GRAINS AND PAHS

INTERSTELLAR DUST GRAINS – AN OVERVIEW

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Abstract. During the last years our knowledge about the structure and chemical composition of cosmic dust grains has very much deepened mainly driven by the rapid progress in infrared observations, laboratory experiments, and a much better theoretical treatment of grain evolution and the microphysical interactions of solid particles with gas, radiation, and with each other. This contribution will review the progress in the understanding of cosmic grains especially concentrating on the different grain populations, the physical processes which they link together, and the morphological and chemical structure of the particles.

1. Introduction

The study of cosmic dust grains is essential in understanding the dynamical, thermal, and chemical properties of the dense phases of the interstellar medium. Although the interstellar dust contributes only a minor amount to the total mass of our and other galaxies it strongly interacts with the stellar and gas components. The upper mass limit of newly formed stars and the stellar winds in distinct classes of evolved stars are directly related to the presence of solid particles (Yorke & Henning 1994, Sedlmayr 1994). Dust opacity effects may drive or influence instabilities in protostellar flows and accretion disks (Noh et al. 1991, Duschl 1993, Lenzuni et al. 1995). In addition, dust particles are both a sink and a source for gas phase molecules and play an important role in interstellar chemistry (Wagenblast & Williams 1993, Herbst 1993). The dust grains can carry a substantial fraction of the charge in dense, weakly ionized cosmic plasmas and, therefore, influence the electrodynamics of these regions (Havnes et al. 1987, Ciolek & Mouschovias 1993).

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Thermal continuum emission from dust grains at infrared and submillimetre/millimetre wavelengths serves as an important indicator for the presence of cold protostars, of circumstellar disks and envelopes around young stellar objects and stars in their later evolutionary stages, and of tori around active galactic nuclei (André 1994, Beckwith 1994, Henning 1996a,b, Urry & Padovani 1995).

There is still another aspect of cosmic dust research. The interstellar grains are a special system of nano- and microparticles (Bohren & Huffman 1983). Therefore, many bridges to solid-state physics, chemical physics, and quantum chemistry exist. The study of novel forms of carbon was triggered by astrophysical questions (Kroto et al. 1985, Krätschmer et al. 1990, Ugarte 1995), the investigation of polycyclic aromatic hydrocarbons got a new impetus from astrophysical studies (Léger et al. 1987), and new methods for the interaction of light with irregular, anisotropic, and fluffy grains were developed by astrophysicists (Draine & Flatau 1994, Henning et al. 1995, Stognienko et al. 1995, Michel et al. 1996).

In this review, I will discuss dust models for both the diffuse and molecular phases of the interstellar medium. Cosmic abundance constraints and new data from the analysis of primitive material in the solar system are included in the discussion. A more complete review about the dust metamorphosis in the galaxy is given by Dorschner & Henning (1995), the properties of dust around young stellar objects are covered by Henning (1996a,b), and dust in late stages of stellar evolution is reviewed by Sedlmayr (1994).

2. Cosmic dust - a multicomponent system

The cosmic dust consists of several well-distinguished populations typical of the special environments in which they are formed and/or modified (Dorschner & Henning 1995). Each population is a multi-component system containing grains or grain ingredients of different chemical composition and physical structure. There are at least four main populations:

- 1. Stellar outflow dust (stardust)
- 2. Dust in the diffuse interstellar medium (interstellar dust)
- 3. Dust in dense cool clouds (molecular cloud dust)
- 4. Circumstellar dust around young stellar objects (YSO dust).

Cool high-luminosity stars, in particular AGB and post-AGB stars, are the primary suppliers of stardust if the poorly understood process of dust formation in supernovae is not more efficient (Sedlmayr 1994, Jones & Tielens 1994).

In the diffuse interstellar medium, grains from various sources are well mixed. Because of the frequent reprocessing of grains due to the passage of shocks, adsorption of gaseous species, irradiation by the interstellar UV field and cosmic rays and being in the molecular cloud phase for several periods, the interstellar dust should develop into a homogeneous sample. Destruction mechanisms connected with SN shocks are thermal and non-thermal sputtering and grain-grain collisional vaporization/shattering (Tielens et al. 1994, Jones et al. 1994, Borkowski & Dwek 1995). The calculations by Jones et al. (1994) resulted in grain lifetimes of 4×10^8 yr (carbonaceous grains) and 2.2×10^8 yr (silicate grains) which are much shorter than the stardust injection timescale of 2.5×10^9 yr. Because most of the Si atoms are depleted in silicates, this would mean that an efficient grain growth process in the interstellar medium must exist and interstellar dust is not dominated by stardust injection. However, before a final conclusion can be drawn, the dust formation rate by supernovae and the grain destruction efficiency of porous grains and particles shielded by refractory mantles must be better known.

In the dense regions of molecular clouds, adsorption of gas phase species and surface chemistry leads to the formation of ice mantles. Theoretically (and partly proven by observations), one can expect mantles composed of H_2O , CH_3OH , CO, CO_2 and some other simple molecules with admixtures of impurities such as carbonaceous particles (Whittet 1993, 1996). Grain coagulation will modify the size distribution and leads to larger composite and fluffy grains (Ossenkopf 1993, Ossenkopf & Henning 1994, Weidenschilling & Ruzmaikina 1994). Similar processes but at a much higher rate are expected in the very dense protostellar cores. In protoplanetary disks including the solar nebula, the gases and grains were at least partially reprocessed by chemical reactions. In addition, dramatic changes of the grain properties due to coagulation, collisional and chemical destruction, sublimation and condensation can be expected (Morfill & Völk 1984, Mizuno 1989, Sterzik & Morfill 1994, Duschl et al. 1996, Schmitt et al. 1996).

3. Grain diagnostics

Cosmic dust grains have been studied from X-ray to radio wavelengths. Typical grain diagnostics consists of (Mathis 1993, Dorschner & Henning 1995):

- 1. X-ray haloes (Predehl & Klose 1996)
- UV/VIS/NIR extinction and polarization curves including the absorption feature at 217.5 nm (Cardelli et al. 1988, 1989, Martin & Whittet 1990, Whittet et al. 1992, Jenniskens & Greenberg 1993, Kim & Martin 1995)
- 3. Extended red emission observed in reflection nebulae, H II regions, and planetary nebulae and peaking between 650 and 700 nm (Witt & Schild 1988, Witt & Boroson 1990, Furton & Witt 1992)

- 4. Infrared emission and absorption features including the polarization in the features (Whittet 1993, 1996, Henning & Stognienko 1993, Henning 1996a)
- 5. Infrared and (sub)millimetre thermal continuum emission (Beckwith & Sargent 1991, Sodroski et al. 1994, Henning 1996a,b).

The diffuse interstellar bands at optical wavelengths (Herbig 1995, Tielens & Snow 1995, Salama 1996, Freivogel et al. 1994) and the infrared emission features (Allamandola et al. 1989, Puget & Léger 1989, Sellgren 1994) are generally not attributed to dust grains but related to C-bearing molecules (e.g. PAHs).

In the following, we will concentrate on some results of the infrared spectroscopy. The presence of the 10 and 18 μ m features in the spectra of a wide variety of objects (compact H II regions, Herbig Ae/Be stars, T Tauri stars, Vega-like objects, AGB stars) and along lines of sight going through the diffuse interstellar medium is generally attributed to silicates and shows their wide distribution (Little-Marenin & Little 1988, 1990, Simpson 1991, Ossenkopf et al. 1992, Jäger et al. 1994, Dorschner et al. 1995). Evidence for other refractory components such as carbides, sulfides, and oxides is mainly based on the detection of one single band in the spectra of circumstellar envelopes around evolved stars and doubts are, therefore, reasonable (see Tab.1). The ISO spectra of dust shells around evolved oxygen-rich stars revealed the presence of several new emission features between 20 and 45 μ m which are not yet reliably identified with special carriers (Waters et al. 1996).

A $3.4-\mu$ m feature has been observed in several IR sources in the Galactic Centre region, in the heavily obscured "hypergiant" Cyg OB 2 No.12, in some supergiants, and in some Wolf-Rayet stars of the types WC 9 and WC 10 (see, e.g., Pendleton et al. 1994, Sandford et al. 1995). The feature is generally attributed to C-H stretching vibrations of saturated aliphatic hydrocarbons present in the diffuse interstellar medium. Here we should note that there is no evidence that interstellar hydrocarbon grains contain a lot of oxygen. That means that the organic grain mantles may actually have a structure quite similar to HACs which may also form by other chemical routes via the direct condensation on pre-existing cores in the diffuse interstellar medium (Duley 1993) or the modification of amorphous carbon by reactions with atomic hydrogen (Furton & Witt 1993).

Infrared spectra of the Galactic Centre show absorption features at 3.0, 3.4, 5.5, 5.8, 6.1, 6.8, 9.7, and 19 μ m (Roche & Aitken 1985, Roche 1988, Tielens et al. 1996). The 3.0 and 6.1- μ m features can be attributed to the presence of H₂O as part of an incompletely hydrogen bonded network (Tielens et al. 1996). These features are probably produced in the molecular



Figure 1. ISOPHOT-S spectrum of the massive young stellar object W33 A

clouds associated with the Galactic Centre sources. They are not observed along other lines of sight through the diffuse interstellar medium.

Infrared spectroscopy revealed numerous bands of cosmic "ices" between 2 and 15 μ m in the spectra of deeply embedded molecular cloud sources (for reviews see Schutte 1996, Whittet 1993, 1996). The most abundant mantle molecule is H₂O with a pronounced feature at 3.08 μ m. This fundamental O-H stretch vibration has been observed in a wide variety of objects. Apart from the 3.08- μ m feature, the weaker O-H bending vibrations at 6.0 μ m are observed. Lacy et al. (1984) detected solid CO by its stretching vibration at 4.67 μ m in the infrared spectra of deeply embedded and luminous YSOs. CO is present in both polar and non-polar matrices (see, e.g., Chiar et al. 1995). A catalogue of optical depths in the CO feature for a larger number of YSOs is given by Whittet & Duley (1991). Solid CO₂ was first detected by its bending vibration at 15.3 μ m in the IRAS LRS spectra of a few

Wavelength	Component	Sources	References
11.3 µm	SiC	Carbon-rich CSE	Baron et al. 1987
13 µm	Al ₂ O ₃	Oxygen-rich CSE	Sloan et al. 1996, Begemann et al. 1996b, Koike et al. 1995
21 μm	SiS ₂	Carbon-rich CSE (PPNe)	Kwok et al. 1995, Henning et al. 1996, Begemann et al. 1996a
30 µm	MgS	Carbon-rich CSE	Omont et al. 1995, Begemann et al. 1994

TABLE 1. Carbides, oxides, and sulfides in circumstellar envelopes

embedded infrared sources (d'Hendecourt & Jourdain de Muizon 1989). ISO observations unambiguously demonstrated the presence of the C–O stretching vibration of the CO₂ molecule at 4.27 μ m in quite a number of YSO spectra (Gürtler et al. 1996, de Graauw et al. 1996, Whittet et al. 1996). Another ice component which seems to be much less important is CH₃OH with vibrations at 3.08 μ m (OH stretching mode), 3.35 and 3.53 μ m (CH stretching modes), 6.85 μ m (CH₃ deformation mode), 9.75 μ m (CO stretching mode), and at 8.9 μ m (CH₃ rocking mode). Recent results can be found in Allamandola et al. (1992) and Skinner et al. (1992). The feature observed at 6.85 μ m is probably a blend of different absorption components because otherwise the CH₃OH abundance derived from the 6.85 μ m feature would be much higher and would contradict the values obtained from the 3.53 μ m and 9.75 μ m feature.

4. Cosmic abundance constraints

Element abundances have been widely used to constrain dust models. The fractional abundances of the elements directly lead to the main dust-forming species: oxygen, carbon, iron, silicon, and magnesium. That means that the dust grains are mainly made up of carbonaceous solids, silicates, and other iron/magnesium oxides. New determinations of gas phase abundances with the Goddard High Resolution Spectrograph aboard the Hubble Space Telescope and the NLTE analysis of B-star atmospheres point to tighter limits for the carbon and oxygen present in dust grains (Snow & Witt 1995,

Abundances	C/H [ppM]	О/Н [ppM]
Solar	355 ± 50	740 ± 90
abundances	(Grevesse & Noels 1993)	(Grevesse & Noels 1993)
Cosmic	225 ± 50	350 ± 50
abundances	(Snow & Witt 1995)	(Kilian et al. 1994)
(young stars)		480 ± 180
		(Gies & Lambert 1992)
Interstellar gas	140 ± 20	310 ± 20
abundances	(Cardelli et al. 1996)	(Sofia et al. 1994,
		Cardelli et al. 1996)
Cosmic grains	100 - 400	150 ± 30
	(different models)	(Fe, Si, Mg in
	50 ppM of graphitic carbon	completely
	are needed to produce the	oxidized
	are needed to produce the	
	217.5 nm bump;	state)
	217.5 nm bump; 140 -155 ppM sufficient to	state)
	217.5 nm bump; 140 -155 ppM sufficient to explain IS extinction including	state)

TABLE 2. Cosmic abundance constraints

Mathis 1996a, b, Cardelli et al. 1996). The B-star abundances are much less than the solar values traditionally assumed as a reference for the interstellar medium (see Table 2). If the lower abundances are typical for the "cosmic" abundances and we take into account that about 50 ppM of graphitic carbon are needed to produce the 217.5 nm bump, not much carbon is left to produce the interstellar extinction curve. Even if we use the solar value for the fractional abundance of carbon, many dust models require too much carbon (300-400 ppM) in the solids if the new gas phase C/H values are considered. The oxygen in the dust grains could completely account for the difference between the gas phase value and the reduced reference abundance. We should note that there may be still systematic errors in the B-star abundance determinations or that the heavy elements may not be completely incorporated into stars during massive star formation.

5. Primitive material in the solar system

The detection of stardust grains in primitive meteorites and interplanetary dust particles as well as new data from interplanetary spacecrafts are important sources of information concerning the nature of interstellar dust grains. The isotopic analysis led to the identification of presolar diamond, carbides, graphite, corundum, and silicon nitride grains (Anders & Zinner 1993, Ott 1993 a,b, Zinner et al. 1995, Nittler et al. 1995). Up to now, silicate grains with a typical AGB star isotopic signature have not been detected in primitive solar system solids. However, Bradley (1994 a,b) found non-stoichiometric grains of silicate glasses with depletions of magnesium and silicon relative to oxygen and inclusions of iron-nickel metal and iron sulfides (GEMS = Glasses with Embedded Metal and Sulfide). These are strong indications for a pre-accretional origin where strong irradiation strips the cations with the weakest band strengths from the grains. GEMS are a special subgroup of polyphase grains occuring in anhydrous interplanetary dust particles. The sizes of these basic subunits range from 0.1 to 0.5 μ m. The GEMS share many properties with interstellar silicate grains (Martin 1995, Goodman & Whittet 1995) although it cannot be excluded that they are early nebular condensates.

Interstellar dust grains with sufficiently low charge-to-mass ratios can penetrate the heliopause and enter the solar system. The detection of an interstellar dust component in the solar system by the Ulysses dust detector (Grün et al. 1993, 1994) opened a direct way for the investigation of such particles. The mean mass of the particles was 3×10^{-13} g with even more massive particles present.

6. Grain models

Grain models for the diffuse interstellar medium are mainly based on an analysis of interstellar extinction and polarization curves taking into account cosmic abundance constraints (see Mathis 1993, Dorschner & Henning 1995). Recent dust models are summarized in Table 3. Here, the grain composition is given by AC (amorphous carbon), GRA (graphite), HAC (hydrogenated amorphous carbon), I (iron), PAH (polycyclic aromatic hydrocarbons), RO (refractory organics), and SIL (silicates). The size distribution is described by d (discrete size or very small size interval), exp (exponential law), g (giant grains in the order of magnitude 10 μ m), p (power law), and vs (very small grains).

All current dust models share some common features: (1) they contain silicate and carbonaceous material, (2) they include very small grains and/or PAHs, and (3) they all claim to be able to fit the observed extinction curves. The last item is indicative of the non-uniqueness of the model predictions. With the non-uniqueness of the models, we mean that integral quantities (extinction) are fitted which contain both the size distribution and the optical properties of the grains. Better constraints of the models can be obtained if both the extinction and polarization curves are simultaneously modelled and spatial/temporal variations of the curves are taken into account.

The properties of the dust population in molecular cloud cores, circumstellar envelopes around YSOs, and protoplanetary disks can be considerably different from those of the dust in the diffuse interstellar medium and the envelopes around evolved stars. There are two main processes which modify the grains in the colder regions: the formation of molecular ice mantles and the coagulation of grains leading to fluffy and inhomogeneous aggregates. The optical properties of coagulated particles are a sensitive function of the assumed structure and chemical composition of the clusters (for reviews see Henning et al. 1995, Henning 1996b). In protoplanetary disks including the solar nebula, the gases and the grains were at least partially reprocessed by thermochemical reactions and shock chemistry (Prinn 1993). This may explain the wide-spread existence of FeS (troilite) in primitive bodies of the solar system. During the evolution of protoplanetary disks, dramatic changes of the opacity due to coagulation, collisional destruction, sublimation, and condensation of grains can be expected (see, e.g., Morfill & Völk 1984, Mizuno 1989, Sterzik & Morfill 1994, Schmitt et al. 1996).

Comprehensive dust models for protostellar cores and protoplanetary accretion disks were recently provided by Pollack et al. (1994), Henning & Stognienko (1996), Krügel & Siebenmorgen (1994), and Ossenkopf & Henning (1994). The latter authors treated the dust evolution in cold molecular cloud cores together with the evolution of the optical properties of the particles self-consistently. The fluffy structure of the aggregates produced during the coagulation process was explicitly included in their calculations. The main components of this dust model are silicates, amorphous carbon, and an ice mixture. Pollack et al. (1994) considered the material composition and the element abundances in molecular cloud cores and accretion disks in detail. They are partly based on the chemical composition of primitive material found in the solar system. The authors included olivine, orthopyroxene, volatile and refractory organics, water ice, troilite, and metallic iron as major grain species. In contrast to the earlier model by Pollack et al. (1985), they did not consider hydrated silicates and magnetite. A detailed investigation of the influence of particles with a fluffy structure on the disk opacities was performed by Henning & Stognienko (1996). A major result of this study was that the iron abundance in the different dust species plays a crucial role for the optical properties of the protoplanetary dust popula-

Authors (year)	Grain type Composition	Size distr. function	217.5nm carrier
Draine and Lee (1984)	bare grains SIL, GRA	р	GRA
Chlewicki and Laureijs (1988)	core-mantle + bare grains core: SIL, mantle: RO, bare: GRA, I, PAH	exp, d	GRA
Greenberg (1989)	core-mantle + bare grains core: SIL, mantle: RO, bare: GRA	exp, d	GRA
Williams (1989), Duley et al. (1989)	core-mantle + bare grains core, bare: SIL, mantle: HAC	p, vs	SIL
Mathis and Whiffen (1989)	coagulated + bare grains coagulated: SIL, GRA, HAC bare: GRA	р	GRA
Wright (1989)	fractal	· · · · · · · · · · · · · · · · · · ·	GRA
Désert et al. (1990)	core-mantle + bare grains core: SIL, mantle: RO, bare: AC, PAH	p, vs	carbon. material
Sorrell (1990)	bare grains porous SIL, AC, GRA	d	GRA
Rowan-Robinson (1992)	bare grains SIL, AC, GRA	d, g	GRA
Siebenmorgen and Krügel (1992)	bare grains SIL, AC, GRA, PAH	р	GRA
Aannestad (1995)	core-mantle + bare grains core: SIL, mantle: GRA, AC, RO, bare: Diamonds, carbon. grains, SIL, PAH	p, vs	GRA
Mathis (1996b)	coagulated + bare grains coagulated: SIL, carbon, oxides, bare: GRA	p, exp	GRA

TABLE 3. Dust models for the diffuse interstellar medium

tion. The next model step will be the self-consistent calculation of the dust evolution, optical properties, and re-coupling of the evolving opacities to the disk dynamics (Schmitt et al. 1996).

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Discussion

Pecker: When one considered "spherical" grains to be typical, a lot of discussion was made about *lifetimes* of grains, taking into account growth factors, destruction factors (sputtering) and "expulsion" by the radiation field. Dust was found to stay a short time near hot stars, a longer time in the ISM, and finally the smaller dust grains were expelled from the galaxy by galactic radiation. The size spectrum of grains in the ISM was then rather *narrow* (A&A, 1974, Pecker, and other papers). What is the present situation?

Henning: Recent models of grain sputtering in interstellar clouds indicate grain lifetimes of a few 10^8 years, which are considerably shorter than the stardust injection timescale.

Williams: First, a comment: Cesare Cecchi-Pestellini and I have developed a model of dust that is consistent with the new abundance constraints. My question is: would you not agree that the materials of which dust is composed may change their nature in response to the local conditions, and so variations in the interstellar extinction curve (and other observational parameters) may be caused by such changes, in addition to possible changes in grain size distribution?

Henning: We cannot exclude this possibility at the moment. Dramatic changes of the optical properties can be expected during the growth of particles (Ossenkopf & Henning 1994, Schmitt et al. 1996). In addition, we expect the presence of different carbon modifications depending on the hydrogen content and the radiation field of the environment.