Solid State Astrophysics
Probing Interstellar Dust and Gas Properties with X-rays

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Julia C. Lee\textsuperscript{1}, Randall K. Smith\textsuperscript{2}
C. R. Canizares\textsuperscript{3}, E. Costantini\textsuperscript{4}, C. de Vries,\textsuperscript{4} J. Drake\textsuperscript{2}, E. Dwek\textsuperscript{5}, R. Edgar\textsuperscript{2}, A. M. Juett\textsuperscript{5}, A. Li\textsuperscript{6}, C. Lisse\textsuperscript{7}, F. Paerels\textsuperscript{8}, D. Patnaude\textsuperscript{2}, B. Ravel\textsuperscript{9}, N. S. Schulz\textsuperscript{3}, T. P. Snow\textsuperscript{10}, L. A. Valencic\textsuperscript{11}, J. Wilms\textsuperscript{12}, J. Xiang\textsuperscript{1}

\textsuperscript{1}Harvard University
\textsuperscript{2}Smithsonian Astrophysical Observatory
\textsuperscript{3}Massachusetts Institute of Technology
\textsuperscript{4}SRON-NL
\textsuperscript{5}NASA/Goddard Space Flight Center
\textsuperscript{6}University of Missouri
\textsuperscript{7}Johns Hopkins University Applied Physics Laboratory
\textsuperscript{8}Columbia University
\textsuperscript{9}NIST
\textsuperscript{10}University of Colorado
\textsuperscript{11}Johns Hopkins University
\textsuperscript{12}Universität Erlangen-Nürnberg-Germany
Abstract

The abundances of gas and dust (solids and complex molecules) in the interstellar medium (ISM) as well as their composition and structures impact practically all of astrophysics. Fundamental processes from star formation to stellar winds to galaxy formation all scale with the number of metals. However, significant uncertainties remain in both absolute and relative abundances, as well as how these vary with environment, e.g. stellar photospheres versus the interstellar medium (ISM). While UV, optical, IR, and radio studies have considerably advanced our understanding of ISM gas and dust, they cannot provide uniform results over the entire range of column densities needed. In contrast, X-rays will penetrate gas and dust in the cold (3 K) to hot (10^8 K) Universe over a wide range of column densities ($N_H \sim 10^{20-24} \text{cm}^{-2}$), imprinting spectral signatures that reflect the individual atoms which make up the gas, molecule or solid. X-rays therefore are a powerful and viable resource for delving into a relatively unexplored regime for determining gas abundances and dust properties such as composition, charge state, structure, and quantity via absorption studies, and distribution via scattering halos.

Introduction

Understanding astrophysical processes, from galaxy evolution to star formation to stellar or AGN outflows, requires an understanding of the metal abundances in the surrounding medium, in gas and dust phases. As the primary repository of metals in the interstellar medium (ISM), dust plays a major role in the chemical evolution of stars, planets, and life. Although it makes up only $\sim 1\%$ of the baryonic mass of our Galaxy, it accounts for virtually all of the UV/optical extinction, in scattering and absorption. This extinction is so efficient that only 1 in $10^{12}$ of the optical photons created in the Galactic Center reaches us.

In addition, ISM dust and molecules store the heavy elements needed for making Earth-like planets, while their physics and chemistry play an important role in giant molecular clouds, where dust acts as a catalyst in the formation of the organic compounds vital to the development of life (Whittet 2003). Accurate measurements of the distribution of gas and dust phase abundances in galactic environments are therefore crucial for improving our understanding of a wide range of astrophysical processes from nucleosynthesis to planet formation.

Despite extensive multi-wavelength studies (primarily in radio to IR bands), we have a limited understanding of dust grain size distributions, their elemental and crystalline composition, and their distribution in astrophysical environments ranging from the cold ISM to the hot disks and envelopes around young stars and compact sources. One immediate difficulty arises from our incomplete knowledge of the overall material available in the gas and dust phases (Fig. 1). Dust abundances are traditionally...
inferred from the observed depletion of the gas phase relative to the assumed standard solar abundances (or some linear fraction of them), rather than directly measured. The best direct measurements of gas abundances thus far have come from optical & UV absorption-line studies of diffuse interstellar clouds (e.g. Savage & Sembach 1996). However, these results are limited to low opacity sightlines, and cannot penetrate dense molecular clouds. IR and radio spectroscopy can see into dense clouds to measure many ISM molecules and compounds (mostly polycyclic aromatic hydrocarbon or PAHs, graphites, certain silicates, and ice mantle bands). Yet, since these spectral features come from probing complex molecules as a whole through rotational or vibrational modes originating from e.g. the excitation of phonons (rather than electrons), they require sophisticated modelling efforts or matching to laboratory spectra. Reproducing the exact IR spectral features observed has proven difficult in many cases, making robust abundance and structure determinations for these molecules dependent upon assumptions about their physical properties (Draine 2003b).

The power of X-ray ISM studies of dust and gas

X-rays probe all ions from neutral atoms to hydrogenic ions, including H-like Fe xxvi (Fe+25), thereby providing a unique window into the cold (3 K) to hot (10^8 K) Universe, over a wide range of column densities (N_H ~ 10^{20-24} cm^{-2}), not possible in any other waveband (see Paerels & Kahn 2003 and references therein). Detailed X-ray studies of the ISM began with Schattenburg & Canizares (1986), who first detected photoelectric edges along with a tentative detection of an atomic O i line. Fifteen years later, the Chandra and XMM gratings have facilitated stringent ISM abundance measurements of individual ionic species, from e.g. O i-vii (e.g. Paerels et al. 2001; Juett et al. 2004; Juett et al. 2006). To draw similar parallels, the improved spectral resolution and throughput available to future studies will allow us to routinely use X-ray spectra to determine the quantity and composition of dust, where such studies are now pushing the limits of extant satellite capabilities (see Lee et al. 2009a). These important studies can be facilitated as additional bonus science spawned from targeted studies of X-ray bright objects whose lines-of-sight also intersect with inter- and intra-stellar gas and dust with enough opacity to imprint their unique spectral signatures. For the remainder of this white paper, we focus on the unique means by which X-
ray studies can be used to combine condensed matter/solid state theory and atomic physics techniques to the study of astrophysical gas (in photoionized and collisional environments), and dust (composition, quantity, structure, and distribution), that is highly complementary to other wavebands and fields (e.g. planetary science, chemistry, geology, and experimental physics, as relevant to laboratory astrophysics). As such, we can expect such studies to have relevant applications which span the Galactic to Cosmological.

An X-ray absorption method for determining gas-to-dust ratios

Both gas and dust (when $\lesssim 10\mu m$) are semi-transparent to X-rays. Therefore, these high energy photons can be used to make a direct measurement of condensed phase chemistry via a study of element-specific atomic processes, whereby the excitation of an electron to a higher-lying, unoccupied electron state (i.e. band/molecular resonance) will imprint signatures in X-ray spectra that reflect the individual atoms which make up the molecule or solid. In much the same way we can identify ions via their absorption or emission lines, the observed spectral modulations near photoelectric edges, known as X-ray absorption fine structure (XAFS) provide unique signatures of the condensed matter that imprinted that signature. Fig. 2 shows how XAFS signatures of different molecules and solids can be identified by their unique structure and wavelength. With high X-ray spectral resolution, and throughput, one can easily assess these details to determine astrophysical dust and molecular properties. At the current highest spectral resolution (R=1000) of the Chandra HETGS, one can discern at high confidence between $\text{Fe}_2\text{O}_3$ (red) and $\text{FeSO}_4$ (green), but not between e.g. $\text{Fe}_2\text{O}_3$ and $\text{FeO(OH)}$‡, as would be possible at the $R = 3000$ spectral resolution of Fig. 2. Furthermore, higher throughput and spectral resolution than currently available will provide additional important knowledge about grain structure (i.e. bond lengths and charge states). Therefore, X-rays should be considered a powerful and viable resource for

‡We note that, while XAFS theory is quite mature, the study of XAFS is still largely empirical. Therefore, the success of such a study will require that space-based measurements be compared with empirical XAFS data taken at synchrotron beamlines to determine the exact chemical state of the astrophysical dust.

Fig. 3.— A 15ks Chandra HETGS observation of Cygnus X-1 (black) zoomed in on the $\sim 700eV$ ($\sim 17.7\text{Å}$) FeL spectral region shows that at the current highest available spectral resolution, we can discern at high confidence between $\text{Fe}_2\text{O}_3$ (red) and $\text{FeSO}_4$ (green), but not between e.g. $\text{Fe}_2\text{O}_3$ and $\text{FeO(OH)}$ (dark blue). In light blue is continuum absorption by Fe L from both gas and solids (CM). In addition, even for a source as bright as Cyg X-1, a 15 ks integration is require to achieve a S/N $\sim 5$ per bin. Future missions with higher throughput will allow us to engage in such studies with more sources, and accompanying higher spectral resolution as e.g. that shown in Fig. 2 will enable more involved studies of dust structure, not currently possible.
delving into a relatively unexplored regime for determining dust properties: composition, charge state, structure, quantity (via absorption studies; see Lee et al. 2009a for discussion on how to determine quantity and composition), and distribution (via scattering halo studies; e.g. Xiang et al. 2007 and references therein; details to follow).

Chandra and XMM have begun this work but have been limited by the available effective area at high spectral resolution (e.g. Lee et al. 2001, 2002; Takei et al. 2002; Ueda et al. 2004; deVries & Costantini 2009). As such, condensed matter astrophysics (i.e. the merging of condensed matter and astrophysics techniques for X-ray studies of dust) is now possible, albeit difficult due primarily to the need for more S/N. As stated, for more involved studies of grain structure, higher spectral resolution than currently available is also needed.

To illustrate the complementarity of X-ray studies with those in other wavebands, consider Lee et al. (2009b)’s Spitzer IR and X-ray study of the line-of-sight toward the BH binary Cygnus X-1 which shows different grain populations: IR detections of silicates versus X-ray studies ruling out silicates. This brings to bear intriguing questions relating to grain sizes and origin: e.g. does the IR probe a population of large silicate grains that are opaque to the X-rays, or are we probing truly different origins, or is it something more complex? Another example arises from Spitzer IRS studies of the star HD 113766, which shows tantalizing evidence for dust associated with terrestrial planet formation (Lisse et al. 2008). Analysis of the IR spectra provided knowledge of the mineralogy, but could not determine overall abundance ratios, e.g. the amount of Mg vs Fe depleted into grains, to better than a factor of 2. This information can be extracted from X-ray studies of XAFS spectra with sufficient S/N and spectral resolution. These examples highlight the power of an orthogonal approach using X-rays to complement other wavebands: (1) by probing dust properties missed by other detection techniques, and (2) by being sensitive to the range of sub-micron to \( \sim 10 \ \mu m \) size dust in \( N_H \sim 10^{20-24} \text{cm}^{-2} \) environments. Such multi-wavelength studies, especially if achieved with high throughput and spectral resolution in the X-ray band, will add significantly to our knowledge of the mineralogy and distribution of nascent and interstellar dust populations and therefore the environments from which they originate, be they outflows or star forming regions.

Despite the power of using X-rays for dust studies, this energy band has not been fully exploited for spectral studies of gas, dust and molecules, due largely to the unavailability of instruments with both good throughput and spectral resolution \( (R \gtrsim 1000) \). Missions such as IXO can push the frontiers of such studies by enabling high-precision elemental abundance measurements of gas and dust towards hundreds of sightlines, both in our Galaxy and beyond (see Figure 4[Right]). Simulations based on IXO’s target spectral resolution and area show that a S/N=10 per bin can be achieved for over 200 sources in 30 ksec or less, while the higher spectral resolution will allow us to realize the previously-discussed studies of dust structure that are not currently possible.

IXO’s energy coverage will allow us to study in detail photoelectric edges near C K, O K, Fe L, Mg K, Si K, Al K, S K, Ca K, and Fe K, and therefore all gas-phase as well as molecules/grains containing these constituents, covering all the important species with
IXO: 3–10% measurements

Percent Error Abundances

Chemical Element

Fig. 4.— [Left] Potential abundance measurement accuracy from spectra with 50 ksec exposures using the Chandra ACIS-S, LETG (circles), XMM-Newton RGS (squares) and IXO calorimeter (triangles) for \( N_H \) values of \( 5 \times 10^{20} \) cm\(^{-2}\) (green), \( 5 \times 10^{21} \) cm\(^{-2}\) (blue), and \( 5 \times 10^{22} \) cm\(^{-2}\) (red). [Right] Sightlines to bright AGN or X-ray binaries for which IXO will be able both study the source and determine abundances to better than 10%.

high depletion rates onto dust. These studies, when applied to different astrophysical environments, Galactic or extragalactic, will enable probes of the gamut of outstanding issues ranging from NS and BH (stellar and supermassive) evolutionary histories, to the hot accretion flow in dust enshrouded accretion systems (e.g. Sgr A* and similar AGN and star formation systems; see Lee et al. 2009a for discussion), to cosmological implications (e.g. Type Ia SNe light curves are affected by line-of-sight dust), all using X-rays.

X-ray spectra can also determine abundances in different ISM environments (Yao & Wang 2006), thereby opening a window on the study of grain evolution and cycling between diffuse and dense or dark clouds. The current uncertainties for Chandra and XMM abundance measurements usually exceed 20%, due primarily to the low effective area of the spectrometers. As a result, these results do not constrain ISM abundances with more accuracy than using stellar photospheres or UV/optical data. Over 1800 sources (Fig. 4[Right]) have high enough X-ray fluxes \( \gtrsim 5 \times 10^{-12} \) ergs cm\(^{-2}\)s\(^{-1}\) for IXO to make high precision (3–10%) O, Mg, Si, and Fe abundance determinations for both diffuse and dense sightlines, including molecular regions where \( N_H > 5 \times 10^{22} \) cm\(^{-2}\) (see Figure 4[Left]). Along the less dense sightlines with X-ray and UV-bright sources, UV/optical gas-phase abundance measurements can be combined with X-ray determinations of the total abundances to extract the ratio of gas-to-dust directly (e.g. Cunningham et al. 2004). X-ray observations will also probe abundances beyond the Milky Way: between 10-100 ultra-luminous X-ray sources (ULXs) have X-ray fluxes that will allow robust abundance measurements beyond our Galaxy. With spectral resolution \( R > 1000 \), the Galactic and distant contributions can be separated simply using known velocity separations.

With the additional XAFS studies of dust composition possible for over 200 sources along different sightlines, we can also discriminate between different grain models. With these many sight-lines, we will obtain valuable information on the chemical uniformity of the ISM, including mixing and enrichment.
Dust-induced X-ray Scattering

Scattered X-rays also provide information on dust grain sizes, positions, and composition, via imaging studies of the arcminutesc ale halos around X-ray bright sources created by small-angle scattering in interstellar dust grains (Draine 2003). In some cases, we can even use such studies to more accurately determine distances to compact objects or even other galaxies (see Trümper & Schönfelder 1973 for a description of the method; Predehl et al. 2000; Draine & Bond 2004; Xiang et al. 2007 for applications). Measuring the location and size of grains – seen most dramatically in the dust-scattered rings around X-ray bursts (Vaughan et al. 2004) – provides information about the grain environment and their formation processes when combined with composition and abundance studies discussed previously.

The intensity of the halo created by small-angle scattering of X-rays by dust is especially sensitive to the large end of the grain size distribution, as these grains dominate the scattering cross section ($\sigma \propto \rho^2 a^4$). In addition, every IXO observation of 20 ksec or longer of a moderately bright source ($>10^{-11}$ erg s$^{-1}$ cm$^{-2}$) with $N_H \gtrsim 10^{21}$ cm$^{-2}$ will contain a detectable X-ray dust halo. By measuring the total scattered halo intensity as a function of energy in bright sources – absorption features from the elemental grain composition can be measured (Costantini et al. 2005), as shown in Figure 5 for an IXO simulation. These X-ray halos will directly measure the composition of the large grains.

Existing interstellar grain size distributions have been developed through information gathered from UV/optical/NIR extinction, polarization, IR emission, and depletion. By combining measurements towards hundreds of sight-lines, modelers have constrained the composition, shape, and grain size distributions from tens of Å up to ~0.5 µm; above this size, grains act as size-independent “gray” particles in these wavebands. Despite the lack of detailed information, the models agree that even in the diffuse ISM, grains larger than 0.1µm contain most of the dust mass in the ISM. Moreover, most interstellar dust resides in dense molecular clouds, where UV/optical observations are difficult to impossible.

Early interstellar grain models used an approach consisting of a population of bare silicate and graphite grains in a simple power law size distribution, designed to reproduce the “average” Galactic UV extinction curve (Mathis et al. 1977). Since that time, many workers have developed models that were constrained by data from different wavelength regimes, as more information became available (e.g. Dwek et al. 1997; Li & Greenberg 1997; Li & Draine 2001; Weingartner & Draine 2001; Zubko et al. 2004). However, a mismatch of
up to $\sim 30\%$ between the total grain mass and the available metals remains in many models (see Figure 1; Draine 2003b; Zubko et al. 2004). It is not yet clear if the solution will involve changes to the ISM abundances or to the grain models. Halos seen with Chandra and XMM have already shown that adjusting the grain porosity does not solve the problem (Smith et al. 2002; Smith 2008; Valencic & Smith 2008); more accurate abundance data are sorely needed.

Amongst other advantages, X-ray studies will afford us a window into giant molecular clouds, which are opaque to UV and optical light. While grains may coagulate there and/or grow envelopes of ices and organic material (e.g. Clayton & Mathis 1988; Vrba et al. 1993; Whittet et al. 2001), what little we know about these chemical warehouses come from observed molecular transitions in the IR and microwave, which are primarily sensitive to ice and organic compounds. Theoretical work by Cho & Lazarian (2005) offer that far-IR and sub-millimeter polarization studies may shed light on grain sizes in dark clouds ($A_V > 10$), although this remains to be demonstrated. By capitalizing on the well-known sensitivity of X-ray scattering halos on grain sizes, X-rays can be used to provide, again, an orthogonal means by which we can assess dark cloud cores to compare with studies in the IR. The halos of bright objects behind these clouds will let us examine the grain growth processes which heretofore have been shrouded in mystery, while the observed fine structure near photoelectric absorption edges discussed above will provide valuable information on the composition and growth of organic mantles.

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