Modeling Galactic Extinction with dust and “real” PAHs

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Abstract. We elaborated an interstellar dust model assuming a distribution of core–mantle grains and a collection of single polycyclic aromatic hydrocarbons. Exploiting this model, we are able to reproduce a very large sample of galactic extinction profiles with very different flavours, proving that a polycyclic aromatic hydrocarbons population can reproduce extinction curve features in the ultraviolet range. Dust grains are composed by an hollow silicatic core and a carbonaceous mantle (this description is mutated by the cycle of carbon in the interstellar medium); molecular population is represented by 54 molecules in four charged states and, despite the large number of free parameters (we have 9 parameters to represent grain distribution and $54 \times 4$ column densities to reproduce the molecular contribution to the extiction), we are able to determine some global properties for molecular ensemble and we found that these properties are indipendent by specific species which we use in our model.

1. Introduction
Interstellar dust grains are an important component of the interstellar medium (ISM). Deducing their nature is a very important step in the understanding of chemistry, dynamics and thermodynamics of the interstellar medium in the Milky Way and in external galaxies [1].

There are many lines of evidence of interstellar dust presence in the ISM, from which astronomers can deduce different dust properties. A strong indication for dust presence is the reddening of stellar light, caused by the absorption and scattering by dust grains. This reddening is wavelength-dependent, so an interstellar extinction curve can be derived by comparing the spectrum of an unreddened star with the one of a reddened star of the same spectral class. Other indicators of the nature of interstellar dust are: elemental depletions, polarization of stellar light, absorption and emission features [2].

The extinction curve is the observational tool most frequently used to infer dust properties. There is a basic similarity in the shapes of these curves: a general rise in normalised extinction from low values in the infrared to high values in the far ultraviolet, a near linear portion in the optical region, and a pronounced and broad “bump” near 217.5 nm. Hypothesis on the origin of this feature require Carbon, due to the presence, in the same spectral range, of the electronic transition $\pi^* \leftarrow \pi$ typical for aromatic carbon. By modelling interstellar extinction curves, we can deduce the grain size distribution. By depletion data we know that important components
in interstellar dust are silicates [3] and carbonaceous materials, both in graphitic \((sp^2)\) and in polymeric \((sp^3)\) valences [4].

During the last thirty years, different models have been elaborated, mostly based on the model by [5] in which dust grains are represented with a double population (graphite and silicate grains) following a power law size distribution (the Mathis-Rumpl-Nordsieck “MRN” distribution).

A model with significant differences from [5] model has been developed by researchers at Cagliari and Messina [6, 7]. In this model, astronomical silicates and solid carbon are present, but these components form a single population of dust grains in which carbon is assumed to be deposited on bare silicatic cores following description of [4] model. According to this model, dust grains are composed by bare silicatic cores, covered by a layer of solid carbon with a rate depending on gas density and temperature. This carbon, initially hydrogen-rich and \(sp^3\) bonded, is then converted to \(sp^2\) bonding at a rate (the so-called photodarkening rate) proportional to the intensity of the radiation field. The other component, which completes this model, is represented by Polycyclic Aromatic Hydrocarbons (PAHs), which can be modeled with a double Lorentzian or with “real” cross–sections for a sample of these molecules. Using the model in its simplified version (two Lorentzian profiles to represent PAHs contribution) [8] were able to fit a wide variety of peculiar galactic extinction curves.

In this paper, which is mainly based on [9], we use the model both in its simplified version and in including “real” PAHs cross-sections to fit the whole sample of extinction curves parametrized by [10]. We present the model in section 2, a collection of results in section 3 and we draw our final remarks in section 4.

2. The model

Our interstellar dust model has two components

- classic component, represented by a distribution of silicatic core grains covered by a carbonaceous mantle;
- molecular component, represented by a population of Polycyclic Aromatic Hydrocarbons (PAHs).

We developed the model in two ways, differing only in the molecular representation (see section 2.2): in the simplified version we use a double Lorentzian approximation to reproduce the molecular contribution, while in the detailed version we use photo–absorption cross–sections of 54 PAHs in 4 charged states.

2.1. Classic component

This component is the same for both model versions and it is represented by dust grains with four concentric spherical layers: the core which is composed by a central void, to simulate the porosity, covered by a silicatic shell, and a double carbonaceous mantle with the inner layer composed by carbon \(sp^2\) bonded and the outer layer composed by carbon \(sp^3\) bonded. This particular composition takes into account the carbon galactic cycle in the interstellar medium according to the description by [4] and the cosmic abundances inferred by gas phase elements depletions.

We assumed that the mantle thickness must be the same over the whole grain distribution as the mantle accretion in the interstellar medium suggests [11]. Likewise, the vacuum fraction in volume is a variable fit parameter, but it is independent of grain size and it is the same for all grains. We adopted a power law distribution for dust grains size \((a + w)^{-q}\), in which \(a\) is the outer silicatic core radius and, in our model, it ranges from 5 to 1000 nm, \(w\) is the mantle thickness and it is free to vary from 0 to 3 nm, \(q\) is the exponent of the power law distribution, it is a free parameter and its value is around 3.45. This distribution allows for a gap in particle size dividing small grains by large ones, hence characterizing them by a lower and upper size
limit. These two populations have no qualitative differences and the components are the same for both.

2.2. Molecular component
By the particular shape of PAHs cross–sections from UV to FUV range, we can infer that these molecules can contribute to the interstellar extinction in that spectral range. Futhermore these molecules are responsible for IR emission bands which are observable along different lines of sight and their contribution to the extinction is consistent with the observed emission in the IR bands.

In our model PAHs are represented in two ways: i) with a double Lorentzian, ii) with “real” cross–sections of a mixture of 54 PAHs in four charge states.

In the simplified version, the PAHs contribution to the extinction is approximated with a double Lorentzian profile following the description of [6]. The first Lorentzian mimics the $\pi^* \leftarrow \pi$ resonance in PAHs and reproduces the characteristic bump at 4.6 $\mu m^{-1}$ of interstellar extinction curve; the second Lorentzian mimics the low energy tail of the $\sigma^* \leftarrow \sigma$ resonance, reproducing the far ultraviolet non linear rise in the interstellar extinction curve. An exponential cut–off on the low energy tail of the $\sigma^* \leftarrow \sigma$ resonance has been introduced to take into account the lower contribution of PAHs to extinction at low energies compared to the contribution of double Lorentzian profiles. We calibrated double Lorentzian on cross–sections of a mixture of 54 PAHs in four charge states: 0, ±1, +2.

In the detailed version, we used a linear combination of computational photo–absorption cross–sections of a sample of 54 PAHs in the same charge states which we used to calibrate double Lorentzian. In this representation, a number of 216 free parameters (4 charge states for each PAH) have been considered.

3. Results
Using both the model in the simplified version and in the detailed version, we fitted the full set of [10] interstellar extinction curves. We used a modified version of C MPFIT implementation of Levenberg–Marquardt non linear least squares algorithm to perform the fits. This iterative procedure seeks to minimize numerical $\chi^2$ starting from a first guess of free parameters, staying on parameters constraints. A possible problem with this procedure is that our fit could fall on the nearest minimum which could be reached in a saddle point. Therefore, to avoid a similar problem and to evaluate the covariance matrix, after performing a fit on original data, we perturb them with a Gaussian noise proportional to the errors and we performed a fit on these perturbed data. In some cases the perturbed fit was better than for unperturbed data, showing that the first fit falled on a local minimum or a saddle point.

Figure 1 shows two interstellar extinction curves representative for the whole set and their fit using the detailed model. The model is able to fit the remarkable variety of interstellar extinction curves: from bumpless curves to curves similar to the galactic average one. Therefore PAHs could be considered as a solution to reproduce ultraviolet extinction features.

Some of the classical parameters are constant across the whole sample of fitted curves. This is the case for the exponent of the power law distribution, which is almost always very close to 3.45, and for the minimum size for small grains (it is nearly always fixed on the limit value of 5 nm, then the fit, if unconstrained, would in most cases try to move towards smaller grains). The upper limit for large grains size shows little variations, suggesting that our fit is insensitive to the population of bigger grains. Carbonaceous mantles are mostly 1 nm thick and they are mostly aromatic. In some cases we obtain bare silicatic grains (only with simplified model): in these lines of sight we expected that very small grains would emit in the silicate bands when transiently heated by the absorption of energetic photons, but such emissions are not observed. Futhermore a small number of lines of sight has mantle tickness values of 3 nm (our upper limit).
It is likely that, if left free, these fits would have converged to somewhat larger values for mantle thickness.

Regarding the molecular component, we are able to determine from our fits some global properties for PAHs, for example column density and average charge for the PAHs mixture. On the other hand the PAHs detailed composition is largely unconstrained by the fit, so our results are not dependent by the specific species used for the fit. Although the two versions of the model have the same classical component and double Lorentzian, in the simplified version, are calibrated on the same PAHs mixture photo–absorption cross–sections that we used in the detailed version, comparing fit results of the two versions for the same line of sight, we found some differences both in PAHs abundances and in classical part. This is due by the different flexibility of the two versions of our model: i) the two Lorentzians have complete freedom to vary their relative intensity but their shape must be strictly Lorentzian, ii) PAHs can vary the particular shape of their extinction contribution but the intensity ratio between two resonances has limited variability. As a consequence, when we fit the same extinction curve, especially if it is a peculiar one, classic dust must compensates these differences on molecular contribution to the extinction (see figure 2), resulting in the observed difference in classical dust distributions between the two models.

We also searched a correlation between the average charge per carbon atom and the ratio of $c_4$ and $c_3$ parameters of parametrization introduced by [10]. These two parameters represent the FUV rise intensity and the bump intensity respectively. Indeed it is known that PAHs with an increasing positive ionization have a larger gap between the $\pi^+ \leftrightarrow \pi$ and the $\sigma^+ \leftrightarrow \sigma$ resonances.
We found a positive correlation with some scatter, which confirms that PAH charge plays a role in determining the ratio between bump and FUV rise intensities but it does not solely determine it.

The amount of required Carbon locked in both solids and molecules is consistent with the interstellar budget for F and G stars, but too much Si is required by our model to fit interstellar extinction curves (see Fig. 14 of [9]).

4. Conclusions

With our model we are able to fit the whole sample of 328 galactic interstellar extinction curves of [10], using both the simplified version and the detailed version. Usually interstellar dust models are applied only to the average Galactic interstellar extinction curves or to a few individual lines of sight.

We determine some global properties for PAHs mixture, as average charge per Carbon atom and column density, but individual properties for the molecules are unconstrained. With our model we also find that bumpless interstellar extinction curves are not necessarily lines of sight devoid of PAHs and we do not need particular exotic dust properties to fit them.

Our fitting algorithm tries to reach the best match with observations regardless of abundance constraints, so we obtained that our model requires too much atoms (especially Si) to fit interstellar extinction curves. Actually, to reduce the required abundances, we are performing new fits with an increasing $\chi^2$ penalty term for abundances increasingly exceeding constraints.

The next step will be to extend the analysis with our model to external galaxies, starting from closest galaxies as the Small and Large Magellanic Clouds, to learn more about the cosmic history of the dust.

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