Composition and evolution of grains

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Aussois, March 2006

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Processes Cosmic rays Thermal annealing UV photons Surface reactions

Size modification

Coagulation MAC with size Distributions gas phase accretion coagulation sedimentation

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Class 0-III



extract from Bam Acke thesis 2005, see ref. cited

In terms of observability of dust composition, outside the solar system, limited to IR and MM.

 will lead to observational biases Composition and evolution of grains

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Dust sources : from production to evolution

EVOLUTIO

DUST LIFECYCLE_4-

SOURCES

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Contributions of Stardust Sources in the ISM



after Jones et al., 2001, Phil. Trans. R. Soc. Lond. A, 359, 1961

Mass loss rates inject a large fraction of dust

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Schematic view of a cooling/expanding flow



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Chemical effect : composition driven by the $\ensuremath{\mathsf{C}}\xspace/\ensuremath{\mathsf{O}}\xspace$ ratio



Ebel, 2000, JGR 105, 10365.

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Physical effect : evolution of the flow rates



Molster et al. 2002, Posch et al. 2002, Cami 2002 ...

 Correlation between wind density and condensates Low loss mass : Simple oxides (quenching) High loss mass : Amorphous silicates like ISM ones Even higher : Cristalline silicates

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Reality : condensation sequences



+ binarity

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Silicates "astromineralogy"

Olivines $(Mg_{2x}Fe_{2-2x}SiO_4)$	Formula	Name
	Mg_2SiO_4	Forsterite
	Fe_2SiO_4	Fayalite
Pyroxenes $(Mg_xFe_{1-x}SiO_3)$	Formula	Name
	$Mg_2Si_2O_6$	Enstatite
	$Fe_2Si_2O_6$	Ferrosilite
		(hypersthene)
	$CaMgSi_2O_6$	Diopside
	$CaFeSi_2O_6$	Hedenbergite

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Silicates



Pyroxene



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2. (µm)

Jaeger et al. 1998

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100

100

Compositions



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Carbonaceous material : versatile bondings

- sp (alkanes, carbon chains)
- sp² (graphite, fullerene, nanotubes, Polycyclic Aromatic Hydrocarbons (PAHs))







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mixed bondings: (Hydrogenated) Amorphous Carbons (HAC)



Dartois et al. 2005

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■ Large number of phases

PAHs (coronene)



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PAHs emission is not thermal



Léger (in this room !) Puget 1984

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PAHs emission



Extracted from ISO database

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Padgett et al. 1999

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Disks models : the simplest flat passive case



e.g. Lynden-Bell & Pringle 1974; Adams, Lada, Shu 1988

Power absorbed by dS ≈ \$\frac{\sigma T_*^4 R_*^2}{r^2} sin(\alpha) dS\$
≈ \$\frac{\sigma T_*^4 R_*^2}{r^2} dS \frac{R_*}{r}\$
Power radiated by dS ≈ \$\sigma T^4(r) dS\$
\$T(r) ≈ \$T_*(\frac{r}{R_*})^{-3/4}\$

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Passive disks : integration

Flux emitted $L_{\nu}/4\pi d^2 = \nu F_{\nu}$ $= \nu \int_{Rint}^{Rext} 2\pi r B_{\nu}(T(r)) dr$

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Flat disk SED



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Chiang & Goldreich, 1997

Passive disks : flared disk

e.g. Kenyon & Hartmann 1987

- Expected due to hydrostatic equilibrium that gas/dust scale height and therefore α increase with radius.
- $\alpha_{flared} > \alpha_{flat}$, intercept more stellar flux

г

• $T(r) \propto r^{-2/5}$

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Flared disk SED



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Flared disk radiative equilibrium



Chiang & Goldreich 1997

- Stellar light absorbed in the upper layer where $au_V \approx 1$
- T(surface) > T(blackbody) (flaring + $\kappa(\nu)$ V>> $\kappa(\nu)$ IR)
- ▶ IR emitted by surface outward detected ($\tau_{IR} \ll \tau_V$)
- ▶ IR emitted inward absorbed if $\tau_{IR} \approx 1$ (still related to α !!!).

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SED flat disk + transfer



Chiang & Goldreich 1997

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SED flared disk + transfer



Chiang & Goldreich 1997

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With features ...!!!...



Chiang & Goldreich 1997

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A hole in the SED



Will produce fluxes deficits in the NIR-MIR range

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Observations show near infrared excess



Natta et al. 2001

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Quantify NIR excess



Natta et al. 2001

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- up to \sim 25% of total stellar flux
- poorly compatible with disks reaching stellar surface

An geometry change near the dust sublimation ?



Dullemond, Dominik & Natta 2001

- Interface cavity/dust sublimation zone.
- Puffed-up and hotter rim (directly exposed to stellar flux).
- Will affect the shadowed region just behind (Mid-ir suppression).

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Effect on the SED



Dullemond et al. 2001

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SED need for this inner disk wall



Natta et al. 2001

- Some SED show infrared deficit "Clearing" (DM Tau, GM Aur, Calvet et al. 2005)
- SED evidence of gaps in the first 10's AU ?

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Interferometry in the IR



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Interferometry in the IR

"Optically-thin Cavity" Disk Model



 Lower luminosities compatible with the puffed-up inner wall.

e.g. Monnier et al. 2005, see also Eisner et al. 2004, Millan-Gabet et al. 2001 and co-workers for more details on IRI.

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NIR Excess observed at all disk angles

Not a wall !



Isela & Natta 2005

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- smoother inner puffed-up rim.
- Less sensitive to disk orientation as observed.

Other mecanisms to take into account for SED



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Observations of PAHs and Silicates

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Observations: PAHs and Herbig-Ae/Be with ISO

Acke & van den Ancker 2004

- PAHs detected in 26 over 46 Herbig-Ae/Be (57%)
- ▶ 6.6µm in 25/46
- ▶ 7.7µm in 19/46
- ▶ 8.6µm in 16/46
- ▶ 3.3µm in 12/46

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Correlation with Silicates



Acke & van den Ancker 2004

• PAHs poorly or uncorrelated with $10\mu m$ silicates

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Dize modification Coagulation

Distributions gas phase accretion coagulation redimentation

Luminosity emitted/absorbed



Acke & van den Ancker 2004

- absorption/emission decreases with increasing UV flux
- efficiency of PAH abs/em decreases ?
- Hardness play a role?

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Insights ?

- ► No correlation between 850 or 1300 µm excess and PAHs features
- Not correlated with the disk mass but the surface ?
- No correlation between relative PAHs features strength and UV
- $3.3/6.6\mu$ m flux ratio varies from 9% to 94%
- and is apparently independent of stellar UV field
- Sources with faintest 60μ m means faintest PAHs
- ► No correlation disk mass with PAHs emission ⇒ surface layers excitation ?

Acke & van den Ancker 2004

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Spitzer's spectra of Herbig Ae/Be



Sloan et al. 2005

- 6.2 μ m and 7.7 μ m shifted to higher wavelengths
- 2 out of 4 sources display aliphatic emission
- Variation in the 7.9µm/11.3µm ratio : ionisation state ?

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Spitzer's spectra of T Tauri



LkH α 330, C2D program, Geers et al. 2005, Protostars and Planets V

- Confirmed detection of PAHS in about 15% of observed sources.
- ... but may be up to 45%
- Difficulty to observe the 7.7 and 8.6µm features, blended with silicates.

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Modele de PAHs dans les disques



Habart et al. 2004

- Model "standard" idem au modele ISM
- Nc = 100, Teff = 10500K, L = 32L ⊙, M* = 2.4M ⊙, Mdisk = 0.1M ⊙, Rin = 0.3AU, Rext = 300AU, Flared

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Modele de PAHs dans les disques



Other parameters :ionized PAHs (lower CH

modes)

 dehydrogenated PAHs (lower CH modes, enhance CC modes)

Habart et al. 2004

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Modele de PAHs dans les disques



Other parameters :

 lower sizes (Nc=40 instead of Nc=100)

Habart et al. 2004

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Comparison with some obs



Habart et al. 2004

- Objects with strong
 UV have weak 3.3µm!
- The authors propose PAHs are destroyed or disk dissipated.
- integrated spectra are not good (need spatial resolution)
- compatible with large neutral or small ionized
- If present, provide an additional source of opacity and chemical reactant, should expect differences wrt silicates disks

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Spitzer's spectra of T Tauri

- Ground based obs start to resolve the PAH emission.
- Emission originate at (up to ?) 100-150 AU
- ► Geers et al. 2004; van Boekel et al. 2004; Habart et al. 2004
- If coming from 1AU would produce much higher fluxes
- Line flux for T Tauri 1-2 orders of magnitude higher than expected disk + ZAMS models (without taking into account UV form accretion shocks)
- Inner disk PAH abundance lower because destroyed (multi-photon process)

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Silicates in Herbig Ae/Be and T Tauri



Meeus et al. 2001

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Spectra of group I and II



Meeus et al. 2001

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Models of group I and II



Dullemond and Dominik 2004

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Grain growth : infrared evidence in T Tauri



Ground based, ISO; Przygodda et al. 2003, Bouwman et al. 2001

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Grain growth : infrared evidence in Ae/Be



van Boekel et al. Acke & van den An-2003 cker 2004 Composition and evolution of grains

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Spitzer's evidence in T Tauri



Kessler-Silacci 2006

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- Fast grain growth in the surface
- Not correlation strength/shape with age.
- Correlation strength/shape with spectral type ?

Compositional fits for Ae/Be

Must take simultaneously into account mineralogy AND grain growth



Van Boekel et al. 2005

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Some correlations



Grain size versus Crystallinity

Van Boekel et al. 2005 and ref therein

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Implications ?

- Silicates in the ISM are almost 100% "amorphous"
- (<0.4% Kemper et al. 2004)
- and in the Rayleigh limit (small)
- all sources display at least 30% of big grains
- In disks observed, there is removal of small grains (otherwise we would see them !)
- grains are bigger than ISM (sensitivity bias, maybe even bigger)

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coagulatio

Some correlations



Mass fraction in Enstatite versus total crystal

Van Boekel et al. 2005 and ref therein

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Implications ?

- crystal/amorph. $\leq 35\%$
- ▶ higher stellar mass → more crystal
- sources with crystal. sil. have more large grains
- Forsterite (Mg₂SiO₄) / Enstatite (MgSiO₃) Low crystallinities/ High cristallinities
- All sources with more than 2.5M^O have a high fraction of big grains.

Van Boekel et al. 2005 and ref therein

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Radial processing ?



Van Bokel et al. 2004

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Suggest differential processing :



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Differential processing : Enstatite/Forsterite



Gail & Seldmayr 2004

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crystal to amorphous ratio



Bockelée-Morvan et al. 2002

Radial Distance r

- If the radial mixing is efficient on timescale << disks life ...
- ... and the vertical mixing also
- then [cryst]/[amorph] might represent the global dust processing
- ► Forsterite band at $33.5\mu m$ Vandenbussche et al. 2004 with ISO \rightarrow crystal at distance > 10 AU.

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A few processes affecting grains

Cosmic rays

- Thermal evolution (e.g. radial mixing)
- UV photolysis (stellar, ambient field, cosmic rays induced), X-Rays
- Surface reactions, accretion

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$30 \text{keV He}+ \text{ irradiation of Forsterite } (Mg_2SiO_4)$



Optical depth [arb. unit.]

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Brucato et al. 2004

20-50keV He+ irradiation of Enstatite (MgSiO₃)



Demyk et al. 2004, Carrez et al. 2002

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Energy dependence



Stopping power Forsterite, Brucato et al. 2004

high-energetic cr (E > 10MeV) pass through

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Astrophysical timescales



Irradiation doses, Brucato et al. 2004, Jager et al 2003

- low energy ions dose is about 10 ions cm⁻².s⁻¹ during a few 10⁸ years Jones et al. 1996
- Grains receive therefore the equivalent of 10²⁵⁻²⁶ eV.cm-1 from SN ejecta
- Can fully amorphize 40 Angstrœ m grains, can explain ISM amorphous feature.

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Thermal annealing of Mg_2SiO_4 smokes at 1000 K



Fabian et al. 2000

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Thermal annealing keV amorphised Mg_2SiO_4 at 1030 K



Djouadi et al. 2005

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Activation energies for Mg₂SiO₄

$$\frac{1}{\tau} = \nu_0 \, \exp(-\frac{E_a}{kT})$$

- Ea/k = 45500 K vapor phase + vacuum annealing (Hallenbeck et al. 1988)
- Ea/k = 39100 K laser smoke silicates + vacuum annealing (Fabian et al. 2000)
- Ea/k = 40400 K Laser vaporization + vacuum annealing (Brucato et al. 2002)
- Ea/k = 41700 K vapor phase + vacuum annealing + keV amorphization + vacuum annealing. (Djouadi et al. 2005)
- Activation energies not much altered by irradiation
 No "metastable" state as suggested by e.g. Molster et al. 1998

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Implication: radial mixing in disks !



- ► Cristalline silicates (Tform.≈1000K) mixed with ices (Tsubl.≈100K)
- Radial mixing, reprocessing, X ray

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coagulation sedimentation

UV photons versus cosmic rays





UV photons

- Photochemistry (break specific bonds)
- Penetration depth mixture dependant
- Stopped by a few molecular layers
- Ionise species

Adapted from Gerakines et al. 2001

- Cosmic Rays
- Break bonds
- Penetration depth depends on stopping power
- Goes through the grain
- Ionise and generate secondary electrons

Composition and evolution of grains

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Size modification

The existence of some surface reactions

Much before class II, Field stars probe the onset and distribution of ices



Murakawa et al. 2000

- τ H₂0 (ν_1 , ν_3) = α (Av Ath)
- Abundance 10^{-4} - 10^{-5} N_H \neq Gas phase timescales
- surface reactions involving atomic oxygen needed
- well known for the formation of H₂ that surfaces required

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Grain surfaces indirect influence



Ices : inhibitors/promotors for gas phase chemistry.

 Coupling of gas and dust chemistry (need for grains to reform H₂ efficiently at the surface layer)

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Grain surfaces indirect influence



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From diffuse to dense media: structuration of the ISM, intermediate phases

e.g. Cirrus cloud L1780



Miville-Deschênes et al. 2003



- Spectacular decrease of 6.7µm/100µm intensities
- ... but not due to extinction as the cloud is thin

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- variations attributed to PAHs decrease versus VSG increase.
- No spectral info on silicates.
- Signs of dust processing, coagulation, but also protection

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Gas accretion and coagulation



Cambresy et al. 2001

 \blacksquare $au(200 \mu {
m m})/{
m A_V}$ for ${
m A_V} \lesssim$ 6 $> au(200 \mu {
m m})/{
m A_V}$ diffuse

e.g. Boulanger et al. 1996, Bernard et al. 1999, Stepnik et al. 1999, del Burgo et al. 2003

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Grain growth in class 0-1 ?



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Grain growth in class 0-I



size effects on line profiles

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Observed with line ice mantles profiles ?



Dartois 2006

influence on a weighted size distribution may be present.

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Global effect on a distribution



amin~50nm

amax~0.25micron

Mathis Rumpl Nordsieck 1977; Draine & Lee 1984

... slope changed wrt the dense clouds observed.

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coagulation sedimentation



- low size parameter $(2\pi a/\lambda << 1) \kappa \propto$ volume
- intermediate size parameter (2πa/λ ≈ 1) κ highest (best coupling of wave vector to grain size)
- \blacktriangleright low size parameter $(2\pi a/\lambda >> 1)~\kappa \propto$ surface

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A jump into disks in the mm : spectral index β



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A jump into disks in the mm : spectral index eta

- Flux received from a disk in the mm:
- Optically thin: $F(\nu) \propto \kappa(\nu) [cm^2.g^{-1}] B_{\nu}(T_{dust}) M_{dust} / d^2$
- Rayleigh-Jeans limit: F(ν)∝ ν² κ(ν)[cm².g⁻¹] T_{dust} M_{dust} / d²
- Outside the solid material strong absorption bands If $\kappa(\nu) \propto \nu^{\beta}$ then $F(\nu) \propto \nu^{\beta+2}$ The β of dust can be inferred from the observed flux slope minus 2.

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mm dust index change in disks wrt ISM



Beckwith & Sargent 1991 Consequences:

- Some grain properties have changed.
- With β, Mass determination and slope changes.
- The Dynamical masses requires this change in mass abs coeff (e.g. Hogerheijde et al. 2003; ref in talk by A.D., S.G.), otherwise unstable disks

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$eta~pprox {f 1}$ in the mm for circumstellar disks, Why ?

- Large fluffy grain ?
- Grain with sizes of the order of the wavelength ?
- Chemical composition ?
- Optical thickness effect ?
- Temperature effects ?

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Optical thickness

- If the disk is not fully optically thin at mm wavelengths
 β ≈ (1 + Δ)(α − 2)
- with Δ ratio of thick to thin (Beckwith & Sargent 1991)
 it makes β higher

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Composition

- Various components tested by e.g. (Pollack et al. 1994)
- authors say silicates and organics are dominant sources of grain opacities
- H₂O ice (also present in spherical cores and beta almost the same)
- Low k and n at long wavelength, a moderate effect if pure
- but may be important if allow to stick together high n,k material (H₂O matrix effect).

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Fluffyness ?

Investigated theoretically and experimentally, e.g;



e.g. Dominik & Tielens 1997, Wurm & Blum 2004

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Shape and Fluffyness ?

- $\blacktriangleright \kappa$ ten times higher in the geom. regime.
- κ same in the Rayleigh regime (volume)
- κ smoother in the intermediate regime
- Increases the size parameter and coupling of the grains.
- Make an antenna if one dim. large for the same volume.





FIG. 4. Mass opacities (in cgs units) of single-sized compact dust particles (f = 1) for various radius a (0.01 μ m to 100 m) composed of the intimate mixture of silicate and H₂O-ice, where the abundances of dust particles with respect to the H₂ gas are assumed to be solar. Curves for $a \le 10$ am are almost identical at $\nu \le 10^{-35}$ H₂.



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Temperature variation of β ?



Fayalite 295,200,160,100,24Ke.g. Mennella et al 1998

Dust index change for the same material, then T,M vary.

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T variation of β



• MAC for 1.5μ m silica spheres

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 Temperature dependence of β MAC for various silicates in the 10 – 20cm⁻¹ range. Composition and evolution of grains

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T variation of MAC

Temperature (K)	10	30	100	200	300
Silica spheres (1.5 μ m)	0.33	0.36	0.73	1.79	5.66
Fumed silica	0.45	0.51	1.26	2.18	3.75
MgSiO ₃ glass	0.22	0.25	0.37	0.53	0.75
MgSiO ₃ sol-gel	0.12	0.15	0.32	0.59	0.98

Table: Mass absorption coefficient at $10cm^{-1}$ ($cm^2.g^{-1}$)

e.g. Boudet et al 2005

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At very low temperatures



e.g. Agladze et al. 1996

- Turnover in the MAC between 10 and 20K.
- Two Level Systems.

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A summary of abs. coeff.



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Draine 2006

A summary of abs. coeff.



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coagulation sedimentation

Effect of the size distribution

• $\kappa_{\nu} = \frac{\int_{amin}^{amax} (dn/da) Cabs(a,\nu) da}{\int_{amin}^{amax} (dn/da) V(grain) \rho da}$ • $dn/da \propto a^{-3.5}$ • $amin = 3.5 \text{\AA}$ Composition and evolution of grains

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MRN size distribution effect on β



Draine 2006

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Draine 2006

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MAC with size Distributions gas phase accretion coagulation sedimentation

Carbonaceous material

other large size distributions



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Coagulation MAC with size Distributions gas phase accretion

coagulation sedimentation

Modification of some grain size distribution

Somme insight with the hands for discussion

- Once defined a power law size distribution with $n(a)da \propto a^{\alpha}da$ between a- and a+
- and with fixed total mass (Mgas+Mdust=Cte)
- case a : gaz phase accretion
- case b : coagulation
- case c : sedimentation

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Coagulation MAC with size Distributions gas phase accretion coagulation

Size increase by gaz phase accretion

$ightarrow ho_{gas}/ ho_{dust} \lessapprox 100$

- ▶ but only a few 10⁻³ to 10⁻² in mass is accretable (i.e. not in H, H₂, He ...)
- increase almost independent of initial grain size (i.e. each grain acquire the same small thickness)
- small (tiny) increase of large size
- In large increase of small sizes

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Size increase by gaz phase accretion



moderate influence on lowering UV extinction.

cannot account for mm emissivities.

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Size distribution modification : coagulation



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Dize modification Coagulation MAC with size

gas phase accretio coagulation sedimentation

et al. 2006

Increase of the upper size cut-off @ fixed mass

Size distribution modification : coagulation

- large disappearance of the small grains.
- strong influence on UV properties.
- possibility to grow to mm sizes without cosmic abundance limit.
- Counterbalancing mechanism ?
- If grains in disks have grown bigger than ~1cm, one need for a change in size distribution slope @ large grain radius, otherwise inconsistent

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Some effects of coagulation on gas chemistry



Hily-Blant et al. 2006, see also ref therein

Coupled to a PDR code Le bourlot et al. 1993

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Hily-Blant et al. 2006

- Increasing a+ affects more than increasing UV flux.
- The CO photodissociation occurs deeper in the disk.

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Hily-Blant et al. 2006

- ¹²CO/¹³CO/initial(¹²C/¹³C) @ 100,400,800 AU
- Affects also vertically the ¹²CO/¹³CO ratio

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Hily-Blant et al. 2006

▶ then the integrated ¹²CO/¹³CO ratio

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Sedimentation



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Size modification

- Phase separation
- Affects largest grains in a distribution
- Therefore affect much less the transfer in the UV !



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