Grain Physics in Cloudy

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Outline

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- The physical effects of grains on their environment
- Interstellar extinction
- Grain size distributions and the photoelectric effect
- Stochastic heating of grains
- Grain formation and destruction
- Grains in Cloudy

Physical effects (1)

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Grains play an important role in the physics of ionized gas, as well as in the PDR. The main micro-physical processes involving grains are the following:

- Extinction: grains will absorb radiation. Especially in high metallicity environments this can have a substantial influence on the radiative transfer.
- Photoelectric heating: when energetic photons are absorbed, the grain may be ionized (photoelectric effect) and part of the photon energy is carried away by the electron, heating the gas.
- Collisional heating / cooling: when gas particles collide with the grains, they can loose or gain energy, depending on whether the grains are cooler or hotter than the gas.
- Charge exchange: when an ion and a grain collide, the ion may be neutralized by the grain. In rare cases the electron may also move in the opposite direction. This process is very important in fully molecular regions where ions and electrons are rare.

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Physical effects (2)

- Grain surface reactions: grains may act as catalysts for molecular reactions. The most well known example is the formation of H_2. When a hydrogen atom collides with a grain, it can bond with the grain (physisorption, chemisorption). It can also hop around on the grain from one bonding site to another. That way two H atoms can come together and form an H_2 molecule. This is the dominant formation mechanism as gas phase reactions are very slow. Other reactions can also be sped up considerably by this mechanism.
- Molecule freeze-out: grains can act as seeds for molecular freeze-out, thus removing the molecules from the gas phase and impeding reactions with them. The ice mantles can also change the optical properties of the grains, thus altering the radiative transfer in these regions. This only happens in very cold, fully molecular gas ($T_g < 20$ K).
- Thermal emission from grains can pump vibrational transitions in molecules. For most molecules this is currently not implemented in Cloudy.

Interstellar extinction (1)

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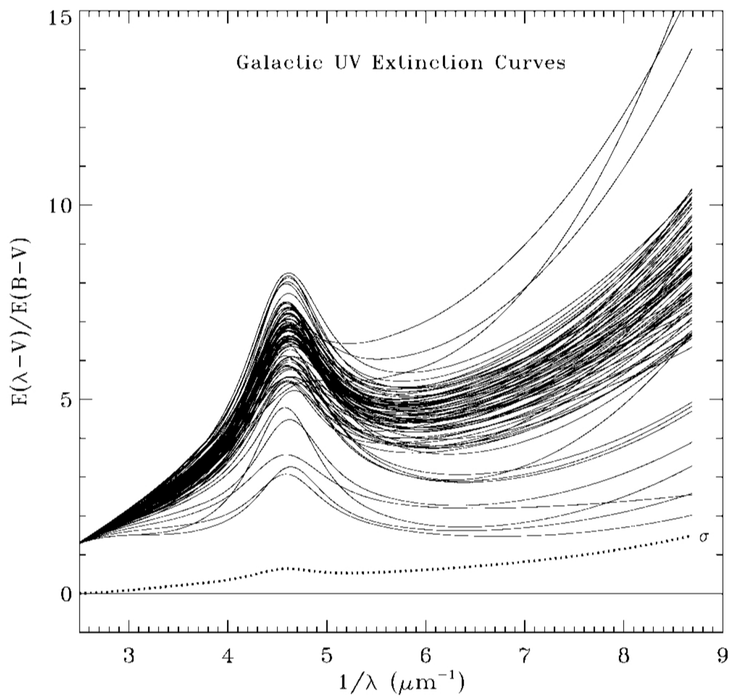

FIG. 2.—Examples of 80 Galactic UV extinction curves derived from *IUE* satellite observations. Analytical fits to the curves are shown, based on the work of Fitzpatrick & Massa (1990). The curves are taken from the Fitzpatrick & Massa catalog, with the addition of the lines of sight toward HD 210121 from Welty & Fowler (1992) and HD 62542 from Cardelli & Savage (1988). This figure demonstrates the enormous range of properties exhibited by UV extinction in the Milky Way. The dotted line, labeled "σ," shows the standard deviation of the sample scaled to the value $\sigma(1500\ \mathring{A}) = 0.74$, as derived from *ANS* satellite data (see § 3 .1).

Image credit: Fitzpatrick (1999)

Grains are responsible for interstellar extinction. The properties of interstellar extinction in the UV vary greatly for different sight lines, but are roughly the same in the optical regime (just visible at the left edge of the plot). Interstellar extinction is usually parametrized by a single parameter R_V (the total to selective extinction ratio) ranging from roughly 2.75 to 5.5, but this is clearly already a simplification... These differences are caused by different size distributions and compositions of the grains.

Note that extinction curves in external galaxies can look quite different from the Milky Way (e.g LMC and SMC).

Interstellar extinction (2)

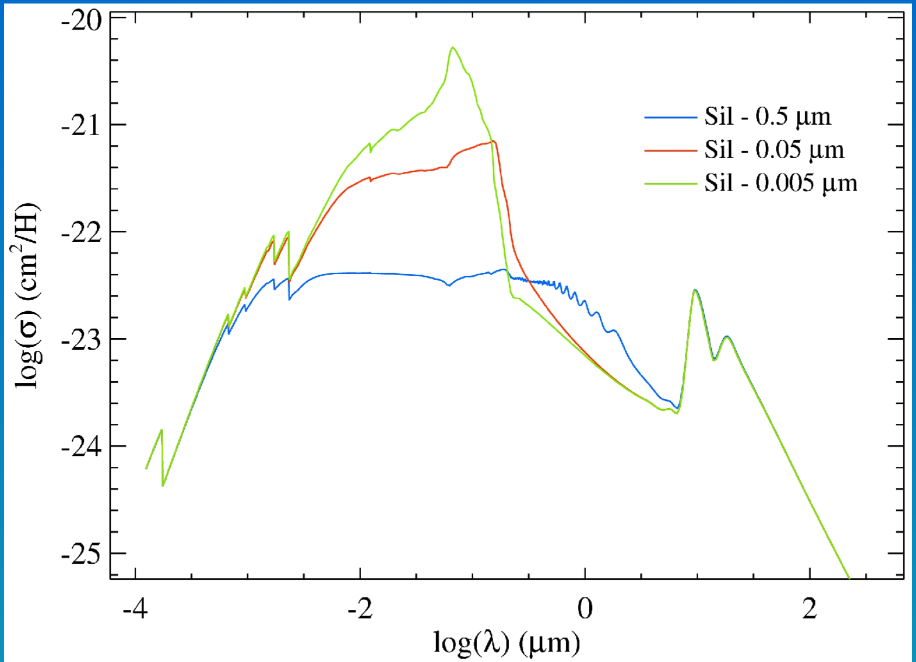

Image credit: P. van Hoof, unpublished work.

Interstellar grains are assumed to consist of a mix of astronomical silicate, graphite and/or amorphous carbon and PAHs (polycyclic aromatic hydrocarbons). The graphite and/or the PAHs are responsible for the strong extinction peak near 220 nm that we saw in the previous plot.

The strong difference in extinction for different R_V values can be understood if we look at this plot of the opacity of astronomical silicate for different grain sizes.

The PE effect

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Photo-Electric Heating in Ionized Regions 3

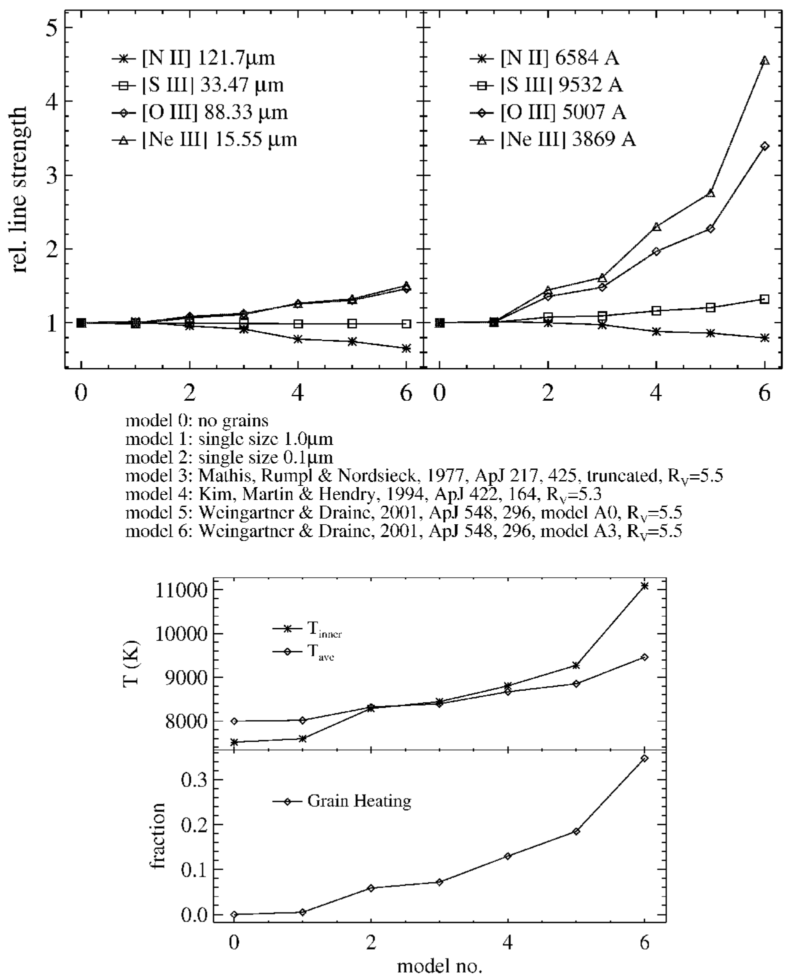

Figure 1. Paris H II region models. In the top left panel we show the relative line strengths for selected infrared fine-structure lines. These are expected to be mostly insensitive to electron temperature and therefore show the difference in the overall ionization structure. The line strengths are normalized to the line strength in the dust-free model. In the top-right panel we show optical/UV forbidden lines of the same species. In the bottom panels we show the electron temperature at the inner edge, as well as averaged over the ionized region, and the fraction of the total gas heating that is due to the photo-electric effect.

Image credit: P. van Hoof et al. (2004) ASP Conf. Series, vol. 313, p. 380.

When UV radiation removes a photon from the grain, part of the photon energy will be carried by the electron as kinetic energy which heats the gas. This is the photoelectric effect. It is an important heating source in the ionized region and the PDR.

The magnitude of the effect depends strongly on the size distribution: small grains have a larger surface area per unit mass and contribute more.

The models on the left all have the same dust mass, only the size distribution is different! The effect is clearly visible.

Unfortunately, the grain size distribution is often poorly known.

Grain size distributions

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Several papers have attempted to determine the size distribution of the grains in the ISM:

Mathis, Rumpl & Nordsieck (1977) ApJ 217, 425 (often called the MRN size distribution): appropriate for the R_V = 3.1 extinction curve (called “ism” in Cloudy).

Baldwin et al. (1991) ApJ 374, 580: truncated version of MRN, appropriate for the R_V = 5.5 extinction curve (called “orion” in Cloudy).

Kim, Martin & Hendry (1994) ApJ 422, 164: give size distributions both for R_V = 3.1 and R_V = 5.3.

Weingartner & Draine (2001) ApJ 548, 296: give a range of size distributions for R_V = 3.1 and R_V = 5.5 (with varying PAH content) as well as the LMC and SMC. Updates in Li & Draine (2001) and Draine & Li (2007)

Abel et al. (2008) ApJ, 686, 1125: PAH size distribution (called “ab08” in Cloudy).

Stochastic grain heating (1)

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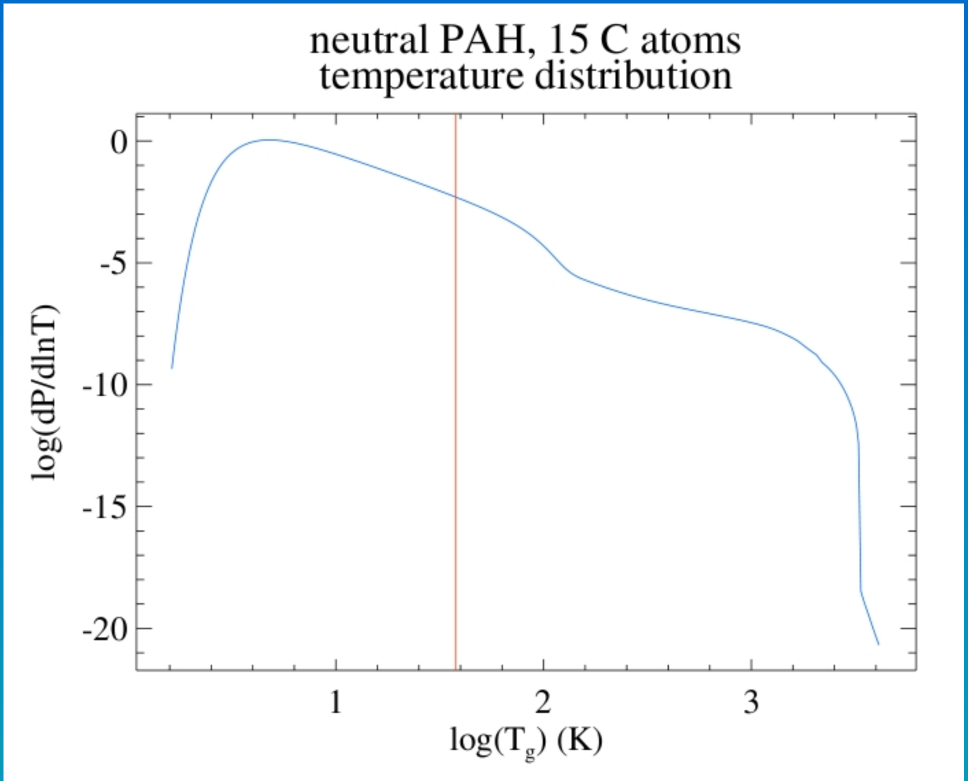

Image credit: P. van Hoof, unpublished work

When a very small grain (VSG, radius less than 100 Å) absorbs a single energetic photon, this will raise the temperature of the grain substantially (by up to several thousand kelvin) since the enthalpy of the grain is very small. The grain will then start to radiatively cool until the next photon is absorbed. If that takes a long time, the grain may cool to very low temperatures. Given the grain enthalpy, the grain optical properties, and the incident spectrum, you can calculate what the probability distribution over temperature of the grain will be. The red vertical line indicates the equilibrium temperature.

Stochastic grain heating (2)

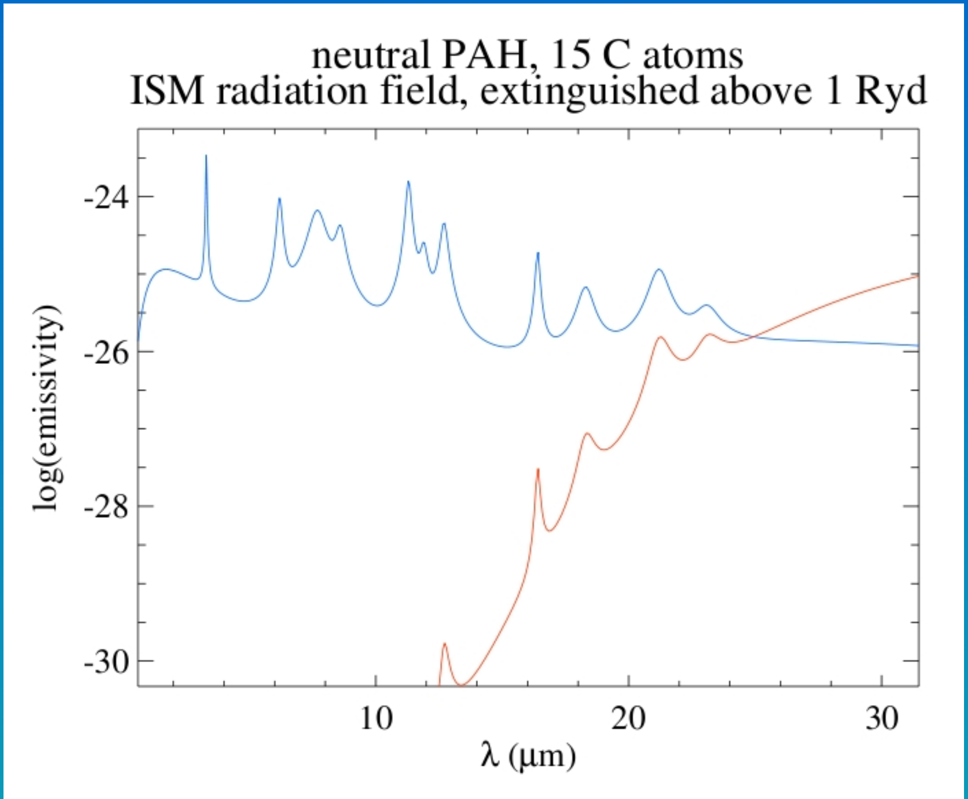

Image credit: P. van Hoof, unpublished work

Since thermal emission is a very non-linear function of temperature (exponential in the Wien tail) having these brief excursions to high temperatures significantly alters the emitted spectrum, even after averaging over time. The short wavelength end of the spectrum (blue curve) will be much stronger compared to the assumption that the grains are constantly at the equilibrium temperature (red curve). This is an important effect in the ISM.

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Grain formation

Grains typically form in dense outflows of evolved stars:

- AGB stars
- Late type WR stars
- Supernovas (efficiency still under debate)

These objects typically only form carbon-rich dust or oxygen-rich dust depending on whether C/O > 1 or C/O < 1. Some mixed-chemistry sources are known.

In the general ISM you will always find a mix of dust from various sources, so using both carbon-rich and oxygen-rich dust is appropriate.

In circumstellar environments the dust can be locally produced. In that case you need to choose between carbon-rich and oxygen-rich dust (e.g. AGB stars, planetary nebulae)

Grain destruction

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Grains can be destroyed by the following processes:

- Sputtering: collisions with energetic particles gradually erode the grain.
- Sublimation: the grain is heated to temperatures where it simply evaporates.
- Coulomb explosions: the grain is charged so high that not enough electrons remain to maintain the molecular bonds (only important for PAHs).
- Shocks: strong shocks can destroy grains, but non-equilibrium calculations are needed to get reliable destruction rates.

In general it is true that small grains are more easily destroyed than larger grains. The most well-known effect of this is that PAHs cannot survive inside the ionized region. They are abundant in the PDR region, but what happens deep in the molecular region is not yet clear.

Grains in Cloudy (1)

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Cloudy has a built-in Mie code for spherical grains. This allows you to calculate grain opacities for arbitrary grain materials and size distributions.

Several frequently used grain opacity files are pre-compiled and included in the data directory.

There are also several refractive index and size distribution files ready to use in the data directory.

You can also create your own refractive index and size distribution files. The syntax of the files is described in Appendix A of Hazy 1.

Several abundance commands **automatically** include grains in the simulation (e.g. the **abundances ISM** command). There is a complex interplay between grains set with the **abundances** command and the **grains** command. See Section 7.8.2 of Hazy 1 for details. Check your output to see if you get all the grains you expect! (especially if you use **abundances planetary**)

Use size-resolved opacity files. These give better results. Usually 10 size bins will be a good choice.

Grains in Cloudy (2)

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For all grains other than PAHs, Cloudy by default assumes that the grain abundance is constant as a function of radius.

You can set the abundance as a multiplication factor on the **grains** command, or using the **metals grains** command. The resulting absolute abundance can be found in the main output above the output of the first zone, or in the section giving the mean properties (the mean dust-to-gas mass ratio). If sublimation can occur in the inner regions, use the keywords **sublimation function** on the **grains** command.

For PAHs the grain abundance is assumed to vary as a function of radius. The default law is to scale the abundance as $n(H^0)/n(H)$. Using the **set PAH "H,H2"** command you can choose a law that scales as $(n(H^0)+2n(H_2))/n(H)$. This keeps the PAH abundance constant deep inside the molecular region.

You can code up your own abundance law in the routine GrnVryDpth() at the end of grains.cpp. Use the keyword **function** on the **grains** command to enable this routine.

Grains in Cloudy (3)

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Cloudy treats the grain physics in a self-consistent manner! There are **no free parameters** in the grain physics (other than the choices you make in the Mie code).

- The grain opacities are defined from the X-ray to the radio regime. The grain temperature is calculated from the amount of energy absorbed in the UV / X-ray assuming thermal balance.
- The optical constants are taken from lab experiments (or atomic data in the X-ray regime). We do not use beta laws or other approximations.
- The grain charge distribution is calculated self-consistently from the PE effect (including Auger cascades) as well as electron capture and charge exchange with ions in the gas. Grain charging is done fully self-consistent with the charge state of the gas. This is an important effect in fully molecular regions where grains tend to “soak up” the free electrons which can have a big effect on the chemistry.