An X-ray view of gas and dust in the diffuse interstellar medium

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Abstract

In this work we study the diffuse interstellar medium in the soft X-ray band (<1 keV). We use XMM-Newton and Chandra observations to study the gas and dust absorption features present in the X-ray spectra of bright X-ray binaries. In particular, we study the oxygen K and iron L-edges in a sample of sources along the Galactic plane. We use newly calculated dust extinction cross sections which include dust compounds with different chemical compositions and crystallinity. We find that the Mg-rich amorphous pyroxene (Mg_{0.75}Fe_{0.25}SiO_3) represents the largest fraction of dust towards most of the X-ray sources, about 70% on average. The second most dominant compound in our modelling is the amorphous olivine (MgFeSiO_4), which covers about 25% of the total amount of dust in the different lines of sight. We also confirm that the iron is heavily depleted from the gas phase, more than 95% of iron is in dust. The depletion of neutral oxygen is lower, it is ranking between 10-25% depending on the line of sight.
4.1 Introduction

Interstellar dust (ID) is ubiquitous and plays an important role in our Galaxy. Dust appears at every stage of stellar evolution, from evolved stars and supernovae to protoplanetary disks. ID is the primary repository of metals in the interstellar medium (ISM) and acts as a catalyst for the formation of complex molecules (Whittet 2003). The properties of dust grains in different regions of the ISM can give insights into their production and destruction mechanisms and reveal the evolution history of our Galaxy.

Dust grains are characterized by their chemical composition, morphology and size. Abundant elements such as carbon, oxygen, silicon, iron and magnesium are the main constituent of cosmic dust. Elements such as titanium, calcium and aluminum can be found in smaller quantities and are highly depleted from the gas phase (Jenkins 2009). ID can be divided into carbonaceous and silicate grains. Additionally, dust can consist of oxides (FeO or SiO), carbides and metallic iron (Draine 2011).

The structural properties of dust grains vary depending on the configuration of the atoms in the grain. Crystalline materials are characterized by a periodic long-range order of atoms, while amorphous dust grains do not show periodic structures and present a 3D disordered network of atoms. Crystalline dust is unlikely to survive the harsh environment of the ISM. Studies of the 10 µm silicate feature in the mid-IR band showed that silicate dust is mostly in amorphous form, and in particular olivines and Mg-rich pyroxenes (Kemper et al. 2004, Min et al. 2007). Moreover, it has been recently found from X-ray absorption studies of interstellar dust that amorphous olivine represents most of the dust in the dense environment of the ISM (see Zeegers et al. (2019) and Rogantini et al. (2020)).

Historically, interstellar dust has been studied in the infrared and millimeter wave spectral range. Nonetheless, the launch of XMM-Newton and Chandra X-ray satellites and their high-resolution spectrometers opened up a new window for the study of the ISM and the dust mineralogy. The photoabsorption edges of some of the most abundant elements in the Galaxy, such as oxygen, iron, neon or silicon, are present in the X-ray spectra. Bright X-ray binaries are used as background lights enabling the study of the spectral features of atomic and solid species of the ISM. In particular, from the X-ray band we are able to distinguish the gas and solid phase abundances of selected elements as well as to investigate the chemical composition of dust in the ISM.

Oscillatory modulations, known as X-ray Absorption Fine Structures (XAFS), are observed near the photoelectric absorption edges and they provide unique fingerprints of dust. These modulations happen when an X-ray photon interacts with a dust grain and gets absorbed by an atom in the dust particle. The ejected photo-electron interacts with the neighboring atoms. This interaction modulates the wave-function of the photo-electron due to constructive and destructive interference between the
outgoing and backscattered electron waves. The shape of the spectral modulations is
determined by the local-scale atomic structure of the grain and it therefore imprints
its chemical composition and structure (see also Newville (2004) for a detailed ex-
planation). Therefore, modelling the XAFS enables the study of the dust chemical
composition and crystallinity.

In the literature models of XAFS for multiple photoelectric edges are available. In
particular, the K-edge of iron has been studied by Rogantini et al. (2018) and Lee &
Ravel (2005) using synchrotron radiation. Synchrotron measurements have been also
performed in order to characterize the K edges of silicon (Zeegers et al. 2017, 2019)
and magnesium (Rogantini et al. 2019). For the soft X-ray band, the oxygen K-edge
(Psaradaki et al. 2020, henceforth, Paper I) and the iron L-edges (Chapter 3) have
been studied using electron energy loss spectroscopy (Egerton 2011). Additionally,
studies of the iron L edges have been performed by Lee et al. (2009) and Westphal
et al. (2019). Elements such as carbon or of lesser abundance in the ISM such as
aluminum and sulfur have been presented in Costantini et al. (2019).

In this paper we are interested in the iron and oxygen in the ISM. Both elements
are very abundant and therefore it is very important to understand the amount that
has been locked up in dust grains (i.e their depletion). Iron is known to be heavily
depleted in interstellar dust as more than 90% of the total iron is believed to be locked
up in dust grains. Iron is primarily formed in supernovae type Ia and core collapse
supernovae. It is believed that more than 65% of the iron is injected in the ISM in
the gaseous form and therefore most of its depletion is expected to take place in the
ISM (Dwek 2016). The exact composition of Fe-bearing grains is still unclear. Poteet
et al. (2015) found that almost all the Mg and Si atoms reside in amorphous silicate
grains, while a substantial amount of iron resides in other compounds than silicates.
Iron is expected to be present in silicate grains but it could also exist in pure metallic
nanoparticles (e.g. Kemper et al. 2002) or even as metallic inclusions in glass with
embedded metal and sulphides of interstellar origin (e.g Keller & Messenger 2013).
Oxygen is one of the most abundant elements in the Galaxy. As discussed in Paper
I, the total budget of oxygen in the ISM is largely uncertain (Jenkins 2009). Oxygen
is missing from the gaseous phase at a rate that cannot be fully explained yet. The
combined contributions of CO, ices and silicate/oxide dust cannot fully account for
the missing oxygen in the ISM. At the interface between diffuse and dense phases,
about 30% of the oxygen is unaccounted for (Whittet 2010). The aim of this inves-
tigation is to give insights into the depletion of oxygen and iron into dust and the
observed abundances of these elements into gas and dust along different lines of sight
in the Galaxy. We further investigate the chemical composition of cosmic dust in the
diffuse regions of the ISM.

We fit simultaneously the O K- and Fe L-edges using the available XAFS models
presented in Paper I and Chapter 3 to fit the dust features. In the literature there are
several studies of these elements using high resolution X-ray observations. Absorption
features around these edges due to atomic and solid phase were found previously in the spectra of several sources (Paerels et al. 2001, Juett (2004), de Vries & Costantini 2009, Kaastra et al. 2009, Lee et al. (2009), Costantini et al. 2012, Pinto et al. 2010, 2013 and references therein). Here, we study a sample of X-ray sources along the Galactic plane using data from the high-resolution X-ray spectrometers on board XMM-Newton and Chandra satellites. We aim to characterize the dust species along different sight lines in the Galaxy and determine the depletion of iron and oxygen into solids. This paper is organized as follows. In Section 4.2 we present the sample of X-ray binaries and in Section 4.3 we show the X-ray data used for this work. The methodology used for the spectral fitting of the ISM is explained in Section 4.4. Finally, in Section 4.5 we discuss our results.

4.2 Sample of sources

We select eight low-mass X-ray binaries as background sources which are suitable for the study of both oxygen K and iron L edges. We selected sources with a column density between $\sim 1 - 5 \times 10^{21}$ cm$^{-2}$ in order to guarantee a large optical depth of the oxygen and iron edges.

For our analysis it is important that the sources have both Chandra and XMM-Newton archival data. Therefore, another selection criterion is the availability of data from the public archives. To further ensure high signal-to-noise ratio we consider observations with enough exposure time. The selected sample of sources as well as their column densities and distances are listed in Tables C.2 & C.1. In Fig. 4.1 we present the projection of the X-ray sources on the Galactic plane.

4.3 Data and reduction

In order to best study the narrow absorption features of gas and dust present in the soft X-ray band (< 1 keV) we combine the capabilities of currently available high-resolution X-ray spectrometers on board XMM-Newton and Chandra satellites. To study the oxygen K-edge we use the Reflection Grating Spectrometers (RGS, den Herder et al. 2001) of XMM-Newton which has a resolving power of $R = \frac{\lambda}{\Delta \lambda} \gtrsim 400$ and an effective area of $\sim 45$ cm$^2$ in this spectral region. For the iron L-edges we use Chandra data. Chandra carries two high spectral resolution instruments, the High Energy Transmission Grating (HETGS, Canizares et al. 2005) and the Low Energy Transmission Grating (LETGS, Brinkman et al. 2000). Here, we use the High Energy Grating (HEG) and Medium Energy Grating (MEG) of HETGS. MEG has an effective area of $\sim 7$ cm$^2$ and a resolving power of $R = \frac{\lambda}{\Delta \lambda} \gtrsim 760$ around the iron L-edges which makes it the most suitable instrument to study the XAFS in this spectral region. A similar approach using combined information from XMM-Newton
4.3 Data and reduction

and Chandra data has been already presented in Costantini et al. (2012). All the data used in this paper are listed in Appendix C.

4.3.1 XMM-Newton

We obtain the RGS data from the public archive. We reduce the data using the Science Analysis Software, SAS (ver.18). We first run the rgsproc command to create the event lists. Then, we filter the RGS event lists for flaring particle background using the default value of 0.2 counts/sec threshold. We exclude the bad pixels using keepcool=no in the SAS task rgsproc. In bright sources, some areas of the grating data may be affected by pile-up which can change the shape of the spectrum. To avoid the pile-up we ignore the region of the spectra below 19 Å. Moreover, when the spectral shape of a certain source does not vary through different epochs and the spectra can be superimposed, we combine the first-order spectra using the SAS command rgscombine. This allows us to obtain a single spectrum with higher signal-to-noise ratio.

\footnote{1http://nxsa.esac.esa.int/nxsa-web/}
4.3.2 Chandra

The Chandra observations used in this work were downloaded from the Transmission Grating Catalogue\(^2\) (TGCat, Huenemoerder et al. 2011). For each observation, we combine the positive and negative orders of dispersion using the X-ray data analysis software, CIAO (version 4.11, Fruscione et al. 2006). Depending on the availability of the data, we use observations taken in either timing mode (TE) or continuous clocking (CC) mode. In bright sources, to avoid pile-up we ignore the region of the spectra below 10 Å. Moreover, if the persistent emission of a certain source is steady, we combine the different observations using the CIAO tool combine_grating_spectra. The Chandra data used here can be found in Table C.2.

4.4 Spectral fitting of the ISM

4.4.1 The two-edge fit

In this work, we fit simultaneously the O K- and Fe L-edges. For our modelling we use the software SPEctral X-ray and UV modelling and analysis, SPEX, version 3.06.01\(^3\) (Kaastra et al. 1996; Kaastra et al. 2018). We fit the Chandra, MEG data in the range of 10-19 Å and the XMM-Newton spectrum between 19-35 Å. The XMM-Newton and Chandra data of each source were obtained at different epochs and therefore the continuum shape might be different. To take into account the continuum variability we use the sectors option in SPEX. Each dataset is allocated to a specific sector and the continuum parameters can vary freely. Because we use a narrow energy band for each observation, the continuum shape cannot be fitted with physical models. For this reason, we use a phenomenological power law (\texttt{pow} in SPEX) and a black body component (\texttt{bb}) that best describes our continuum in this energy range.

The data are binned by a factor of 3. We adopt C-statistics ($C_{\text{stat}}$) to evaluate the goodness of our fit (Cash 1979, Kaastra 2017). Also, in our analysis we adopt proto-Solar abundance units from Lodders & Palme (2009). A step-by-step description of our spectral fitting procedure is presented in the section below.

4.4.2 Fitting procedure

In order to model the gas and dust features, we follow a similar fitting procedure for all the sources presented in Table C.1.

\(^2\)http://tgcat.mit.edu/tgSearch.php?t=N
\(^3\)http://doi.org/10.5281/zenodo.2419563
The multi-phase gas modelling

To characterize the neutral galactic absorption, we adopt the multiplicative component, hot model of SPEX (de Plaa et al. 2004). For a given temperature and set of abundances, the model calculates the ionisation balance and then determines all the ionic column densities by scaling to the prescribed total hydrogen column density. At low temperatures (∼ 0.001 eV) it represents the neutral gas. The free parameters here are the hydrogen column density ($N_H$) and the temperature ($kT$) as well as the relative abundance of oxygen, iron, silicon and magnesium.

Two additional hot models have been used in order to take into account the weakly and mildly ionised gas. In this way, we probe the different ISM phases along the line of sight of each source. The column densities and temperatures of the hot components derived from our spectral fitting are listed in Table 4.1. The first component (hot#1) refers to the neutral gas and represents the bulk of the material in all lines of sight. The second and third components (hot#1 & hot#2) account for the mildly ionised gas (O$_{II}$ − O$_{V}$).

We further take into account the absorption from the hot gas (O$_{VI}$ − O$_{VIII}$) using the slab model in SPEX. It calculates absorption by a slab of optically-thin gas, where the column density of ions are fitted individually and are independent of each other. For GX9+9 and SwiftJ1910.2-0546 the hot gas has been modeled using the 3rd hot component instead of a slab. Therefore the temperature of hot#3 for these two sources is higher than for the other sources.

The dust modelling

In addition to the gas components, we take into account the dust contribution by adding the amol model of SPEX. This model calculates the transmission of a dust component and the free parameter is the column density. Here, we use the recently implemented dust extinction models for the oxygen K-edge presented in Paper I. The models were calculated from accurate laboratory measurements of interstellar dust analogues assuming a Mathis-Rumpl-Nordsieck dust size distribution (MRN, Mathis et al. 1977). For the iron L-edges we use the models calculated in Chapter 3, computed from the same laboratory measurements. In Table 4.2, we summarize the dust models used in this work and we specify their chemical formula and crystallinity.

The amol model allows us to test four different dust compounds at a given fitting run. Following the method presented in Costantini et al. (2012), we test all the possible combinations among the 13 samples assuming that the dust mixture can be described with at most 4 components. We obtain 715 different models to fit for each source.
Table 4.1: Best fit parameters of the ISM gas-phase components.

<table>
<thead>
<tr>
<th>Source</th>
<th>hot # 1</th>
<th>hot # 2</th>
<th>hot # 3</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$N_H$</td>
<td>$kT$</td>
<td></td>
</tr>
<tr>
<td>Cygnus X–2</td>
<td>1.90 ± 0.04</td>
<td>0.047 ± 0.005</td>
<td>0.030 ± 0.005</td>
</tr>
<tr>
<td></td>
<td>0.001</td>
<td>2.6 ± 0.6</td>
<td>14.8 ± 0.1</td>
</tr>
<tr>
<td>4U 1820–30</td>
<td>1.8 ± 0.1</td>
<td>0.08 ± 0.01</td>
<td>0.023 ± 0.005</td>
</tr>
<tr>
<td></td>
<td>0.001</td>
<td>3.3 ± 0.3</td>
<td>14.4 ± 1.1</td>
</tr>
<tr>
<td>4U 1636–536</td>
<td>4.20 ± 0.04</td>
<td>0.9 ± 0.1</td>
<td>0.09 ± 0.03</td>
</tr>
<tr>
<td></td>
<td>0.001</td>
<td>0.17 ± 0.06</td>
<td>12.1 ± 0.1</td>
</tr>
<tr>
<td>4U 1735–44</td>
<td>2.7 ± 0.1</td>
<td>0.20 ± 0.04</td>
<td>0.07 ± 0.02</td>
</tr>
<tr>
<td></td>
<td>0.001</td>
<td>1.3 ± 0.2</td>
<td>10.6 ± 0.1</td>
</tr>
<tr>
<td>GX 9+9</td>
<td>2.1 ± 0.1</td>
<td>0.10 ± 0.02</td>
<td>0.027 ± 0.005</td>
</tr>
<tr>
<td></td>
<td>0.001</td>
<td>2.6 ± 0.8</td>
<td>210 ± 23</td>
</tr>
<tr>
<td>Ser X–1</td>
<td>5.5 ± 0.1</td>
<td>0.4 ± 0.1</td>
<td>0.12 ± 0.05</td>
</tr>
<tr>
<td></td>
<td>0.001</td>
<td>2.8 ± 0.4</td>
<td>14 ± 1</td>
</tr>
<tr>
<td>SWIFT J1910.2–0546</td>
<td>3.25 ± 0.05</td>
<td>0.03 ± 0.01</td>
<td>0.020 ± 0.005</td>
</tr>
<tr>
<td></td>
<td>0.001</td>
<td>13 ± 1</td>
<td>145 ± 10</td>
</tr>
<tr>
<td>XTE J1817–330</td>
<td>1.50 ± 0.01</td>
<td>0.09 ± 0.01</td>
<td>0.03 ± 0.01</td>
</tr>
<tr>
<td></td>
<td>0.001</td>
<td>3.1 ± 0.6</td>
<td>11 ± 2</td>
</tr>
</tbody>
</table>

The dust mixture that represents our data best presents the minimum C-statistic value. In Figures 4.2 and 4.3 we present, for all the sources, the best fit in the oxygen K- and iron L-edges. In Table 4.3 we list the dust mixture of the best fit with the relative column densities. In Figure 4.4 we present the best fit for a selected source (SWIFT J1910.2–0546) in detail. In the bottom panel we show the transmission of gas and dust components used in the fit. It is clear that the Fe L-edge shape is dominated by the dust absorption, while in the oxygen the dust covers a broad region around the edge.

Following the methodology used in Paper I and in Rogantini et al. (2020), we evaluate the best fit among the various dust mixtures using the Akaike Information Criterion (AIC, Akaike 1974). AIC provides a robust and fast way to select the models that are statistically similar to the best fit. This method allows a quick comparison of the candidate’s models by comparing the C-statistic value of every fit with the best one. We calculate the AIC difference ($\Delta$AIC) over all candidate models with respect to the model that has the lowest AIC value. Models with $\Delta$AIC < 2 are considered...
4.5 Discussion

4.5.1 Dust mineralogy and crystallinity

In Figures 4.5 and 4.6 we present the relative fraction of column density for each dust compound, considering models with $\Delta$AIC < 2. Our analysis of the 8 X-ray binaries shows that the Mg-rich amorphous pyroxene ($\text{Mg}_{0.75}\text{Fe}_{0.25}\text{SiO}_3$) is the dominant comp-

The samples 2,5,11 are natural and 8,10,12 are commercial products. Samples 1,3,4,6,7,9 are instead synthesized in the laboratories at the Astrophysikalisches Institut, Universitats-Stenwarte (AIU), and Osaka University. We adopted the metallic iron presented by Lee 2010.

comparable and can fit equally well the spectrum, while models with $\Delta$AIC > 10 can be ruled out (Burnham & Anderson 2002). In Figures 4.5 and 4.6 we present the relative fraction of the dust compounds using the AIC criteria. In particular, in the bar chart we show the results for the models with $\Delta$AIC < 2. It includes all the fits (about 60 on average) with similar significance compared to the best fit. The errors on the bar charts have been considered by calculating the variance of the column density of the compound corresponding to each bar.

### Table 4.2: List of dust samples.

<table>
<thead>
<tr>
<th>#</th>
<th>Compound</th>
<th>Chemical Formula</th>
<th>Form</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Olivine</td>
<td>MgFeSiO$_4$</td>
<td>amorphous</td>
</tr>
<tr>
<td>2</td>
<td>Olivine</td>
<td>Mg$<em>{1.56}$Fe$</em>{0.4}$Si$_{0.91}$O$_4$</td>
<td>crystalline</td>
</tr>
<tr>
<td>3</td>
<td>En60fe40</td>
<td>Mg$<em>{0.6}$Fe$</em>{0.4}$SiO$_3$</td>
<td>amorphous</td>
</tr>
<tr>
<td>4</td>
<td>En60fe40</td>
<td>Mg$<em>{0.6}$Fe$</em>{0.4}$SiO$_3$</td>
<td>crystalline</td>
</tr>
<tr>
<td>5</td>
<td>Enstatite</td>
<td>MgSiO$_3$</td>
<td>crystalline</td>
</tr>
<tr>
<td>6</td>
<td>Enstatite</td>
<td>MgSiO$_3$</td>
<td>amorphous</td>
</tr>
<tr>
<td>7</td>
<td>Fayalite</td>
<td>Fe$_2$SiO$_4$</td>
<td>crystalline</td>
</tr>
<tr>
<td>8</td>
<td>Forsterite</td>
<td>Mg$_2$SiO$_4$</td>
<td>crystalline</td>
</tr>
<tr>
<td>9</td>
<td>En75fe25</td>
<td>Mg$<em>{0.75}$Fe$</em>{0.25}$SiO$_3$</td>
<td>amorphous</td>
</tr>
<tr>
<td>10</td>
<td>Magnetite</td>
<td>Fe$_3$O$_4$</td>
<td>crystalline</td>
</tr>
<tr>
<td>11</td>
<td>Troilite</td>
<td>FeS</td>
<td>crystalline</td>
</tr>
<tr>
<td>12</td>
<td>Pyrit Peru</td>
<td>FeS$_2$</td>
<td>crystalline</td>
</tr>
<tr>
<td>13</td>
<td>Metallic iron</td>
<td>Fe</td>
<td>-</td>
</tr>
</tbody>
</table>
The symbol α refers to amorphous compounds and c to crystalline. In the last row we present the \( C^{\text{stat}} \) of the best fit in every source compared to the degrees of freedom (f.o.d.).

<table>
<thead>
<tr>
<th>Compound</th>
<th>Dust Compound</th>
<th>C^{\text{stat}}/f.o.d.</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.01/0611</td>
<td>72/1911</td>
<td>1518/1056</td>
</tr>
<tr>
<td>0.01/0611</td>
<td>72/1911</td>
<td>2970/2282</td>
</tr>
<tr>
<td>0.01/0611</td>
<td>72/1911</td>
<td>1933/1591</td>
</tr>
<tr>
<td>0.01/0611</td>
<td>72/1911</td>
<td>1590/1321</td>
</tr>
<tr>
<td>0.01/0611</td>
<td>72/1911</td>
<td>2099/1667</td>
</tr>
<tr>
<td>0.01/0611</td>
<td>72/1911</td>
<td>1012/787</td>
</tr>
<tr>
<td>0.01/0611</td>
<td>72/1911</td>
<td>2122/1837</td>
</tr>
<tr>
<td>0.01/0611</td>
<td>72/1911</td>
<td>1190/1002</td>
</tr>
</tbody>
</table>

\( \text{f.o.d.} \)
4.5 Discussion

Figure 4.2: Best fit in the O K and Fe L-edges.
Figure 4.3: Best fit in the O K and Fe L-edges.
Figure 4.4: Best fit in the O K and Fe L-edges for SWIFT J1910.2–0546 and the relative transmission for the gas and dust components. The transmission of the gas has been multiplied by a factor of 2.5 and 4.5 for iron and oxygen respectively for display purposes.

pound in most of the sources, with amorphous olivine (MgFeSiO₄) to be the second dominant. Only in the line of sight towards GX9+9, amorphous olivine seems to be the dominant compound. On average we find that ~70% of the total amount of dust in the different line of sights is amorphous pyroxene, while about 25% is amorphous olivine.

This result is consistent with previous studies in the infrared band. Min et al. 2007 studied the spectral shape of 10 µm interstellar extinction feature towards the Galactic center and they find that interstellar silicates are magnesium rich and that the stoichiometry lies between pyroxene and olivine types. Also, they argue that the high magnesium content of amorphous silicates provides an explanation for the relatively high amount of magnesium rich silicates found in cometary and circumstellar grains. Other infrared studies have also showed that the silicate feature can be modeled with a mixture of Mg-rich olivines and pyroxenes (Molster et al. 2002, Chiar & Tielens 2006).

Previous X-ray studies of Rogantini et al. (2020) and Zeegers et al. (2019) in the silicon and magnesium K-edges showed that amorphous olivine represents most of the dust in the dense environments of the ISM (~10²² cm⁻²). The authors used the same dust samples as used in this study. Here, we probe more diffuse regions of the ISM (~10²¹ cm⁻²) and different lines of sight and therefore variations in the results are
Demyk et al. (2001) performed irradiation experiments exposing crystalline olivine and pyroxene materials to high energy ions. They found that under He$^+$ irradiation the olivine loses Mg and O and therefore the silicate composition is evolving from olivine to pyroxene. Our lines of sight probe regions with typical gas densities that are an order of magnetite lower than those of Rogantini et al. (2020) and Zeegers et al. 2019. It is possible that the degree of processing of silicates along these different sightlines differs. Our sight lines could represent a population of dust that is losing oxygen and magnesium atoms to the gas phase, which could lead to a more pyroxene like stoichiometry. In other, higher density environments this process may be less efficient, or accretion of atoms to dust grains may become important. From our analysis we find an upper limit on the crystallinity of 20%. Our values are much higher than the ones observed in the infrared. The shape of the $\sim 9\mu$m and $\sim 18\mu$m features suggest that the upper limit of crystallinity is constrained to 2.2% (Kemper et al. 2004). Rogantini et al. (2020) and Zeegers et al. (2019) studied the crystallinity of interstellar dust from the X-ray band and found higher values than those revealed from the infrared, $\sim 0 - 30\%$. This discrepancy between the infrared and the X-ray band could be attributed to the nature of X-rays. X-rays are sensitive to a short range order of atoms and therefore we may observe crystallinity in partly glassy materials (for details see Rogantini et al. 2020, Zeegers et al. 2019).

### 4.5.2 Abundances and depletions

In Table 4.4 we present the abundances and depletions of oxygen and iron towards different lines of sight along the Galactic plane. In the first column, we list the sources used in this study. In the second ($N_{gas}$) and third column ($N_{dust}$), we list the column density of the neutral gas (O1) and dust respectively. In the next two columns we show the abundances of the neutral gas and dust with respect to hydrogen. Column 6 shows the total abundance of gas and dust with respect to proto-Solar abundances of Lodders & Palme 2009 and in the last column we present the depletion of each element into dust i.e. the fraction of oxygen and iron that has been locked up in dust grains with respect to the total.

We find that about (10-25)% of the neutral oxygen is depleted into dust. This result is consistent with previous X-ray studies in the oxygen K-edge (Costantini et al. 2012, Pinto et al. 2013). Iron is heavily depleted into dust at a rate of $> 90\%$.

Moreover, we find that oxygen in most line of sights is over-abundant compared to the proto-solar value of Lodders & Palme (2009). We find that that total abundance of oxygen is about 0.9-1.3 times the Solar value, depending on the line of sight. Surprisingly, iron seems to be under-abundant compared to the Solar value. This can be attributed to the fact that we find a very low amount of metallic iron, as described Section 4.5.4 and in Chapter 3. Additionally, in the fits here we are missing
4.5 Discussion

Figure 4.5: Relative fraction of column density for each dust compound. The fraction has been calculated considering models with $\Delta AIC < 2$. The symbol $a$ refers to amorphous compounds and $c$ to crystalline.
**Figure 4.6:** Relative fraction of column density for each dust compound. The fraction has been calculated considering models with $\Delta AIC < 2$. The symbol $a$ refers to amorphous compounds and $c$ to crystalline.
the contribution of the large grains which could possibly improve our fits and increase
the abundance of iron in the results (see Zhukovska et al. 2018 and Chapter 3).

4.5.3 The oxygen budget

A long standing problem is the oxygen budget in the ISM. It has been found that in
dense environments of the ISM \( (n_H > 7 \text{ cm}^{-3}) \), oxygen is missing from the gas phase
at a rate that cannot be explained only with its depletion into dust and therefore ad-
tional reservoirs should be found (Jenkins 2009, Whittet 2010). In our work we find
on average that 10-25 % of oxygen is depleted into dust. Our values are consistent
with Poteet et al. (2015). They studied the IR absorption spectra in the line of sight
of Zeta Oph and found that about 21% of oxygen is in dust. According to the authors
an amount of oxygen is still missing from the gas phase. A substantial fraction of
interstellar oxygen could reside in other reservoirs, such as ices (\( \text{H}_2\text{O} \)) or CO.

In our study, the abundances of oxygen (i.e. both in gas and dust) along the different
lines of sight are around Solar. We measure total abundances of oxygen between
0.9-1.3 times the Solar value compared to Lodders & Palme (2009). Given the typical
distances to our sources of 3-8 kpc (Table C.1), we can derive an average hydrogen
density of \( \sim 0.1 \text{ cm}^{-3} \). This number should be used with caution however, because
we have no direct information about the spatial distribution of interstellar gas along
our sightlines. Nevertheless, it is interesting to compare this value to the expected
partitioning between gas and solids in Whittet (2010). They studied the oxygen reser-
voirs in a wide range of interstellar environments. They found that the oxygen budget
problem start to be significant for hydrogen densities above \( 7 \text{ cm}^{-3} \). For densities
below \( 0.1 \text{ cm}^{-3} \) the oxygen reservoir does not appear to be a problem. Our result
confirms this scenario and therefore we conclude that in this study we do not need
an additional reservoir of oxygen (such as \( \text{H}_2\text{O} \)).

Moreover, the detection of dust absorption in the oxygen K-edge has been a puzzle
for the last few years. Gatuzz et al. (2016) studied the oxygen K-edge using only gas-
phase oxygen. They find under-abundance of oxygen towards most of their sightlines.
In this study, we account also for dust and we result into Solar abundances of oxygen,
or above. Our result is consistent with previous studies of Costantini et al. (2012)
and Pinto et al. (2013), where they considered both gaseous and solid phase oxygen.
We therefore conclude that the oxygen K-edge can be best described by using both
gas and dust models.

4.5.4 Where is the missing iron?

About 90% of the total amount of iron is missing from the gas phase and is believed
to be locked up in dust grains. In this work we find that more that 90% of the total
### Table 4.4: Oxygen and iron column densities, abundances and depletions.

<table>
<thead>
<tr>
<th>Source</th>
<th>Oxygen</th>
<th>Iron</th>
<th>O/H</th>
<th>Fe/H</th>
<th>O/Fe</th>
<th>N/Fe</th>
</tr>
</thead>
<tbody>
<tr>
<td>XTE J1817-330</td>
<td>0.0 ± 0.2</td>
<td>0.8 ± 0.7</td>
<td>0.4 ± 0.7</td>
<td>0.0 ± 0.02</td>
<td>2.4 ± 0.1</td>
<td>0.6 ± 0.2</td>
</tr>
<tr>
<td>SWIFT J1910.2-0546</td>
<td>0.0 ± 0.2</td>
<td>0.4 ± 0.7</td>
<td>0.0 ± 0.02</td>
<td>2.4 ± 0.1</td>
<td>0.6 ± 0.2</td>
<td></td>
</tr>
<tr>
<td>SETI X-1</td>
<td>0.0 ± 0.2</td>
<td>0.4 ± 0.7</td>
<td>0.0 ± 0.02</td>
<td>2.4 ± 0.1</td>
<td>0.6 ± 0.2</td>
<td></td>
</tr>
<tr>
<td>GX 9+9</td>
<td>0.0 ± 0.2</td>
<td>0.4 ± 0.7</td>
<td>0.0 ± 0.02</td>
<td>2.4 ± 0.1</td>
<td>0.6 ± 0.2</td>
<td></td>
</tr>
<tr>
<td>4U 1636-536</td>
<td>0.0 ± 0.2</td>
<td>0.4 ± 0.7</td>
<td>0.0 ± 0.02</td>
<td>2.4 ± 0.1</td>
<td>0.6 ± 0.2</td>
<td></td>
</tr>
<tr>
<td>4U 1820-30</td>
<td>0.0 ± 0.2</td>
<td>0.4 ± 0.7</td>
<td>0.0 ± 0.02</td>
<td>2.4 ± 0.1</td>
<td>0.6 ± 0.2</td>
<td></td>
</tr>
<tr>
<td>Cygnus X-2</td>
<td>0.0 ± 0.2</td>
<td>0.4 ± 0.7</td>
<td>0.0 ± 0.02</td>
<td>2.4 ± 0.1</td>
<td>0.6 ± 0.2</td>
<td></td>
</tr>
</tbody>
</table>

Note: The table provides column densities of oxygen and iron in interstellar dust as seen by XMM, Chandra, and Swift. The O/H, Fe/H, and O/Fe ratios correspond to the total column density of neutral gas and dust, respectively, for the X element (oxygen or iron). N and N correspond to the total column density of neutral gas and dust (with respect to hydrogen).
iron has been depleted into dust. It has been discussed in the literature that more than 65% of the iron is injected into the ISM in gaseous form. Therefore most of its depletion should take place in the ISM (Dwek 2016). Additional reservoirs of iron other than silicates have been extensively discussed in the literature (Poteet et al. 2015). Ferromagnetic inclusions (Fe$_3$O$_4$) could be possible iron carriers. In particular, ferromagnetic inclusions, such as magnetite composition, in dust grains have been discussed in the view of grain alignment due to their ferromagnetic properties (Hoang & Lazarian 2016).

Moreover, Zhukovska et al. (2018) demonstrated that silicates constitute 70% of interstellar iron. In this study, we find that about > 90% of iron is locked up in silicates and less than 1% in other inclusions, such as metallic iron. We also find a very low amount of iron sulfides, less than 1%. We would like to highlight here that the metallic Fe model has been taken from the literature and therefore the differences in the resolution or the energy calibration of this model compared to our models could possibly have an effect on this results. We discuss this possibility in detail in Chapter 3.

4.5.5 Advantages of the two-edge fit

In this work we performed a simultaneous fit of the oxygen K and iron L edges to constrain the dust absorption in these two edges. In Paper I, we fitted the XMM-Newton spectrum of Cygnus X-2 only in the oxygen K-edge. By studying the two edges simultaneously we are able to break degeneracies that might be present from the fit of a single edge and constrain the dust properties. In Paper I we were able to disentangle the dust and gas contribution in the O K-edge but we could not distinguish among the different dust species. Here, by fitting the two edges we are able to constrain the dust chemical composition.

In Paper I we find that (7 ± 1)% of oxygen is in dust while here we find a higher number of 21 ± 2%. This is consistent with the previous works of Costantini et al. 2012 and Pinto et al. 2013. We therefore conclude that in order to understand the contribution of dust in the O K-edge the simultaneous fit of the Fe L-edges is essential.

4.6 Conclusions

In this work we simultaneously studied the O K-and Fe L-edges using XMM-Newton and Chandra observations. We model the gas and dust features in the X-ray absorption spectrum of a sample of 8 bright X-ray binaries near or along the Galactic center. For the dust modelling we use the calculated extinction models presented in Psaradaki et al. (2020) and Chapter 3. The dust samples include silicates, oxides and iron sulfides. Our results are the following.
• Mg-rich amorphous pyroxene dust composition (Mg$_{0.75}$Fe$_{0.25}$SiO$_3$) represents most of the dust along the sightlines probed in this study. The second most dominant compound is the amorphous olivine (MgFeSiO$_4$).

• Iron is heavily depleted into dust, more than 90% of the iron is in the form of dust grains.

• The oxygen depletion is about 10-25 %, depending on the line of sight.

• The simultaneous fit of the O K- and Fe L-edges can give us insights into both the dust depletions and the chemical composition of grains in the diffuse regions of the ISM.

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