compounds and titanium compounds, would be of most interest. Tab. 3 shows condensed species that may be present in astronomical objects for some combinations of temperature and density, and which should hence be calculated. We will obtain extinction efficiency for various species, using measured optical constants of particles with different radii or data sets for different temperatures. Consequently, we will be able to state whether there is a difference between the theoretical and observational results.

Tab. 3

Species				
MnS	$MgTi_2O_5$	VO	$CaMgSi_2O_6$	$MnSiO_3$
TiC	$Ca_2MgSi_2O_7$	CaS	$KAlSi_3O_8$	$CaSiO_3$
Mg_3N_2	$NaAlSi_3O_8$	Ti_2O_3	$Al_6Si_2O_{13}$	
Ti_4O_7	Cr_7C_3	V_2O_3	$ZrSiO_4$	
Al_2S_3	Mg_2SiO_4	Cr_2O_3	Ca_2SiO_4	

References

[1] Alexander, D.R. and Ferguson, J.W. 1994, Astrophys.J., **437**, 879
[2] Begemann, B., Dorschner, J., Henning, Th., Mutschke, H., Gürtler, J., Kömpe, C., and Nass, R., 1997, Astrophys. J., **476**, 199
[3] Begemann, B., Dorschner, J., Henning, Th., Mutschke, H., and Thamm, E., 1994, Astrophys. J., **423**, L71
[4] Dorschner, J., Begemann, B., Henning, Th., Jäger, C., and Mutschke, H., 1995, Astron. Astrophys., **300**, 503
[5] Dowling, J.M., and Randall, C.M., 1977, *Infrared Emissivities of Micron-Sized Prticles of C, MgO, Al2O3, and ZrO2 at Elevated Temperatures*, El Segundo: The Aerospace Corporation.
[6] Egan, W.G., and Hilgeman, T., 1977, Icarus, **30**, 413
[7] Hudgins, D.M., Sandford, S.A., Allamandola, L.J., and Tielens, A.G.G.M., 1993, Astrophys. J., **86**, 713
[8] Koike, C., Kaito, C., Yamamoto, T., Shibai, H., Kimura, S., and Suto, H., 1995, Icarus, **114**, 203
[9] Mutschke, H., Begemann, B., Dorschner, J., Gürtler, J., Bustafson, B., Henning, Th., and Stognienko, R., 1998, AStron. AStrophys., **333**, 188
[10] Ordal, M.A., Bell, R.J., Alexander, R.W., Newquist, L.A., Querry, M.R., 1988, Appl. Opt., **27**, 1203
[11] Ordal, M.A., Bell, R.J., Alexander, R.W., Long, L.L., Querry, M.R., 1987, Appl. Opt., **26**, 744
[12] Ordal, M.A., Bell, R.J., Alexander, R.W., Long, L.L., Querry, M.R., 1985, Appl. Opt., **24**, 4493
[13] Osenkopf, V., Henning, Th., and Mathis, J.S., 1992, Astron. Astrophys., **261**, 567
[14] Palik, E.D., 1991, *Handbook of Optical Constants of Solids II*, Orland: Academic Press Inc.
[15] Palik, E.D., 1985, *Handbook of Optical Constants of Solids*, Orland: Academic Press Inc.
[16] Pegourie, B., 1988, Astron. Astrophys., **194**, 335
[17] Pollack, J.B., Hollenback, D., Beckwith, S., Simonelli, D.P., Roush, T., and Fong, W., 1994, Astrophys. J., **421**, 615
[18] Querry, M.R., 1985, *Optical Constants*, Maryland: Chemical Research and Development Center
[19] Rouleau, F., and Martin, P.G., 1990, Astrophys. J., **377**, 526
[20] Tamanai, A., 1998, *Low Temperature Opacity*(Thesis: Wichita State University, Wichita, KS USA 67260).
[21] Warren, S.G., 1984, Appl. Opt., **23**, 1206

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Grid (1 , 1)