Extinction by stratified interstellar dust grains

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We compute the optical properties of spherical dust grains composed of hollow silicate cores coated with two carbonaceous layers, the inner layer of mostly graphitic sp^2 carbon and the outer layer of sp^3 polymeric amorphous carbon, and explore the consequences on modelled interstellar extinction curves. A family of curves is created by varying the thicknesses of the sp^2 and the sp^3 layers. The average galactic extinction curve is well matched by one of this family of computed curves.

INTRODUCTION

Dust is almost everywhere in interstellar space, from the expanding envelopes of mass-losing stars where it is formed, to warm gas cooling behind supernova shocks. At least on large scales, the dust and gas are well mixed, with the density of dust tending to be proportional to the density of gas. Although very familiar to the astronomers, the nature of interstellar dust is still elusive after almost 100 years from its discovery.

Various models have been proposed for interstellar dust which may be summarized in three broad classes: (i) the silicate-graphite model [1] (the so-called MRN model) with major upgrades providing the optical constants for "astronomical" silicates [2] and graphites [3], and the natural extension to include a population of small grains, filling the size range between 5 nm (the previous MRN lower limit) and 0.3 nm, the size of large molecules [4] --- these molecules, basically free-flying or stacked PAHs, are described by means of two Drude profiles [5]; (ii) the silicate core carbonaceous-mantle model (e.g., [6, 7, 8]); and (iii) the composite model, which assumes the dust to be low-density aggregates of small silicate and carbonaceous particles ([9], and more recently [10]). While differing in details, all these model categories have certain properties in common, as they also share certain problems. Each model exploits a different (to some extent arbitrary) form for the size distribution of grains, with several free parameters to be determined by fitting the model predictions to the observations. Attempts to determine the optimum size distributions from observational constraints alone have been put forward in the last decade, using the maximum entropy method [11], and regularization techniques [10]. This opens the possibility of determining effective size distributions of grains for individual lines of sight.

Here we adopt a description similar to the one proposed by Jones et al.[7]. Details of the model can be found in Iatì et al.[12]. Carbon atoms and ions are assumed to be deposited on dust grains, partially hydrogenated, and retained on the surface. The newly deposited hydrogen-rich carbon is dominated by the sp^3 bonding. Under the influence of the interstellar radiation field, this aliphatic carbon loses hydrogen and becomes more

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graphitic and aromatic, and is dominated by the sp^2 bonding. The optical properties of these two carbonaceous materials are quite different; for example, the sp^2 material absorbs strongly in the visible, while the sp^3 polymeric material does not. Thus, in this model there are two main types of mantle, an inner layer of older sp^2 material, and an outer layer of more recently deposited sp^3 material.

COMPUTATIONAL APPROACH, MODEL, AND RESULTS

To calculate the optical properties of stratified spheres, we use the extension of the Mie theory to radially non-homogeneous spheres by Wyatt[13]. To preserve the continuity of the refractive index and its radial derivative between two contiguous layers (of refractive indexes n_1 and n_2), a thin transition zone of thickness Δr is placed at the interface. In this zone the refractive index, n varies as a function of δr, the distance from the base of the lower layer, as $n^2(\delta r) = n_1^2 + \left(3s^2 - 2s^3\right) \times \left(n_2^2 - n_1^2\right)$, with $s = \delta r/\Delta r$. The introduction of a transition layer of appropriate thickness may also account for the fact that the upper layer is actually formed by successive deposition of carbon atoms. It is reasonable to think that the first deposited atoms are adsorbed at the surface of the internal layer thus giving origin to a smooth transition from the properties of the internal layer to those of the external layer in formation.

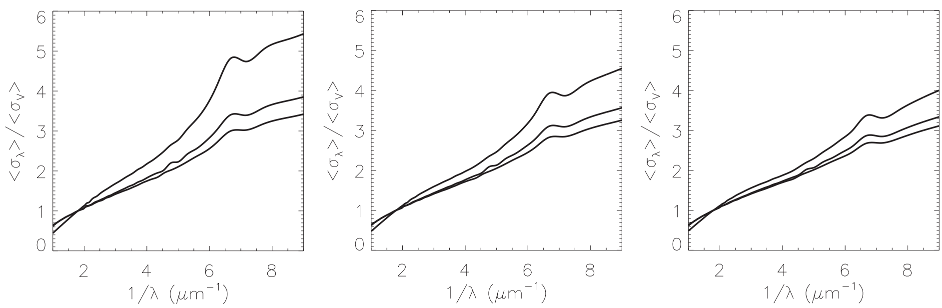

Figure 1. Normalized size-averaged extinction cross section as a function of the wave number. The size distribution is the MRN power-law $a^{-3.5}$. The lower and upper limits of the size spectrum are $a = 5$ and 1000 nm, respectively. The mantle thickness is $w = 2$ nm. The (inner) sp^2 layer has a thickness $w_{sp^2} = 0$ left, 1 central, and 2 nm right panel. In each panel the core vacuum volume fraction is 0, 1/3, and 2/3 (bottom to top).

In our model grain there are 3 concentric components: the silicate shell, the sp^2 layer and the sp^3 layer. Optical constants for the adopted materials are taken from [2], [14] (sample BE), and [15], respectively. To simulate porosity, silicate cores may present a central void, whose volume is a fixed fraction (f_V) of the total core volume, irrespective of the core size. To illustrate the results, we consider a size distribution for the silicate cores given by a power-law $a^{-3.5}$ with $a = 5$ and 1000 nm the lower and upper limits of the distribution, respectively. In Fig. 1 we show the size averaged extinction cross section normalized to its value in the visible. We keep fixed the mantle thickness to $w = 2$ nm over the whole range of grain sizes to simulate mantle accretion in the interstellar medium (e.g., [16]). The increase in the central void volume increases the relative (to the visible) extinction in the UV while, as expected, the UV extinction decreases with increasing sp^2 mantle fraction.

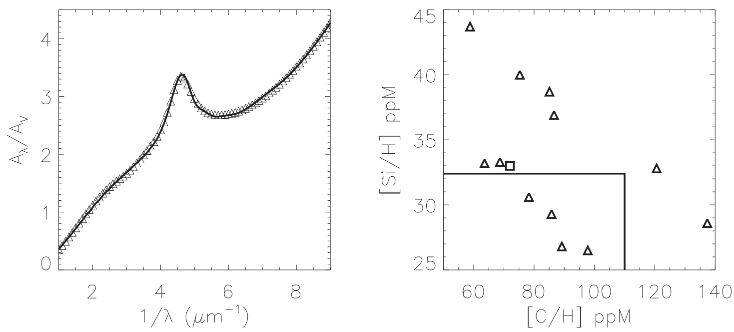

Figure 2. Left panel: model AGE (solid line) compared to the one (triangles) derived by Fitzpatrick and Massa[17]. Right panel: Si and C masses (ppM) locked in grains as functions of the mantle thickness and core vacuum fraction (triangles). The square represents the pair of values derived by the AGE best-fit. Models within the box satisfy the constraints on both Si and C masses.

There is a remarkable variety of IR-through-UV extinction curves. Several decades of work utilizing pair method extinction curves spanning the near-IR through UV spectral domain have provided a good estimate of the average wavelength dependence of the extinction in the Milky Way, summarized in an average galactic extinction (AGE) profile [17]. We fitted the AGE (see Fig. 2, left panel) with two separate populations of grains: core-mantle grains described above, and a collection of single and stacked PAHs summarized through a double Lorentz profile to include both the convolution of individual $\pi \rightarrow \pi^\star$ transitions, as well as the tail of the giant resonance associated with the $\sigma + \pi$ electron plasmon centred at wavelengths shortwards of the Lyman edge. The fit to the AGE by the adopted model is excellent. However, distinct populations of small ($5 \leq a \leq 13$ nm) and large ($80 \leq a \leq 440$ nm) grains are required to achieve this fit: continuous size distributions fail to reproduce the AGE (cf. Fig.1 e.g., the small bump near 6.2 μm^{-1} not present in the AGE). We exploit an MRN-like power-law for the size distribution with $q = 3.53$. The fitting technique then determines $w = 1.2$ nm, $f_V = 0.5$, and $f_{sp^2} = 0.97$. The resulting masses in silicates and carbon are [Si/H] = 33 and [C/H] = 72 ppM. To explore the best dependence on the elemental mass, we generate 12 additional models keeping the mantle thickness and the core vacuum fraction fixed, and derive the corresponding best fit to the AGE and the mass budget. Results are reported in the right panel of Fig. 2. As evident from the figure, the Si mass and the C mass appear to be anti-correlated. Adopting a Si solar abundance of 32.4 ppM [18] and a mean C abundance of 110 ppM [19], we find that there is a wide range of parameters consistent with the mass constraints in the diffuse interstellar medium.

DISCUSSION AND CONCLUSIONS

The interstellar extinction curve may be attributed to a population of layered grains of silicate cores with carbonaceous mantles, as an alternative to the more conventional grain model of separate populations of each materials. Varying the sp^2/sp^3 ratio within the layers generates a family of interstellar extinction curves. The variation of dust optical properties is compatible with a scenario in which carbon is deposited slowly on the surfaces of silicate cores.

The solid carbon is also processed by the interstellar radiation so that its optical properties change with time. The computed interstellar extinction curve for this model thus evolves in time. The variety of observed extinction curves may be interpreted (at least, in part) as due to evolutionary changes of interstellar dust.

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