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A framework for resolving the origin, nature and evolution of the diffuse interstellar band carriers?

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ABSTRACT

The carriers of the diffuse interstellar bands (DIBs) still remain an unknown commodity. Both dust and molecules have been suggested as carriers but none proposed have yet been able to explain the nature and the diversity of the DIBs. Hence, it is perhaps time to review the problem in terms of the intermediate-sized nano-particles. It is here proposed that the DIB carriers are the nm-sized and sub-nm-sized products of the UV photo-fragmentation of hydrogenated amorphous carbon grains, a-C(:H), and their heteroatom-doped variants, a-C:H:*X* (where *X* may be O, N, Mg, Si, Fe, S, Ni, P, …). An interstellar hydrogenated amorphous carbon dust evolutionary framework is described within which a solution to the age-old DIB problem could perhaps be found.

1. Introduction

The diffuse interstellar band (DIB) problem has now been with us for almost 100 years and we still appear to be no nearer discovering the carriers of the DIBs. Hence, it is perhaps opportune to begin to think outside of the box for a solution to this long-standing conundrum. During the course of DIB history our ideas have oscillated back and forth between molecular and dust carriers but perhaps the solution lies in the intermediate domain between these two cases, *i.e.*, in the physics of the nano-particles that lie at the molecule-particle interface?

2. The nature of the DIB carriers

Herbig (1995) gives a comprehensive review of all of the key DIB and DIB-related issues. For a more recent and the state-of-the-art view of this subject the reader is referred to the, shortly to be published, proceedings of the latest meeting dedicated to DIBs (IAU 297, "The Diffuse Interstellar Bands", Noordwijkerhout, 20–24 May 2013). The following provides an incomplete list of the currently known observational constraints on the DIBs observed in the interstellar medium (ISM) and their carriers. The DIBs:

- are generally associated with the diffuse rather than the dense ISM,
- correlate with the dust extinction, $E(B-V)$,
- *show a weak positive correlations with the 217 nm UV bump*,
- *show a weak negative correlation with the FUV extinction*,
- are broader than atomic or molecular lines,
- are weaker in strong UV radiation fields,
- that are broader are less sensitive to UV radiation,
- correlate with small molecules/radicals (but less well than with dust),
- are environment-dependent and
- *generally do not correlate well with each other*.

This list is certainly incomplete and the logical connections between the various constraints on the nature of the DIB carriers have yet to be melded into a coherent model.

3. Amorphous hydrocarbon dust evolution in the ISM

In the condensed matter community it has long been known that hydrogenated amorphous carbons, a-C:H, darken with ultraviolet (UV) irradiation and thermal annealing to form hydrogen-poorer amorphous carbons, a-C (*e.g.*, see Jones, 2012a–c and references therein). This processing leads to a loss of hydrogen atoms from the structure and an evolution from aliphatic-rich towards aromatic-rich materials, *i.e.*, a-C:H → a-C, associated with a closing of the band gap, E_g, of the material. This evolution of the band gap is indeed the key to explaining the observed variations in the a-C(:H) optical and structural properties.

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The interesting physical and optical properties of the full suite of (hydrogenated) amorphous carbon materials {a-C:H : a-C }, or a-C(:H) for short, have resulted in quite some interest in them as a model for the solid carbonaceous matter in the ISM (*e.g.*, Jones et al., 1990; Duley, 1995; Duley et al., 1997; Dartois et al. 2004a,b, 2005; Pino et al., 2008; Serra Díaz-Cano and Jones, 2008; Jones, 2009, 2013; Godard and Dartois, 2010; Godard et al., 2011; Compiègne et al., 2011; Jones et al., 2013), in circumstellar media (*e.g.*, Goto et al., 2003; Sloan et al., 2007) and in the Solar System (*e.g.*, Dalle Ore et al., 2011). In the ISM a-C(:H) grains can undergo rather complex, size-dependent evolution arising, principally, from ultraviolet (EUV-UV) photon absorption leading to photo- and/or thermal-processing (*e.g.*, Jones, 2009, 2012a–c) and incident ion and electron collisions in shock waves and in a hot gas (*e.g.*, Micelotta et al., 2010a,b, Bocchio et al., 2012).

In the ISM the principal process that drives the transformation of the structure and composition of a-C(:H) dust is UV-EUV photo-processing and the relevant time-scales for a-C(:H) photo-processing will be composition- and size-dependent and are of the order of a 10^5–10^6 years for a-C(:H) nano-particles (*e.g.*, Jones, 2012c). Within this framework for the physical, structural and optical properties of a-C(:H) materials (Jones, 2012a–c) it has been possible to construct an interstellar dust model that, for the first time, coherently takes into account the evolution of these materials within the astrophysical context (Jones et al., 2013; Jones, 2013).

Principal among the photo-processes that drive a-C(:H) evolution in the ISM in general, and in photo-dissociation regions (PDRs) in particular, is their photo-fragmentation, which derives from the UV-photo-dissociative rupture of the structure, a process that is enhanced with respect to bulk materials by the small (nm) particle sizes. There is strong observational evidence for the destruction of the IR emission band carriers in intense radiation fields (*e.g.*, $G_0 > 10^3$, Boulanger et al., 1994, where G_0 is the interstellar radiation field intensity normalised to that of the Solar neighbourhood). More recently, Pilleri et al. (2012) found evidence for small carbonaceous grain photo-fragmentation in PDRs. Their study shows that the photo-fragmentation of small carbon grains into IR emission band carriers occurs in relatively dense and UV irradiated PDRs (H atom density $n_H = 10^2$–10^5 cm^{-3}, $G_0 = 10^2$–5×10^4, *i.e.*, $0.5 < G_0/n_H < 1.0$). It is therefore clear from the observational evidence that carbonaceous nano-particle photo-fragmentation and destruction does occur in response to EUV-UV photon irradiation in intense radiation fields.

It is also evident from observations that (photo-)fragmentation can play a role in the more diffuse ISM. For instance, in their carbon depletion study Parvathi et al. (2012) find that the FUV extinction gradually decreases with decreasing density, when normalised by $E(B-V)$, which they interpret as an indication of the preferential fragmentation of small grains in the diffuse ISM. However, this effect can also be explained by the progressive a-C:H to a-C transformation in the diffuse ISM, where the FUV dust cross-section decreases and the UV bump strength increases as the a-C(:H) band gap decreases (see Jones et al., 2013, Fig. 6). The work of Parvathi et al. (2012) therefore suggests that carbonaceous dust undergoes significant processing in the neutral ISM and lends support to the idea that dust mass variations in the small carbonaceous grain population can be driven by photo-processing and/or photo-fragmentation in low density regions.

Thus, photo-fragmentation of a-C(:H) can lead to the liberation of hydrocarbon fragments, such as arophatics (Micelotta et al., 2012), which consist of aromatic clusters linked by aliphatic and olefinic bridging structures. In this context, a-C(:H) nano-particles are particularly susceptible to disruption by EUV-UV photon driven processes that drive arophatic cluster formation and lead to the eventual demise of the fragmentation products as they break down into and liberate daughter molecule/radical/ion species such as H_2, C_2, CN, CCH, C_3, C_3H^+, c-C_3H_2 and C_4H (*e.g.*, Smith, 1984; Duley, 1998; Pety et al., 2005; Jones, 2009; Pety et al., 2012; Jones et al., 2013).

Based on the above and preceding work (Jones et al., 1990, 2013; Jones, 1990, 2009, 2012a–c, 2013) the principal processes in the a-C(:H) dust evolutionary cycle in the ISM can be summarised as follows:

- Dust formation in AGB dust shells leads to the formation of wide band gap ($E_g \sim 2.5$ eV), aliphatic-rich a-C:H dust, which is aromatised in the transition to the ISM (small grains and the outer surfaces of large grains are converted to low band gap a-C, $E_g \sim 0$ eV).
- Dust eroded in the ISM (through the effects of EUV photo-processing, shocks and cosmic rays) is then re-accreted in the denser, molecular ISM ($A_V > 1$) to form wide band gap ($E_g \gtrsim 2$ eV) mantles on all grains. Such accreted mantles may be the glue that cements the grains in aggregates and could also be the source of the observed cloud/core shine (see Jones et al., 2013, and references therein).
- During a-C:H dust (re-)formation by accretion in denser regions hetero-atoms could be incorporated into the structure to form doped materials, *i.e.*, a-C:H:*X*, with the element *X* showing a preference for the aromatic phase and/or aliphatic phase depending upon its chemical proclivity.
- Carbon dust evolution, via EUV-UV ($h\nu \geq 10$ eV) photo-processing, in the ISM/HII regions/PDRs leads to associated de-hydrogenation, aromatisation and a decrease in band gap (all manifestations of the chemical evolution of the structure), and can also lead to photo-fragmentation.
- EUV-UV photo-fragmentation in intense radiation fields, perhaps aided by grain–grain collisional fragmentation in turbulent regions of the ISM, is a trickle-down process that leads to a wide range in the a-C(:H) grain size distribution, which includes:
  - FUV extinction carriers ($a \sim 3$ nm, a few 1000s of C atoms),
  - UV bump carriers ($a \sim 1$ nm, a few 100s of C atoms),
  - emission band carriers ($a \sim 0.5$ nm, a few 10s of C atoms),
  - molecules/radicals (C_2, CN, CCH, l-C_3, l-C_3H^+, c-C_3H_2, l-C_4H, …l/c-C_nH_m, $m \lesssim n$).
- Photo-fragmentation of a-C(:H) grains yields aromatic-rich fragments or sub-grains with 10–1000 C atoms, and molecules and radicals with < 10 C atoms. The resulting fragment distribution will be incorporated into the ambient ISM where, in comparison, it will be subject to only relatively minor modifications.

The size distribution determined by the photo-physics in HII regions and PDRs then determines and sets the small carbonaceous grain size distribution in the diffuse ISM, where the radiation field and hence the effects of photo-processing are significantly reduced.

Among the smallest a-C(:H) species, containing less than a hundred carbon atoms, there will be a rather wide isomeric variation, which is nevertheless limited by the bonding configuration in arophatic clusters and is therefore probably based upon a limited set of common 'backbone' species.

4. The Red Rectangle: a case in particular

The Red Rectangle (RR) is an interesting object because it allows us to qualitatively test some of the EUV-UV photo-processing aspects outlined above. The RR is a proto-planetary nebula that exhibits a spectacular display of red luminescence, the