Dust evolution in photon-dominated regions

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• Dust is involved into environments such as galaxies, star-forming regions, protoplanetary disks, ... Through different processes:
  • Gas heating by photoelectric effect on dust grains.
  • Interaction with the radiation field and the magnetic field.
  • Formation of molecules on grain surface, ...
• These processes strongly depends on the dust properties (i.e. size, composition, and shape) hence the necessity to constrain those properties.

• **Problem**: The wide disparity in the physical conditions (density and irradiation) throughout the interstellar medium (ISM) triggers an evolution of the dust properties through accretion, coagulation, fragmentation, photo-destruction, ...

• **Objective**: Understand how interstellar dust evolves as a response to the physical conditions.

• **How/Where**: We study dust evolution in regions where the physical conditions are strongly contrasted and are spatially resolved by our instruments: photon-dominated regions.
What are photon-dominated regions (PDRs)?

- PDRs are the surface layers where the radiation field can dissociate $\text{H}_2$ but cannot ionise H.
- They are therefore located at the interface of HII regions and molecular clouds.
- The radiation field coming from nearby stars regulates the chemical and physical evolution of the gas.
- Physical quantities ($n_\text{H}, T_{\text{gas}}$) vary widely on small spatial scales.

→ PDRs are therefore a unique place to study dust evolution as a response to the physical conditions.
Three well-known photon-dominated regions (PDRs)

- Observations with Spitzer and Herschel in 10 photometric bands (3.6, 4.5, 5.8, 8, 24, 70, 160, 250, 350, 500 μm) of:
  - Horsehead: Irradiated by a star at 35000 K and $G_0 = 100$.
  - IC63: Irradiated by a star at 25000 K and $G_0 = 1100$.
  - Orion Bar: Irradiated by a star at 38000 K and $G_0 = 26000$. 

Horsehead at 3.6 μm (Schirmer+2020).
IC63 at 3.6 μm (Schirmer+2022).
Orion Bar at 3.6 μm (Schirmer+2022).

Three well-known photon-dominated regions (PDRs)
Models and tools

- An interstellar dust model: THEMIS (Jones+2013, Jones+2017)
- Model dust emission in optically thin regions: DustEM (Compiegne+2011)
- Model dust emission in optically thick regions (radiative transfer): SOC (Juvela+2019)

![Size distributions](Schirmer Thesis 2020).

![Dust emission and relative contributions](Schirmer Thesis 2020).

![Grains in the THEMIS model](Jones+2013).

- **Fragmentation**: Power-law distribution of a-C nano grains (NG, \(a < 20\) nm) emitting in the near and mid-IR.
- **Coagulation**: Log-normal distribution of large a-C:H and a-Sil grains emitting in the Far-IR.
Influence of the nano-grain (NG) abundance ($M_{a-C}/M_H$) on dust emission

**Left:** Dust size distributions of a-C grains for $M_{a-C}/M_H$ varying from $0.01 \times 10^{-2}$ to $0.20 \times 10^{-2}$. **Right:** Associated spectra computed with DustEM for $G_0 = 100$ (Schirmer+2020).

- A decrease in $M_{a-C}/M_H$ implies a decrease in the nano-grain population that is responsible for the emission in the near and mid-IR thus:
  - Dust emission in the near ($\lambda \sim 1 - 5 \, \mu m$) and mid-IR ($\lambda \sim 5 - 25 \, \mu m$) **increases** with an increase in $M_{a-C}/M_H$.
  - Dust emission in the far-IR ($\lambda \sim 25 - 500 \, \mu m$) is **not affected** by variations in $M_{a-C}/M_H$. 

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Influence of the NG minimum size \( (a_{\text{min}, \text{a-C}}) \) on dust emission

**Left:** Dust size distributions of a-C for \( a_{\text{min}, \text{a-C}} \) varying from 0.4 nm to 0.9 nm. **Right:** Associated spectra computed with DustEM for \( G_0 = 100 \) (Schirmer et al. 2020).

- A increase in \( a_{\text{min}, \text{a-C}} \) implies a **redistribution** of the grain mass from the smallest NG (near-IR emission) to the largest NG (mid-IR emission):
  - Dust emission in the near-IR **decreases** with an **increase** in \( a_{\text{min}, \text{a-C}} \).
  - Dust emission in the mid-IR **increases** with an **increase** in \( a_{\text{min}, \text{a-C}} \).
  - Dust emission in the far-IR is **not affected** by variations in \( a_{\text{min}, \text{a-C}} \).
Influence of the NG power-law exponent ($\alpha$) on dust emission

**Left:** Dust size distribution of a-C for $\alpha$ varying from -7 to -4. **Right:** Associated spectra computed with DustEM for $G_0 = 100$ (Schirmer+2020).

- An increase in $\alpha$ implies a **redistribution** of the grain mass from the smallest NG (near-IR emission) to the largest NG (mid-IR emission) and some large grains (far-IR emission):
  
  - Dust emission in the near-IR **decreases** with an **increase** in $\alpha$.
  - Dust emission in the mid-IR **increases** with an **increase** in $\alpha$.
  - Dust emission in the far-IR is **slightly increase** with an increase in $\alpha$. 

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Example of $\chi^2$ distribution for a given value of $\alpha$ in the 2D-space ($M_{a-C}/M_H$, $a_{\text{min}, a-C}$) for IC63 (Schirmer+22)

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We minimise a $\chi^2$ that quantifies the difference between the dust observed and modelled emission and we obtain:

<table>
<thead>
<tr>
<th>PDR</th>
<th>$G_0$</th>
<th>$T_{\text{eff}}$ [K]</th>
<th>$D$ [pc]</th>
<th>$M_{a-C}/M_H$</th>
<th>$a_{\text{min}, a-C}$ [nm]</th>
<th>$\alpha$</th>
<th>$n_0$ [H cm$^{-3}$]</th>
<th>$z_0$ [pc]</th>
<th>$\gamma$</th>
</tr>
</thead>
<tbody>
<tr>
<td>IC63</td>
<td>1100</td>
<td>25000</td>
<td>1</td>
<td>$(0.1 \pm 0.01) \times 10^{-2}$</td>
<td>$0.70 \pm 0.01$</td>
<td>$-5 \pm 0.1$</td>
<td>$1 \times 10^5$</td>
<td>0.004</td>
<td>2.5</td>
</tr>
<tr>
<td>Horsehead</td>
<td>100</td>
<td>35000</td>
<td>3.5</td>
<td>$(0.02 \pm 0.01) \times 10^{-2}$</td>
<td>$0.77 \pm 0.03$</td>
<td>$-6 \pm 0.5$</td>
<td>$2 \times 10^5$</td>
<td>0.06</td>
<td>2.5</td>
</tr>
<tr>
<td>Orion Bar</td>
<td>26000</td>
<td>38000</td>
<td>0.25</td>
<td>$0.0025 \pm 0.0015 \times 10^{-2}$</td>
<td>$\leq 0.8$</td>
<td>$\leq -5.5$</td>
<td>$1.5 \times 10^5$</td>
<td>0.025</td>
<td>2.5</td>
</tr>
<tr>
<td>Diffuse ISM</td>
<td>1</td>
<td>-</td>
<td>-</td>
<td>$0.17 \times 10^{-2}$</td>
<td>0.4</td>
<td>-5</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>
Constrain $M_{a-C}/M_H$, $a_{\text{min}}$, $a-C$, and $\alpha$ in the Horsehead, IC63, and Orion Bar

Example of $\chi^2$ distribution for a given value of $\alpha$ in the 2D-space ($M_{a-C}/M_H$, $a_{\text{min}}$, $a-C$) for IC63 (Schirmer+22)

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<th>$\alpha$ [°]</th>
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</tr>
<tr>
<td>Orion Bar</td>
<td>3800</td>
<td>58000</td>
<td>0.23</td>
<td>$(0.0023 \pm 0.0015) \times 10^{-1}$</td>
<td>$0.7 \pm 0.5$</td>
<td>$-3.5$</td>
<td>$1.5 \times 10^5$</td>
<td>0.023</td>
</tr>
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<td>1</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
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Final model for the Orion Bar. Dust modelled (observed) emission profiles is shown in blue (green) line. (Schirmer+22)

→ The nano-grain abundance is lower than in the diffuse ISM and strongly varies from one PDR to another (~2 times lower than in the diffuse ISM in IC63 and 60-100 times lower than in the diffuse ISM in the Orion Bar)

→ The nano-grain minimum size increases by a factor ~2 from the diffuse ISM to the PDRs. It barely varies from one PDR to another (~0.7-0.8 nm)
Nano-grain formation: fragmentation of aggregates

- We propose that collisions of dust aggregates due to radiative pressure lead to their fragmentation in nano-grains. To assess whether it is a viable scenario or not, one needs to:
  - The collision velocity needs to be larger than 1 m/s to trigger fragmentation and not sticking (Güttler+2010)
  - Collisions timescales must be lower than the typical time during which dust grains are processed in PDRs (i.e. the advection timescale, \( \tau_{\text{ad}} \approx 10^3 - 10^4 \text{ yrs} \)).

- We use a classical 1D approach and solve the equation of motion of a dust aggregates with size \( a \):
  - Equation of motion: \( m_{\text{dust}} \frac{dV_{\text{dust}}(a)}{dt} = F_{\text{pr}}(a) - F_{\text{drag}}(a) - F_{\text{grav}}(a) \)
  - Gravitational force: \( F_{\text{grav}}(a) = \frac{4}{3}\pi a^3 \rho_{\text{dust}} \times \left( \frac{GM*}{D^2} \right) \)
  - Gas collisions: \( F_{\text{drag}}(a) = \pi a^2 \rho_{\text{gas}} v_{\text{dust}}^2(a) \)
  - Radiative pressure: \( F_{\text{pr}}(a, \lambda) = \pi a^2 Q_{\text{pr}}(a, \lambda) \left( \frac{\pi R_*^2}{D^2} \times \frac{B_\lambda(T_*)}{c} \right) \)
  - The asymptotic solution gives: \( v_{\text{drift}}(a) = \frac{1}{D} \left[ \frac{1}{1.4 m_H n_H} \left( \frac{\pi R_*^2}{c} \left( Q_{\text{pr}} B_\lambda \right) - \frac{4}{3} a \rho_{\text{dust}} GM_* \right) \right]^{1/2} \)
  - The collision timescale is: \( \tau_{\text{coll}}(a_1, a_2) = \left( n_H \sqrt{n_u(a_1)n_u(a_2)} \pi (a_1 + a_2)^2 v_{\text{drift}}(a_1) \right)^{-1} \)

Top: Drift velocities of aggregates for the three PDRs. Bottom: Associated collision timescales (Schirmer+2022)
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We use a classical 1D approach and solve the equation of motion of a dust aggregates with size $a$:

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$a_0 = 0.05 \mu m$ (smallest aggregates that are the most abundant)
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The collision timescale is: $\tau_{\text{coll}}(a_1, a_2) = \left( n_{H} \sqrt{n_{d}(a_1)n_{d}(a_2)} \pi (a_1 + a_2)^2 v_{\text{drift}}(a_1) \right)^{-1}$

$\tau_{\text{frag}} \propto \tau_{\text{coll}} \rightarrow$ Fragmentation efficiency is roughly the same in IC63 and in the Horsehead. More efficient in the Orion Bar.
Nano-grain destruction

- Nano-grains are composed of a mix in different molecular domains, i.e. aromatic domains connected by aliphatic (C-C) and olefinic (C=C) bridges. Photo-destruction of nano-grains is triggered by the photo-dissociation of aliphatic and olefinic bonds. There are at least three processes that can lead to the photo-destruction of nano grains (direct photo-dissociation, photo-thermo dissociation, Coulomb explosion):

  - A decrease in the absorption timescale implies an decrease in the photo-destruction timescale.
  - An increase in the average energy of an absorbed photon implies an increase in the photo-destruction efficiency.

  -> Photo-destruction happens more frequently in the Orion Bar than in the Horsehead.
Decrease in the nano-grain abundance from the Horsehead to the Orion Bar

• The energy of an absorbed photon is roughly the same in the Horsehead and in the Orion Bar ($E_{\text{abs}} \sim 9 \text{ eV}$) → the nano-grain destruction efficiency depends almost solely on the absorption timescale.
Decrease in the nano-grain abundance from the Horsehead to the Orion Bar

**Average energy of an absorbed photon** (Schirmer+2022).

- The energy of an absorbed photon is roughly the same in the Horsehead and in the Orion Bar ($E_{\text{abs}} \sim 9$ eV) –> the nano-grain destruction efficiency depends almost solely on the absorption timescale.

- The absorption timescale is ~100 times lower in the Orion Bar than in the Horsehead ($10^6 \rightarrow 10^4$ s) –> the nano-grain destruction efficiency is ~100 times larger in the Orion Bar than in the Horsehead.

**Absorption timescales** (Schirmer+2022).
Decrease in the nano-grain abundance from the Horsehead to the Orion Bar

- The energy of an absorbed photon is roughly the same in the Horsehead and in the Orion Bar ($E_{\text{abs}} \sim 9 \, \text{eV}$) $\rightarrow$ the nano-grain destruction efficiency depends almost solely on the absorption timescale.

- The absorption timescale is $\sim 100$ times lower in the Orion Bar than in the Horsehead ($10^6 \rightarrow 10^4 \, \text{s}$) $\rightarrow$ the nano-grain destruction efficiency is $\sim 100$ times larger in the Orion Bar than in the Horsehead.

- The collision timescale is $\sim 10$ times lower in the Orion Bar than in the Horsehead ($10^3 \rightarrow 10^2 \, \text{yrs}$) $\rightarrow$ the nano-grain formation efficiency is $\sim 10$ times larger in the Orion Bar than in the Horsehead.
Decrease in the nano-grain abundance from the Horsehead to the Orion Bar

1) Nano-grain destruction is ~100 times larger in the Orion Bar than in the Horsehead. 
2) Nano-grain formation is ~10 times larger in the Orion Bar than in the Horsehead.

\[ \frac{\text{destruction}}{\text{formation}} \text{ is therefore } 10 \times \text{larger in the Orion Bar than in the Horsehead.} \]
Decrease in the nano-grain abundance from the Horsehead to the Orion Bar

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The absorption timescale is $\sim 100$ times lower in the Orion Bar than in the Horsehead ($\tau_{\text{abs}} \rightarrow 10^4$ yrs) —> the nano-grain destruction efficiency is $\sim 100$ times larger in the Orion Bar than in the Horsehead.

The collision timescale is $\sim 10$ times lower in the Orion Bar than in the Horsehead ($\tau_{\text{coll}} \rightarrow 10^2$ yrs) —> the nano-grain formation efficiency is $\sim 10$ times larger in the Orion Bar than in the Horsehead.

This is in accordance with our results: we found that the nano-grain abundance is $\sim 10$ times lower in the Orion Bar than in the Horsehead.

1) Nano-grain destruction is $\sim 100$ times larger in the Orion Bar than in the Horsehead
2) Nano-grain formation is $\sim 10$ times larger in the Orion Bar than in the Horsehead

The ratio destruction/formation is therefore $10$ times larger in the Orion Bar than in the Horsehead.

Average energy of an absorbed photon (Schirmer et al. 2022).

Absorption timescales (Schirmer et al. 2022).

Associated collision timescales (Schirmer et al. 2022).
Dust evolution scenario in PDRs

1. The UV radiation field pushes aggregates through radiative pressure. The velocity drift decreases with depth inside the cloud because of the decrease of the UV field with depth due to dust extinction, leading to collisions hence fragmentation.

2. As the velocity drift of nano-grains is much smaller than that of the larger grains/aggregates, the latter are pushed towards other aggregates that are located in the denser part.

3. Freshly formed small grains are unprotected from the UV radiation field and are therefore photo-processed. The smallest of the nano-grains are photo-destroyed.
We modelled dust emission in three PDRs (the Horsehead, IC63, and the Orion bar) with the 3D radiative transfer code SOC together with the THEMIS dust model.

We perform a $\chi^2$ minimisation in the 3D-space defined by the nano-grain mass-to-gas ratio, the nano-grain minimum size, and the slope of the nano-grain power-law size distribution.

We show that the nano-grain minimum size increases from 0.4 nm to 0.7-0.8 nm in those three PDRs and explain this result as there is a critical dust size limit ($a_{\text{lim}} \sim 0.75$ nm) above which dust grains are unlikely to be (thermo-)photo-destroyed.

We show that the nano-grain mass-to-gas ratio decreases from IC63 $\rightarrow$ Horsehead $\rightarrow$ Orion Bar as the ratio between the destruction and the formation of nano-grain decreases from IC63 $\rightarrow$ Horsehead $\rightarrow$ Orion Bar.

We proposed a viable scenario to explain both the creation of nano-grains through the fragmentation of larger grains and the destruction of nano-grains.

$\rightarrow$ Study the Orion Bar observations with the JWST (Early release science program, PIs: Olivier Berné, Emilie Habart, Els Peeters) and the Horsehead nebula (GTO, to be observed soon: Meriem El Yajouri, Alain Abergel).