IR Observations and Mineralogy of Comet Dust Grains

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with co-Is David E. Harker (UCSD) & Chick Woodward (U. Minn.)
& Deep Impact: Sugita and collaborators
I. Motivation: Comets Probe the Effects of Heating and Radial Mixing of Grains in Our Protoplanetary Disk
Comet grains constrain interstellar and solar nebula processes

Grains from the ISM and the Solar Nebula Contribute to Comet Dust
AGB mass loss donates Mg-rich crystalline and amorphous silicates to ISM

Ion Bombardment changes crystalline silicates into amorphous silicates and reduces FeO in mineral lattices to embedded nanophase Fe.

Recycle dust into stars

Some dust evaporates and recondenses or is annealed in hot regions of the solar nebula.

Comets contain amorphous silicates (ISM) and Mg-rich crystals (solar nebula).
proto-stars: white yellow

3.6 μm
4.5 μm
5.8 μm
8.0 μm
star forming disks in InfraRed light... IR probes deeper, reveals heat of dust and PAH emission excited by stellar UV
star-forming disks in visible light -- emitted & scattered
Low-mass ProtoPlanetary Disk affects its Environment

I Cold Cloud with warm Core

II Infall

III Core warmed by star+disk

IV Bipolar Outflow

V Wind-cloud Bow Shock

VI Accretion shock at disk surface

age < about 100,000 yr
Increasing Complexity of Molecules

Icy Mantles come off Grains

Wooden et al. Comets II
Embedded Outflow in HH 46/47

Spitzer Space Telescope • IRS • IRAC

NASA / JPL-Caltech / A. Noriega-Crespo (SSC/Caltech)

ssc2003-06g
Absorption of protostar light by Amorphous Silicates
Absorption Spectra through ISM Lines of Sight Show ISM Crystalline Silicates are Rare (<1–5%)

Li & Draine 2002; Kemper et al. 2002, 2004
The Mineralogy of Silicate Dust Changes from Amorphous to Crystalline from Protostar Embedded within Core (Class 0 Young Stellar Object) to Exposed Protoplanetary Disk (Class 2 Young Stellar Object)
Crystal Enhancements in Inner Regions of PPDs

Inner Disk compared to whole disk: 2-6 times more crystals at < 2 AU
VLT+MIDI Interferometry
van Boekel et al. (2004)

Inner Disk compared to outer disk: 2-6 times more crystals at < 5 AU
ISO+HIFOGS Spectral Energy Distr.s
Harker, Wooden et al. (2005)
Scenario 1: **Early Delivery of Crystals to Outer Disk**

Warm nebula model: Crystalline Fraction at $r>20$ AU at Time $>5 \times 10^4$ yr

Uniform Crystalline Fraction at $r>2$ AU at Time $>5 \times 10^5$ yr

Bockele-Morvan et al. 2002; similar concepts Dullemoand et al. 2006, $f_{cryst} \sim$ ang. momentum
Initial ProtoPlanetary Disk Composition
= ISM and molecular cloud core

• **RARE Crystalline Silicates**
  < 1% towards Galactic Center (Kemper et al. 2005)
  < 5% line-of-sight in ISM (Li & Draine 2001)

• **Abundant Mg-Fe Amorphous Silicates**
  mostly Olivine and some Pyroxene towards Galactic Center (Kemper et al. 2005)
  ISM absorption spectrum matches comets and an ensemble of GEMS from anhydrous Chondritic Porous Interplanetary Dust Particles of probable cometary origin
  
  *Fe is in the Silicate Dust in Galactic-Disk Clouds, as shown by ISM Depletion Studies [Jones, 2000, JGR]*

• **Abundant Carbon** in aromatic, aliphatic, ‘amorphous’ carbon bonds, also some C in SiC made by carbon stars, 10-15% in PAHs
  
  • organics & ices (often discussed by Charnley & Ehrenfreund)
Scenario 2: Crystal Gradient Evolving still at 1Myr

crystals condense and are annealed, includes grain-gas exchange of Fe

2-D, time-dependent model
Gail 2004, Wehrstedt & Gail 2006

Mdot vs time

crystalline fraction vs heliocentric distance
amor silicates, carbonaceous, ices

condensation

annealing by viscous heat

ISM

age $\approx 3 \times 10^5 - 10^6$ yr
disk no longer shrouded by collapsing core

Comets sample early ProtoPlanetary Disk processes:
heating and radial mixing of grains

age $\approx 10^6 - 3 \times 10^6$ yr
planetesimals evolving and gas is dissipating
Durisen’s crashing wave of gas in the solar nebula:
http://westworld.astro.indiana.edu/movies.html
What Determines Comet Composition?

- **Initial PPD Composition**: Ices, trapped gases & amorphous dust grains
- **Duration of Crystal Formation**: Condensation/Annealing
- **Comet Composition**: Fast vs. slow
- **Rate of Cometesimal Aggregation and Migration**
- **PPD Evolution**: Solar heating/Shocks
- **Efficiency andExtent of Radial Transport**
QUESTIONS from Students at Planetary School 2006, motivated by the Part I Introduction...

In small groups, students formulated questions about comets and the implications comet dust provide for processes in the protoplanetary disk. These questions were then answered using selected slides in the rest of this powerpoint presentation.
Silicate Mineralogy Questions

- Why does the silicate feature appear at 10μm?
- How can we distinguish between olivine and pyroxene in the amorphous silicate phase (in silicates that have amorphous or highly disordered structures)?
- Can we deny the existence of crystalline silicates?
- What is the difference between the constraints on the crystalline silicate fraction in the interstellar medium: “<2% towards the Galactic Center” compared to “<5% towards other lines-of-sight in the ISM”?
PPDisk Radial Transport Questions

- Only tiny particles can couple with the gas and diffuse outwards. Which process is dominant: collisional growth or collisional disruption?
- If outward radial mixing of dust transports only the smallest grains and grains are efficiently aggregating to larger sizes and settling to the disk mid-plane, then does the need to radially migrate out crystals imply that dust aggregates must be actively destroyed to maintain the small grain population?
- What is the origin of shocks in disks?
- What controls the outward transport of crystalline silicates?
- What are the transport mechanisms for the crystalline silicates from the inner disk radii to the outer disk radii?
- How can we test the hypothesis of radial mixing of crystalline silicates?
Comet Nuclei Formation Questions

- Where in the comet nucleus do we find the materials from different radial distances in the disk (cold materials, such as water with ortho/para ratios indicating T<35K from the outer disk and crystalline silicates from the hot inner disk)? In other words, if the comets were formed at 30 AU, the core of the comet nucleus should be dominated by amorphous silicates; if comet nuclei either migrated inwards or radial mixing moved high temperature crystals outwards over time (1 Myr), then nuclear layers accumulated later might be richer in crystalline silicates. Is there evidence for this?

- Do collisions and/or space weathering play a significant role in changing primordial comet composition?

- Do we know when the comets formed? Do the materials inside comets (amorphous silicate grains compared to crystalline silicate grains) have the same formation age?
Comets-PPDisk Questions

• Why do we think amorphous olivine and amorphous pyroxene constitute the initial protoplanetary disk (PPD) composition?

• Could the inner-disk silicate feature rich in crystalline silicates (MIDI observations, van Boekel) be an artifact of optical depth? If the silicates settle to the midplane, then do the observations of crystals only in inner disks imply that can see the midplane at small disk radii (<1–2 AU) but we cannot see the midplane at larger disk radii (>2 AU)?

• Currently, there is a discussion about crystalline versus amorphous minerals in the rocks (refractory minerals). Can future observations lead to a discussion about crystalline versus amorphous water ice and implications for formation and transport at different disk radii? What are the difficulties?
Answers to these questions primarily came from the following slides...
Part II. Silicate Mineralogy - Feature Identifications and Comet Modeling Techniques and Results...
Deriving Grain Properties from IR Observations

Chart showing the computational steps in thermal emission models.

<table>
<thead>
<tr>
<th>Computation Tools &amp; Techniques</th>
<th>Step 1</th>
<th>Step 2</th>
<th>Step 3</th>
<th>Step 4</th>
<th>Step 5</th>
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<td>Mie Scattering</td>
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<td>Radiative Equilibrium</td>
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<td>Solve Flux Integral</td>
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<tr>
<td>Opt. Const. &amp; Radii ${n, k, a}$</td>
<td>Heliocentric Distance $r_h$</td>
<td>Size Distribution &amp; Porosity $n(a), D$</td>
<td>Abundance Multipliers $N_{\text{Mineral}}$</td>
<td>Data SED</td>
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<th>Outputs</th>
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<tbody>
<tr>
<td>$Q_{\lambda, AC}(a)$</td>
<td>$T_{AC}(a, r_h)$</td>
<td>$F_{\lambda, AC}(a, r_h, n(a))$</td>
<td>Model SED $\sum {N_{\text{Mineral}} \ast \lambda F_{\lambda, \text{Mineral}}}$</td>
<td>Best Fit Model SED $\lambda F_{\lambda, \text{Mineral}}$</td>
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<td>$T_{AO}(a, r_h)$</td>
<td>$F_{\lambda, AO}(a, r_h, n(a))$</td>
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<td>$Q_{\lambda, AP}(a)$</td>
<td>$T_{AP}(a, r_h)$</td>
<td>$F_{\lambda, AP}(a, r_h, n(a))$</td>
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<td>$F_{\lambda, O}(a, r_h, n(a))$</td>
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<td>$Q_{\lambda, P}(a)$</td>
<td>$T_{P}(a, r_h)$</td>
<td>$F_{\lambda, P}(a, r_h, n(a))$</td>
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</table>
Crystals

Glasses

Amorphous Olivine

$\text{Mg}_2\text{SiO}_4$

Amorphous Pyroxene

$\text{MgSiO}_3$
The wavelengths of the mid-IR features can show the Mg-content of mineral crystals: shorter wavelengths are Mg-rich, longer wavelengths are Fe-rich. [Chihara et al. 2003; Koike et al. 2002].

**Olivine: Mg-content is**

\[
\frac{\text{Mg}}{(\text{Mg}+\text{Fe})} = 1 \quad \text{Fo 100} \\
0 \quad \text{Fo 0}
\]

(Mg+Fe)  Forsterite  Fayalite
Scattering cross sections

The cross-sections for absorption, scattering, and extinction are expressions of the effective area of the interaction zone for a photon encounter with a particle.

These are often normalized to the geometric cross-sectional area of the particle.

**Scattering Efficiencies**

\[
Q_{\text{abs}} = \frac{\pi a_{\text{abs}}^2}{\pi a^2} \quad Q_{\text{sca}} = \frac{\pi a_{\text{sca}}^2}{\pi a^2} \quad Q_{\text{ext}} = \frac{\pi a_{\text{ext}}^2}{\pi a^2}
\]

extinction = absorption + scattering

\[
\bar{Q} = \int_0^\infty \pi a^2 Q(a) N(a) da
\]

For an ensemble of coma grains, the emissivity is weighted by the grain size distribution N(a).
Comet Comae Grains are in Radiative Equilibrium

- The IR-flux of dust particles at >~3 μm is dominated by re-radiation of the absorbed solar energy.
- The radiated flux depends on nature and composition of the dust particles.

In thermal equilibrium the grain temperature is balanced by the absorbed flux in the UV and visible and the re-radiated thermal flux in the IR:

\[
\int_0^\infty \frac{L_{\odot, \lambda}}{4 \pi r^2} Q_{\text{abs}}(\lambda, a) \pi a^2 \, d\lambda = \int_0^\infty \pi B[\lambda, T(a, r)]Q_{\text{abs}}(\lambda, a) 4 \pi a^2 \, d\lambda
\]

absorbed flux (sunlight) \hspace{1cm} thermally emitted flux

H. Rauer Saas Fee 06
To obtain the total emitted flux integrate over the size distribution of all grains:

\[ F_\lambda = \int_{a_1}^{a_2} \pi B[\lambda, T(a, r)] Q_{\text{abs}}(a, \lambda) a^2 n(a) \, da \]

**Warm grains:** for small grains the efficiency factors at IR wavelengths are smaller than unity and:

\[ B[\lambda, T(a, r)] Q_{\text{abs}}(a, \lambda) \ll B[\lambda, T(a, r)] \]

The measured IR color temperature is very often higher than the black body temperature at the corresponding heliocentric distance → indication for small grains

H. Rauer Saas Fee 06
The dust grain size distribution

The dust size distribution has been measured insitu for comet P/Halley and 81P/Wild 2.

most particles are measured at small radii.

The dust mass is concentrated in few large particles!

The mass is dominated by few large particles!

only few particles, distribution uncertain

no particles detected >10^{-3} m, distribution extrapolated

H. Rauer Saas Fee 06; McDonnell et al. 1989

assumed density: 1 g cm^{-1}
Clusters of particles seen during STARDUST fly-by Comet 81P/Wild 2 - maybe detecting a truncated size distribution?

Fig. 1. Counting rates for all of the eight PVDF channels and the four acoustic channels during the Wild 2 encounter. Those channels that have no counts were excluded from the figure.

r=1603 km

Closest approach: 236.4 km

r=5650 km

- Countings were not uniform throughout the coma: two high activity periods
- during second period almost no particles in acoustic sensor

H. Rauer Saas Fee 06; Tuzzolino et al. 2004, Science 304, 1776
Comet Dust trails show mm-size grain are released

- Large dust particles have small \( \beta \)
- Therefore, they remain on similar orbits than the parent comet
- They form dust trails along the orbit of the comet
- They are observed mainly in the IR (large particles)

Spitzer MIPS views comet trails: 24 μm images show that a considerable mass of rocky materials are released. mm-size grains are released and are seen many months later along the comet’s orbit.
Grain Size Distribution

Typically used size distribution function:

\[ f(a) = \overline{N} \cdot \left(1 - \frac{a_0}{a}\right)^M \left(\frac{a_0}{a}\right)^N \]

(Hanner 1982, in *Cometary Exploration II*)

\(\overline{N}\): scaling factor, \(a\): particle radius

\(a_0\): lower size limit

(smallest building blocks of fluffy aggregates? Typical size of IDP subgrains is 0.1\(\mu\)m.)
Mineralogy from Thermal Emission Modeling of IR Spectral Energy Distributions

Submicron Mg-rich crystals are cooler than submicron Mg-Fe amorphous silicates, so the 11.2μm feature is difficult to detect if crystals are 1/4 of total mass (i.e., equal masses of Amorphous carbon, amorphous olivine & pyroxene, crystalline olivine)

Grain size distribution extending from submicron to 100μm needed to longer wavelength (cooler emission) in SED

Grain size at which size distribution peaks can be constrained:
PPD Opacities depend on grain mineralogy

- iron
- amorphous carbon
- Fe-rich amorphous olivine
- Fe-rich amorphous pyroxene
- Mg-rich amorphous pyroxene
- Mg-rich crystalline olivine

1) Mg-rich crystalline olivine is cooler than Fe-rich amorphous silicates. A single crystal grain produces less flux than an amorphous grain, so more crystals must be present to be detected in spectra.

2) We need better optical constants from visible through far-IR for FeS.

Emitted Flux from Grains:
\[ F_\lambda = \pi a^2 \pi B_\lambda (T_{dust}) Q_{abs} \]
Evolution of Hale-Bopp’s submicron mineralogy with heliocentric distance
Comet Hale-Bopp: Dynamics of coma grains also tells grain size and composition: Comet Nuclear gravity balances Solar Radiation Pressure

Jets produce most coma gases & dust when comet is close (0.93 ≤ r_h ≤ 1.5 AU) to perihelion 9 Apr 1997)
HALE-BOPP in INFRARED: SMALLER GRAINS ARE HOTTER, SHOW STRONGER CONTRAST FEATURES, AND ARE ON LEADING EDGE OF JETS.

**coma structure**

<table>
<thead>
<tr>
<th>T\textsubscript{dust}</th>
<th>silicate feature contrast</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a) March 25.078, N\textsubscript{tot} = 1.786</td>
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<tr>
<td>(b) March 26.056, N\textsubscript{tot} = 3.856</td>
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<tr>
<td>(c) March 26.089, N\textsubscript{tot} = 3.925</td>
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</table>

March 25.099, 11.7 \textmu m

N\textsubscript{tot} = 1.831
Grain composition and size can be investigated from the shape of the coma. $\beta = \frac{F_{\text{radiation}}}{F_{\text{solar grav}}}$.

Arcs are best-fitted by submicron grains. Submicron silicate grains are less affected by radiation pressure than submicron carbon grains: $\beta_{\text{silicate}} < \beta_{\text{carbon}}$. 

10µm INFRARED LIGHT
C/2001 Q4 (NEAT) & Hale-Bopp have similar silicate mineralogy, both have strong jet activity & crystal/amorph.+cryst. ≈0.7
C/2001 Q4 has a smaller & variable silicate-to-amorphous carbon ratio, which lowers the contrast (or ‘strength’) of the silicate feature.
Mineralogy is inhomogeneous: the relative abundances of Amorphous Carbon and Silicates vary in coma, assoc. with ‘jets’.

C/2001 Q4’s silicate **feature drops in contrast** (height) over 1.5 hours, as jets move grains through beam and dust composition changes: there are fewer silicate grains relative to amorphous C grains.
GEMINI+Michelle Full Data Set (every 7min)

“ON NUCLEUS”

“OFF NUCLEUS”

9P/Tempel
1 Review of Gemini results...

1st Amorphous carbon in “OFF”
2nd submicron grains travel together & have more minerals

Smallest grains are ON nucleus and sustained for 30 min, but takes time (>30 min) for these smallest grains to reach maximum 1” OFF into coma.

Grain size dist with smallest grains have 4 minerals or are ensembles of 4 minerals. Larger grains persist longer ON and OFF (move slower), and have 1 or 2 minerals.
Deep Impact Ejecta-Coma: Comparison of Observation-Modeling Results

0.1–1 μm Portion of Grain Size Distribution Relative Mass Fraction

(GEMINI) On-Nucleus

(Subaru) Ejecta-Coma

Grain Surface-Area Weighted Mass Fraction (Spitzer)
Only for Minerals Constrainable with 10μm and with 5–37μm

Time From Impact = TFI = +45 min

pie charts from Wooden, Woodward, Harker 2007 (DI as a world observatory event proceedings)
Where Deep Impact hit comet 9P/Tempel 1 the dominant mineral on the surface is Amorphous Carbon.

This result is not unexpected: Amorphous Carbon is present on the surfaces of outer icy bodies in significant quantities (~10–80%) see summary Table of near-IR reflectance spectra model fits.
What is comet dust made of?

- **Amorphous Fe-bearing silicates:** olivine \((\text{Mg,Fe})_2\text{SiO}_4\), pyroxene \((\text{Mg,Fe})\text{SiO}_3\); porous, aggregate

- **Abundant amorphous carbon,** or highly disordered, dehydrogenated

- **Crystalline silicates** (when detected)
  - submicron in size, not porous
  - Mg-rich \([\text{Mg}/(\text{Mg}+\text{Fe})>0.9]\)
  - comparatively cooler than the amorphous silicates
  - comparatively abundant

Keller & Flynn 2000; Wooden et al. 2006 PPV
Anhydrous CP IDPs provide information about the Composition of COMETARY GRAINS and Thermal Processing of Sub-Grains

Anhydrous Chondritic Porous Interplanetary Dust Particles are highly porous aggregates of disequilibrated minerals: amorphous silicate spherules (GEMS), silicate crystals, FeS crystals, "glued" together with Carbon.

GRAINS AGGREGATED AFTER CRYSTALS FORMED

Aggregate Matrix is Carbon: amorphous, aliphatic, little aromatic

Spectra of acid-etched IDP thin section shows aliphatic bonds
**Comet Dust Mineralogy & Structure from Anhydrous Chondritic Porous IDPs**

- Average of IDPs have 12% C; individual IDPs 5-90% C
- CP IDPs are abundant in Fe-rich Amorphous Silicates: Amorphous Olivine and Pyroxene (GEMS-like grains)
- CP IDPs contain Mg-rich crystals (Fe/Fe+Mg<0.05), often >20% by mass
- Most of Fe is in FeS

Note: Min et al. (2005) deduce FeS content in Hale-Bopp
Low energy cosmic rays (e.g., 4-50 keV He⁺) amorphize and reduce Fe: GEMS and Mg-Fe amorphous silicates have smooth IR spectral resonant shapes, but there are differences. Laboratory amorphous silicates or an ensemble of GEMS better match comet spectra.

He⁺ Ion Bombardment in ISM of Mg-rich crystalline silicates forms porous amorphous silicates and nanophase Fe

Stardust Crystals Amorphized by Ion Bombardment in ISM
Mg-rich Stardust Crystals Annealed by Ion Bombardment in ISM

nano-phase Fe & FeS make grains absorbing
Mineralogy and Structure from STARDUST MISSION Samples

- CAI-type minerals (highest temp solar nebula condensates)
- Mg-rich silicate crystals
- more minerals to be reported...?
- difficult due to aerogel capture: Fe-Mg amorphous silicates carbonaceous/organic

Mineralogy and Structure from Comet Halley
Time-Of-Flight Mass Spectrometer Measurements

- 50% are siliceous+CHON
- 25% are CHON: 8% of grains are C (amorphous?)
- 25% are siliceous: mostly Mg-rich pyroxene, lesser Mg-Fe olivine, silicates containing Sulphur, FeS
- 70% of Fe is in FeS grains, 30% in silicates

Schulze, Kissel, Jessberger 1997 in From Stardust to Planetesimals
Enstatite=Mg-pure Pyroxene - discrete crystal +C layer

Mg/Mg+Fe≈0.75 polycrystalline Olivine

10μm x 10μm x 3μm

Molster et al. 2003 LPS
Formation Mechanisms for Crystalline Silicates are Gas-Phase Condensation and Annealing (Devitrification)

Mg-rich Crystals may Condense from Nebular Gases at ~1400 K

Mg-rich Crystals may be Annealed from Mg-rich Amorphous Silicates at 900K – 1200K

Mg-rich Amorphous Silicate Smoke, formed by laser ablation of melt
Annealed Mg-Olivine Smoke: crystals in amorphous and polycrystalline matrix
## Summary of Annealing Experiments
(Wooden, Harker, Brearley in Chondrites and the PP Disk)

<table>
<thead>
<tr>
<th>Process</th>
<th>Material</th>
<th>Method</th>
<th>Amorphous Properties</th>
<th>T_d [K]</th>
<th>τ_c [hr] start</th>
<th>τ_c [hr] complete</th>
<th>E_a/k [K] start</th>
<th>E_a/k [K] complete</th>
<th>IR crys., features</th>
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<tbody>
<tr>
<td>Fabian et al. (2000)</td>
<td>MgSiO_3</td>
<td>SEM</td>
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<td>quenched melt</td>
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amor silicates, carbonaceous, ices

crystal gas phase condensation

annealing by viscous heat

CAIs

gas CO, CO₂

elemental Carbon

≈20 AU

disk no longer shrouded by collapsing core
t≈3 × 10⁵–10⁶ yr

How do comets sample early protoplanetary disk processes: heating and radial mixing?

evolving planetesimals
gas is dissipating
t≈10⁶–3 × 10⁶ yr
What Determines Comet Composition?

- Initial PPD Composition
  - Ices, trapped gases & amorphous dust grains

- Rate of Cometary Aggregation and Movement
  - Fast vs. slow

- Efficiency and Extent of Radial Transport
  - Solar heating/Shocks

- PPD Evolution

- Duration of Crystal Formation
  - Condensation/Annealing

- Comet Composition
Annealing Mechanisms

- Accretion heating (< 2 AU, mass accretion rate $10^{-7} \, M_\odot \, \text{yr}^{-1}$)
- **Transient mechanisms** that can act over larger disk volumes than accretion
- Shocks
  - Gravitational instabilities in ~10 AU region (Harker & Desch 2002)
  - X-Ray Flares R< 80AU (PPV poster by Nakamoto & Miura)
- Annealing of Mg-pure amorphous grains produces Mg-pure crystalline grains (Brucato et al. 2002; Fabian et al. 2000) [100% efficient]
- Annealing of Fe-containing GEMS produces moderately Fe-rich olivine crystals (Brownlee et al. 2005) [Mg-Fe-crystals rarer in CP IDPs & comets]
- Rapid annealing of Fe-pure amorphous grains produces Fe-pure crystalline grains [Fe-crystals not seen in comets & CP IDPs]
  [Caution: Nuth et al. produce $\text{Fe}_2\text{O}_3$ and $\text{SiO}_2$ that don’t anneal to Fe-rich crystalline olivine, but Nuth et al. calls these products crys. Fe-silicates]
- When annealing abundant Mg-Fe amorphous silicates to Mg-rich crystals, we need a mechanism to get the Fe out amorphous silicates!
Equilibrium (+ Radial Diffusion)

Fe reacts with gas-phase S

Not seen in comets or primitive enstatite chondrite matrices
Transient Heating

- Fe metal blebs?
- Fe+S = FeS?
- needs to be efficient

ISM amorphous Mg-Fe silicates
- Crystalline Mg-Fe silicates
- Crystalline Mg-rich silicates
- Crystalline Pure-Mg silicates
- Crystalline Pure-Fe silicates

Amorphous pure-Mg silicates
- Amorphous FeO + SiO2
- > 1250 K

1000–1400 K
- rapid crystallization
- annealing

>1400–1450 K
- evaporation + rapid condensation
- non-equilibrium

1000–1400 K
- rapid crystallization
- annealing

Silica?
Shock speeds are sufficient in the 5-10 AU region to quickly anneal Mg-rich amorphous silicate grains.

Plateau of higher temperatures (>1000K for 0.5-1 hr) may heat submicron radii grains long enough for annealing & Fe reduction to occur in the same shock -> ~100% efficient so few Mg-Fe crystals remain so no Mg-rich amorphous remain

shock model Harker & Desch 2002, concept discussed in Wooden et al. 2006 PPV
Fe Reduction Experiments: Fe reduction can occur for grains in solar nebula gas because oxygen fugacity \( [fO_2] \) is low enough

\[
\text{Fe}_2\text{SiO}_4 \text{ in olivine} + 2\text{C}_{\text{graphite}} = 2\text{Fe}_{\text{in metal}} + \text{SiO}_2 \text{ amorphous} + 2\text{CO}_{\text{in gas}}
\]

Heating Mg-rich olivine on a carbon substrate forms Fe-metal blebs on surface, increasing Mg-content and leaving silica-rich surface layer.

Lemelle et al. 2001, Amer. Mineralogist, 86, 47

Fig. 7. TEM bright field micrographs. R100 sample; a) general view of a dusty area from an experimentally reduced San Carlos Fe-Mg olivine. Note the preferential ascension of the metal blebs in the olivine matrix. b) edge of an olivine grain. The rim is free of metallic precipitates. The adjacent phases to the olivine contain new spinel and glass intergrowths, see text for explanation.

Leroux et al. 2003, MPS 38, Nr1, 81-94
Reduction of Fe out of Olivine occurs at Mg-Fe Interdiffusion rates, ~10x slower than rates for annealing of pure-Mg amorphous olivine to pure-Mg crystalline olivine.

Wooden et al. 2006 PPV
Starting Material: $\text{Mg}_{1.8} \text{Fe}_{0.19} \text{Ni}_{0.01} \text{SiO}_4$

$\text{Mg}/(\text{Mg+Fe}) = 0.9$

The origin of GEMS in IDPs as deduced from microstructural evolution of amorphous silicates with annealing

C. Davoisse, Z. Djouadi, H. Leroux, L. d'Hendecourt, A. Jones, and D. Deboffe

Fig. 2. TEM micrograph of sample annealed at 970 K (55 h) showing a forsterite crystal (Fo) embedded in a amorphous matrix. Note the dendritic structure at the edge of the grains. Some metal particles are also present in the amorphous phase (some of them are arrowed).
The origin of GEMS in IDPs as deduced from microstructural evolution of amorphous silicates with annealing

yield annealing was $10^{-10}$ bar. The very low oxygen partial pressure ($<10^{-20}$ bar) necessary for the reduction reaction to proceed is probably due to carbon-rich contaminants coming from the pumping system, which consumes oxygen by the reaction $C + 1/2 O_2 \rightleftharpoons CO$ and thus induces metal formation

the samples before their total crystallization. The main characteristic of all the samples annealed (at $10^{-10}$ bar and without $O_2$ circulation) is the presence of widespread iron-nickel nano-particles (Fig. 1) randomly distributed, 2–50 nm in size, for which the compositions are highly variable, from 3 to 50% Ni. The amorphous phase which encloses the metallic globules is free of Fe. This microstructure and microanalyses clearly show that iron, initially in form of FeO, has segregated from the amorphous phase in the form of metallic precipitates. Despite the presence of metallic precipitates, the average composition (amorphous silicate + metallic nano-particles) is found strongly depleted in Fe. A moderate loss of Mg is also observed.
GEMS have silica-rich subgrains and FeS-rich subgrains: a consequence of reduction of Fe out of the grain under solar nebula (low) oxygen fugacity conditions and FeS formation??

Figure 1. A brightfield STEM image of a cluster of GEMS in IDP L2011B10 (top) and the corresponding Mg+Si distribution map extracted from the EDX spectrum image (bottom). The white arrows indicate the numerous compositionally distinct subgrains that comprise the GEMS aggregate grain.

Figure 2. Ternary plot of measured Fe, Si, and S atomic abundances in GEMS subgrains showing the silica-rich (blue) and FeS-rich (red) subgrain compositions. The dashed line defines a field that encompasses previous bulk GEMS grains analyses [3, 8].

Keller, Messenger, Christoffersen 2005, LPS 36, 2088
Inward Migration of Icy Cometesimals/particles can Raise Oxygen Fugacity by water vaporization -> water dissociation -> forms $O_2$ -> raises $f[O_2]$

Fe-rich silicate chondrule rim formation (but small percentage of volume)

Inward Migration of Carbon-Rich Cometesimals/particles can Lower Oxygen Fugacity by C combustion to CO, CO2 -> lowers $f[O_2]$

Mg-rich silicates in enstatite chondrites

ISM

amor silicates, carbonaceous, ices

condensation

crystal

condens. annealing by viscous heat

gas CO, CO2

elemental Carbon

outward radial transport

inward migration

chondrules

crystal condens.

annealing/shocks

CAIs

crystal gas-phase condensation

‘ISM’

disk no longer shrouded by collapsing core

t≅3x10^5–10^6 yr

How do comets sample early protoplanetary disk processes: heating and radial mixing?

evolving planetesimals gas is dissipating

t≅10^6–3x10^6 yr

≈20° AU
Some Controversial Topics...
New JFC Paradigm: **Crystals are Skin-Deep**

- Deep Impact-induced ejecta has silicate crystals (Spitzer, Gemini, Subaru).
- Post-impact (by <1 rot. period) has crystals (VLT).
- Pre- and post-impact dust has no crystals, dominated by amorphous silicate grains (Gemini).
- Dust in coma in May 2006 (activity maximum) has submicron amorphous silicate grains, no crystals (Keck).
- 73P-C/SW-3 and 73P-B/SW-3 have crystals (broken up 2 orbits ago, and breaking up April ‘06) (Gemini)
- **TREND:** JF comet materials from “below their mantles” possess silicate crystals.
- **DIRECTION:** community effort to study mineralogy and organic volatility versus $r_h$ in select JF and OC comets
New Paradigm?: ISM crystals/GEMS rare <1%
How extreme/efficient is solar nebula processing?

Fig. 2. Oxygen isotopic images of a slice of IDP L2005 C13. A presolar grain with a large $^{17}$O excess can be clearly seen in the $^{17}$O image. 

Messenger et al. 2003
New **Annealing** Paradigm?: 60-80% of GEMS are systematically sub-chondritic in S, Mg, Ca, Fe compared to Si


Diane asks: Were most (60-80%) of amorphous silicates annealed by high fluxes ($10^4$–$10^5 \times$ today’s Sun) of low Energy solar cosmic rays? [cosmic rays–Feigelson et al.]
Amorphous vs Crystalline Water Ice

Fig. 1. Spectrum of comet C/2002 T7 (LINEAR) along with synthesized spectra for pure H$_2$O crystalline icy grains (0.1, 1.0, and 10.0 μm, in diameter). The absorption by H$_2$O ice is clearly shown in the cometary spectrum. However, the agreement between the cometary spectrum and the pure H$_2$O spectrum is not good in the J band.

Fig. 3. Comet Hale-Bopp data (heavy solid line) compared with the reflectance calculated for water ice having grain diameters of 1 μm (dashed line), 5 μm (dotted line), and 10 μm (thin solid line).
amor silicates, carbonaceous, ices

crystal gas-phase condensation

 annealing by viscous heat

ISM

disk no longer shrouded by collapsing core

$t \approx 3 \times 10^5 - 10^6$ yr

How do comets sample early protoplanetary disk processes: heating and radial mixing?

evolving planetesimals

gas is dissipating

$t \approx 10^6 - 3 \times 10^6$ yr

CAIs

chondrules

crystal condens

gas CO, CO$_2$

elemental Carbon

inward migration

outward radial transport

annealing/shocks

≈20 AU
Interpretation of DI Dust...

Wooden, Woodward, Harker 2007
DI as a World Observatory Event
Brussels Mtg (submitted)
9P/Tempel
1 Review of Gemini results ...

1st Amorphous carbon in “OFF”
2nd submicron grains travel together & have more minerals

Amorphous Pyroxene
Amorphous Olivine
Amorphous Carbon
Crystalline Olivine

Smallest grains are ON nucleus and sustained for 30 min, but takes time (>30 min) for these smallest grains to reach maximum 1” OFF into coma. Grain size dist with smallest grains have 4 minerals or are ensembles of 4 minerals. Larger grains persist longer ON and OFF (move slower), and have 1 or 2 minerals.
Deep Impact Ejecta-Coma: Comparison of Observation-Modeling Results

0.1–1 μm Portion of Grain Size Distribution Relative Mass Fraction

(GEMINI) On-Nucleus

(Subaru) Ejecta-Coma

Grain Surface-Area Weighted Mass Fraction (Spitzer)
Only for Minerals Constrainable with 10μm and with 5–37μm

Time From Impact = TFI = +45 min
Deep Impact Dust Properties - Summary

• The nuclear subsurface appears to have an inhomogeneous mineralogy yet contains a volume or pocket of submicron grains of relatively homogeneous yet complex mineralogy. In contrast, the surface appears to be dominated by amorphous carbon.

• The effect of gas drag on the grains is to size sort the grains in the coma as a function time from impact (TFI).

• Silicate crystals travel out with the smallest grains and therefore, by velocity-association, crystals are small. However, from TFI=+0.5~hr (Gemini and Subaru) to TFI=+10~hr (Spitzer) the crystalline fraction does not change significantly as the smaller (0.2--1μm) grains clear out and larger grains travel through the beam. Therefore, crystals are not necessarily only associated with the smallest grains (0.2 μm). Future analyses of the Spitzer spectra may yield further results on the relationship between the crystalline fraction and the grain size.
DI V - Possible Reasons the Crystalline Silicates Not Seen in the Normal Coma (versus DI)

- Grain size Distribution does not extend to small enough grain sizes.
- Grain size Distribution slope is too shallow so smallest grains are not dominant enough.
- Crystalline resonances are diminished in contrast (to the point of non-detection) if the crystals are contained within larger aggregate grains.
- The crystals comprise only the smallest grains in the size distribution, which means crystals dominate the grains' surface area but are only a small fraction of the total mass. The mass fraction of crystals is too small for crystals to be detected in the normal coma.
- Normal activity is from mantles (outer layers a few cm to a m deep) that are devoid of crystals. So mantles have a specific composition and mantles are retained. From mantles, crystals are lost; or, in mantles crystals are destroyed.
- The nucleus is inhomogeneous on smaller scales than the DI impact-crater; where DI impacted 9P, the surface is rich in amorphous carbon and rarified in crystals and the subsurface contains zones of amorphous pyroxene and crystals, and amorphous carbon and amorphous olivine.
Look at the Explanations for Differences - A

- Grain size Distribution does not extend to small enough grain sizes.
  NOT TRUE ap=0.3µm May 25, 0.6µm May 17

- Grain size Distribution slope is too shallow so smallest grains are not dominant enough.
  Implies: The crystalline fraction $f_{\text{crys}}$ is grain size-dependent and the size distributions for normal comae were devoid of these smallest grains. NOT TRUE for $a_p \leq 1\mu$m grains; investigate for $a_p > 1\mu$m with Spitzer

- Crystals are hidden within larger aggregates.
  lab spectra of IDPs shows $f_{\text{crys}} < 0.17$ then crystals may be hidden
  Hale-Bopp DDA computations show $f_{\text{crys}} = 0.55$ for 0.1--5µm size particles
  same as for discrete mineral model

- Too Small a total Mass of dust to see Submicron Grains?
  Same Mass of dust in inner coma measured on 2 dates, so:
  $M_{\text{dust}}(\text{DI},+ 0.5 \text{ to } +3.5\text{hr}) \approx M_{\text{dust}}(9\text{P on 17 May}, \text{single measurement})$
Look at the Explanations for Differences - B

- Activity from Mantles Devoid of Crystals
  Implies (1) in Mantles, crystals are destroyed and (2) Mantles are retained

1. In Mantles, Crystals are Destroyed
   Low Energy Solar Cosmic Rays:
   For the young Sun (0–10^6 yr), flares probably produce \( \sim 10^5 \) times more solar cosmic rays (Glassgold et al. 2005; Feigelson, Garmire, & Pravdo 2002 ApJ, 584, 911). If each cometesimal in the layered pile has an amorphous silicate skin (rime), then this implies very rapid amorphization rates at the time of accretion of the outer layers.
   Problem: Low Energy Cosmic Rays penetrate <100 \( \mu m \) depth
   Need: Gardening by micrometeorite impacts or dust sputtering

2. Irradiation of ices creates porous organic residues that “shrink” as sublimation occurs below their surfaces

3. Challenge: 9P water ice subliming from 3 cm below surface
   Q_dust implies loss of 3cm/ROTATION PERIOD (41hr) over surface or 30cm in 10% of the surface
Look at the Explanations for Differences - C

- Nuclear Inhomogeneities on Smaller Size Scales than Topography, on depth scales smaller than 10m deep and 100m wide

(Belton et al. 2006, LPS 37, #1232)
TALPS OR LAYERED PILE MODEL

- the current surface topography is a result of the accumulation of layers of cometesimals
- the early layers are smaller because the modal size of the impacting aggregates is smaller
- the early layers are more compact because impact speeds are higher for smaller bodies
- the late-accumulation layers may be 50 m thick (390~m diameter cometesimal)
- perhaps 500 layers are on top of the nuclear `core'
- except for the surface layers, each layer experienced a mean exposure age of 5000--50,000 yr in the protoplanetary disk, if ~25 layers cover the surface at any particular time in the accumulation process
- probably a number of surface layers are already lost due to sublimation during previous orbits in the inner solar system
- **Dust Results:** accumulating layers are themselves inhomogeneous; inhomogeneities were preserved in collisions of cometesimals during the epochs of growth of nuclei.
Future Directions

Spitzer & Subaru: C/2006 Q1 (McNaught)
Subaru: Jupiter Family Comets
Rimes (somehow) regulate coma dust properties

Dust/gas Ratio declines for comets that come closer to the Sun ($q_{AU}$)

Hypothesis: Rimes of comets that come closer to the Sun lack loose small (<few μm) grains that contribute to Afrho (following A’Hearn et al. 1995).

Lower Afrho means fewer smaller grains...

Are there fewer small grains
- due to preferential loss?
- due to preferential mantle trapping?
- due to some other mantle “mechanics”?

*Are there actually fewer small grains? (add mid-IR to Afrho)*
Rimes (somehow) regulate coma dust properties: ensemble of JFCs have small Active Area fractions

\[ R_{\text{nu}} \text{(km)} \]

\[ R_{\text{AA}} \text{ (km)} \]

Active Area Effective Radius vs \( R_{\text{nu}} \) (km)

\[ y = 0.7625x^{0.1009} \]

\[ R^2 = 0.0052 \]

Active Areas [km\(^2\)] A’Hearn et al. 95; \( R_{\text{nu}} \) Lamy et al. 05 Comets II
Active Area fraction (AAf) not dependent on Dust/Gas Ratio nor critical grain radius $a_{crit}$

Active Area fraction is independent of Gas/Dust Ratio

Active Area fraction is independent of grain sizes $>a_{crit}$ retained against $F_{drag}$

No affect on AAf if smaller grains are retained against $F_{drag}$ ($a_{crit}$ smaller)

No affect on AAf if more grains entrained by escaping gases
Perhaps Active Area Fractions depend on $P_{\text{rot}}$ for $P_{\text{rot}} < 20$ hr. Nuclear Evolution Models predict Active Area fractions (AAf) are higher in comets that rotate more rapidly, because more uniform temperatures over $P_{\text{rot}}$ prevent re-icing or ‘sealing’ at high latitudes (deSanctis et al. 1996). Comet 46P/Wirtanen may be an example.
C/2006 Q1 (McNaught)

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<th>log Afp/CN</th>
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<td>-22.77</td>
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<td>1.9</td>
<td>10.5</td>
<td></td>
</tr>
<tr>
<td>96P/Machholz 1</td>
<td>daytime only</td>
<td>.124</td>
<td>5.90</td>
<td>5.23</td>
<td>---</td>
<td>2.0E-2</td>
<td>3.2</td>
<td>6.38</td>
<td>2 (aerith) 14 (JPL)</td>
</tr>
</tbody>
</table>

Comets are up for more than 2 hours at less than 2 Air Masses (except 96P daytime), and T-mag are ≤12; most have known radii \( R_{\text{nuc}} \) and \( P_{\text{rot}} \).
Future Observational Characterization of JF Comets and their Rimes

Mantle characteristics from Observations of an ensemble of JF comets:
- small active area fractions
- jets
- active areas persistent over > months
- active areas recurring from apparition to apparition
- dust-to-gas ratios [Afp/CN, Afp/OH] are smaller for comets with smaller perihelion distances q_{AU}

0.1–100 μm Grains

Comets with smaller q_{AU}
- have smaller Afp due to lack of small grain scatterers [Afp, a_p >10 μm]

Comets with larger q_{AU}
- have small grain scatterers [Afp, a_p <10 μm]

Coma Gases

- Comets with smaller q_{AU} produce more CN; implying q_{AU}-dependent CN distributed source from grains [CN radial profile]
- Comets with larger q_{AU} have small grain scatters [Afp, a_p <10 μm]

Color Maps

- Grain size
- n,k

Polarization

- Aggregate size
- Composition
- Porosity

IR SEDs

- Peak grain radius (a_p), mineralogy
- Porosity

Coma-trail shapes

- β = temporal activity
- Jet locations

light curves

- Temporal activity

Q_{gas}

- coma composition

Mineralogy of small grains released from SP comet Active Areas

- β

? Fragmentation of small grains

? CN-producing grains do not produce Afp [Afp, CN profiles]

? CN, C_2, C_3 related; NH not related

Interpretation of Colors of nuclei:
- small grains (a_p < 0.5 μm) may yield %/1000Å=0

Resolve degeneracy in interpretation of Spitzer IRS+MIPS of JFCs at large R_{J}:
- small grains or large (>mm) chunks?

Range of SP comet compositions: probe solar nebula conditions; bimodal or continuous range of mineralogies probes nucleus layered pile model & mixing scales

Grain aggregation & composition:
- Submicron CHON grains;
- Organic glue binds silicate subgrains;
- Core-mantle (birdsnest) aggregates vs disequilibrated mineral aggregates

Implications

Active area fractions smaller for comets with smaller q_{AU} [Q_{OH}, R_{me}].