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

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Abstract

Interstellar dust is a small but important fraction of the total interstellar medium. Among the elements constituting dust, the physical and chemical characteristics of iron are particularly difficult to determine. We present the application to astronomical data, namely the bright X-ray source Cyg X-1, of newly acquired experimental models of the iron L-edges, located at \( \sim 0.7 \) keV in the X-ray spectrum. Both Chandra and XMM-Newton high energy resolution spectra are used for the global modeling of the Fe L and O K-edges. The experimental data include silicates with varying Mg:Fe ratios and different degrees of crystallinity. Metallic iron, sulphates and oxides are also part of the suit of models. The analysis takes into account the contribution of both the cold and ionized phases along this specific line of sight. The line of sight of Cyg X-1 is characterized by a multi-temperature gas as well as identifiable dust. Oxygen and iron are \( \sim 16 \) and 86\% depleted, respectively. The abundance of oxygen has been found to be slightly supersolar (1.17), while surprisingly the abundance of iron is about 0.44 the solar value. This discrepancy might be mitigated when the role of large grains is taken into account in the fit. The chemistry of the dust is dominated by forsterite (\( \text{Mg}_2\text{SiO}_4 \)), while amorphous olivine (\( \text{FeMgSiO}_4 \)) provide and acceptable
fit to the iron L-edges. The role of crystallinity is difficult to determine in this study. The role of metallic iron in this, and previous literature analysis, is also discussed.
3.1 Introduction

Interstellar dust (ID) constitutes around 1% of the total content of the interstellar medium (ISM, Spitzer 1978). The majority of the ID mass is taken by five elements: C, O, Mg, Si and Fe (Mathis et al. 1977). While the first four owe their origin mainly to asymptotic giant branch (AGB) stars (e.g. Gail et al. 2009), iron is produced in the aftermath of supernova (e.g. Thielemann et al. 2018 and references therein) and hypernovae explosions (Grimmett et al. 2018). Supernova type Ia should provide most of the iron that should eventually condense in dust (Dwek 2016). A significant contribution should come also from core-collapse supernova (up to 30% of the total iron, Matteucci & Greggio 1986, Kobayashi et al. 2020).

The majority of the produced iron is included in interstellar particles (Jenkins 2009), however, iron inclusion in dust grains is still an open issue. Iron has been associated with silicates (Draine 2003) either in the form of olivines, (Fe,Mg)_{2}SiO_{4}, or pyroxenes (Fe,Mg)SiO_{3}. Following the condensing temperature scale in the AGB stars environment, in the hotter innermost regions the production of iron poor silicates is promoted, while in colder regions (T<600K) iron inclusion in amorphous silicates is expected (Gail & Hoppe 2010, Henning 2010). However, silicates alone are not sufficient to explain the large iron inclusion into ID. With respect to the other two main constituents of silicates, magnesium and silicon, iron is consistently both more- and faster-included into grains as a function of increasing density in the ISM (Jenkins 2009). Theoretical studies (e.g. Zhukovska et al. 2018) point out that around 30% of the iron in solid should take the form of nano metallic particles, while the rest should be accounted for by silicates. These theoretical predictions are starting to be confirmed by, for instance, in situ measurements of loose iron particles (using Stardust data, e.g. Altobelli et al. 2018). Observations along e.g. diffuse sight lines (ζ Oph, Poteet et al. 2015) and AGB stars (Tamanai et al. 2017) reinforce the idea that silicates alone cannot account for the iron depletion, leaving room to iron inclusion in other forms, like metallic iron. However, experimental studies (using microgravity experiments, Kimura et al. 2017) highlight the extreme ineffectiveness of the formation of metallic iron particles, both in gaseous winds of AGB stars and in Fe-rich supernova ejecta. Moreover, once dust particles are outside the circumstellar environment, they may be subject to further reprocessing (Jones et al. 1990). On a time scale of $10^7 - 10^8$ yr, pure iron would be likely transformed into iron oxide (Fe$_3$O$_4$) or iron sulphide (FeS).

The X-ray band (0.1–10 keV) offers a privileged point of view on the iron content in the ISM. In addition to the photoelectric absorption K edges of O, Mg and Si, the X-ray band hosts the Fe K edge at 7.1 keV and the L$_3$ and L$_2$ edges at $\sim$0.7 keV. While the current X-ray instruments have limited sensitivity and resolution to study the Fe K-edge (Rogantini et al. 2018), the iron L complex has been studied using both the XMM-Newton and Chandra X-ray observatory. The ability to interpret the
X-ray spectra in this band went hand-in-hand with our increasing knowledge of the experimental data to compare the astronomical data with. Indeed, early studies could rely only sparse and incomplete information coming from the literature in the field of solid-state physics (Pinto et al. 2010, 2013, Costantini et al. 2012, Valentini & Smith 2013). These works consistently pointed out the large depletion of iron, together with a relatively modest depletion of oxygen, in agreement with what reported at longer wavelengths. Sets of measurements specifically devoted to the iron L edges using compounds of astronomical interest were presented in Lee et al. (2009, hereafter L09), and Westphal et al. (2019, hereafter W19). Both works applied their measurements to the Chandra data of the bright X-ray source Cyg X-1, finding in both cases that a mixture of compounds were necessary to obtain a good modeling of the Fe L edges. However, while L09 reports a predominance of iron-rich silicates and iron oxide, the second experiment reports a best fit with amorphous silicates, possibly with large particles inclusion, and metallic iron (W19).

In this paper we make use of both Chandra and XMM-Newton data of Cyg X-1, using a newly obtained set of measurements of about twenty samples in total (12 in this paper), on all the edges interesting for this study: O (Psaradaki et al. 2020), Mg (Rogantini et al. 2019), Si, (Zeegers et al. 2019), Al (Costantini et al. 2019) and the Fe K edge (Rogantini et al. 2018). In this paper we focus on the spectral region including oxygen and iron (0.3-0.8 keV, equivalent to 16–35Å).

### 3.1.1 Cyg X-1 as a test case

Cyg X-1 is a high mass X-ray binary (HMXB), constituted by a black hole candidate and a blue supergiant star. The orbital period is about 5.6 days (Brocksopp et al. 1999) with a nearly circular orbit (Bolton 1975). The binary system is located at Galactic coordinates $l = 071.33$ and $b = +03.06$. We adopt a distance of 1.86 kpc (Reid et al. 2011). Ever since its discovery, Cyg X-1 has been the target of extensive X-ray studies, by virtue of its variability, from hours- to years-times scale (Grinberg et al. 2015 and references therein). From RXTE long term observations it has been established that the source spends about 10–34% of the time in a high-soft state (Wilms et al. 2006), when the soft X-ray spectrum dominates over the harder spectrum, following the spectral ‘states’ pattern described in Remillard & McClintock (2006).

Associated to this source, variable, multi-ionization, absorption components have been reported. Cold absorption, correlated with specific positions in the orbital phase, has been reported when the source is in a low-hard state (Grinberg et al. 2015). The observed column density of this cold gas may vary dramatically in the range $10^{22}$–$10^{23}$ cm$^{-2}$ (e.g. Balucinska-Church et al. 2000). This extreme absorption is consistent to be caused by clumpiness in the wind of the companion star (Sundqvist &
Owocki 2013). During the soft-high state this extreme absorption by cold gas has never been observed so far (Grinberg et al. 2015). The black hole accretion is regulated by the outflowing wind of the giant companion. Absorption features from highly ionized ions, H-like Ne, Mg, Si and numerous transitions of iron (Fe\textsc{XVIII}–Fe\textsc{XXVI}), have been detected in all spectral states of the source. The complex absorption reveals a multi-zone absorber, where the innermost part is a more collimated wind, with higher outflow velocity than the outer, non-focused components (Miller et al. 2005, Hanke et al. 2009). The gas higher ionization observed during the high/soft state is consistent to be a response to the increased ionizing flux, both in the UV (Gies et al. 2008) and in the X-ray band (Feng et al. 2003). An important spectral feature in this, and other similar Galactic sources is absorption from ionized gas in the ISM itself (Yao & Wang 2005). Absorption associated with Ne\textsc{IX}, O\textsc{VII} and O\textsc{VIII} has been attributed to hot gas with temperature of the order of $10^6$ K (e.g. Rogantini et al. 2021). Lower ionization ions, especially from oxygen and iron, are indicative of a range of temperatures for different gas components along the line sight of Cyg X-1, from cold to mildly ionized gas (Schulz et al. 2002, Juett 2004, Juett et al. 2006, Gatuzz et al. 2016).

This paper is organized as follows. In Sect. 3.2.3 we present the laboratory measurements of the Fe L edges. In Sect. 3.3 the astronomical observations and data reduction are shown. In Sect. 3.4 we focus on the modeling of the absorption features due to gas and dust. In Sect. 3.5 we discuss our findings. The conclusions are reported in Sect. 3.6.

### 3.2 Laboratory data

The laboratory measurements of the iron L-edges has been carried out using the the Titan Cubed Themis 60-300 electron microscope, operated in scanning transmission mode. This facility is located at the University of Cadiz, Spain. The instrument provides an energy resolution down to 0.1 eV over an energy range $\sim$300–800 eV. For this experiment we reached, in about 0.05 seconds for each pixel, an energy resolution of 0.25 eV in the energy range of interest to cover both the O K-edge (Psaradaki et al. 2020), the Fe L\textsubscript{3} and L\textsubscript{2} edges. The samples (Sect. 3.2.1) were positioned on a carbon grid. Every region of interest was scanned, pixel by pixel, in an imaging spectroscopy-mode, that allows to make spacial selection within the region of interest of the sample.

#### 3.2.1 The materials

We present the samples used in this paper in Table 3.1. The origin of the materials is meteoritic or otherwise natural (crystalline olivine, crystalline enstatite and troilite), or simply commercially available (forsterite, magnetite and pyrite). The rest of the
Table 3.1: 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 compound name follow the convention set in previous papers of the series (e.g. Rogantini et al. 2019).

The materials reported in the Table are synthetized at the Astrophysikalisches Institut, Universitäts-Stenwarte (AIU), and Osaka University. Metallic iron is the only compound in the list whose data were taken from the literature (Kortright & Kim 2000 and implemented in L09). These samples were selected as representatives of the ID composition in a large experimental campaign aimed at measuring all the relevant absorption edges of each compound. This allows a consistent approach in the modeling of multi-featured astronomical spectra (de Vries & Costantini 2009, Zeegers et al. 2017, 2019).

3.2.2 The EELS experiment

The energy-electron-loss spectroscopy is a technique that allows to study how an initially monochromatic electron beam interacts with a material (Egerton 2011). The incoming electrons will scatter via Coulomb forces with the constituents of the target atoms. Elastic scattering will happen when the fast electron interacts and is deflected by the positively-charged nucleus. The majority of those electrons however will be scattered where the nucleus influence is weaker, either in relatively distant regions from the nucleus or regions that are shielded by other electrons. The electron will be deflected at relatively small angles and therefore suffer a non appreciable energy
3.2 Laboratory data

Figure 3.1: Electron energy loss spectrum of a silicate material as observed by the Titan Cubed Themis 60-300 microscope. The most important features are highlighted: the zero-loss peak, which gathers all the events without energy exchange with the incoming beam; the plasmon peak, a broad feature that represents the interaction of the beam with outer-shell electrons. At higher energies the inner-shell electrons exchange energy with the beam, giving rise to features characteristic of the specimen composition.

loss in this process. Inelastic scattering will be instead experienced by the incoming electrons that interact with the electrons in the target. This generally results in an exchange of energy: the incoming beam will lose energy, while the atom will be left in an excited state. What is measured in the EELS is then the loss of energy experienced by the electrons in the beam after their interaction with the material. The transmitted electrons are then sorted according to their kinetic energy by a high-resolution spectrometer, showing a typical scattered intensity distribution that is proportional to the imaginary part of the negative inverse of the dielectric function (Schlemmer et al. 2014). Therefore the loss spectrum can be used to ultimately derive the extinction cross section of the material.

The total spectrum for one of our measurements is showed in Fig. 3.1, where the main features are highlighted. The first peak (zero-loss peak) represents the amount of undeflected electrons, as defined above. The second peak (plasmon peak) is instead the total of inelastic scattering interactions of the electron beam with the outer-shell electrons. With increasing energy, the beam electrons which were inelastically scattered by the inner-shell electrons are characterized by saw-tooth peaks, arising sharply at the ionization threshold of the specific atom.
3.2.3 The EELS data post-processing

We treated the raw data using first the HyperSpy (ver. 1.6.1) procedure, a general interactive program to analyse multidimensional datasets\(^1\). For each region of interest, we inspected the \(t/\ell\) ratio, where \(t\) is the thickness of the specimen and \(\ell\) is the mean free path for all inelastic scattering. We restricted our selection to \(t/\ell < 0.3\) (Egerton 2011). This ensures that the transmitted electrons do not suffer multiple scattering which would produce artefacts in the observed profile (Egerton 2011). For each compound we performed 6–9 measurements in different regions of interests. Our strict selection on \(t/\ell\) however lead to the discard to some (about < 20%) of the measurements, due to lack of sufficient "thin" area in the sample. After this selection, we averaged the remaining measurements to increase the signal to noise in the data. Subsequently, we corrected for the zero-loss peak position, that is the sum of all the events (elastically scattered) that did not suffer any energy loss during transmission (Fig. 3.1). We proceeded in subtracting the instrumental background. In the case of iron, also the curvature produced by the oxygen profile has been subtracted with this action. Last, we performed a principal component analysis (e.g de la Peña et al. 2011) as a control check on the homogeneity of the selected sample area (for details Psaradaki et al. 2020). Near the oxygen profile, an instrumental feature can be identified in almost all measurements. This is seen often in laboratory measurements and attributed to \(O_2\) liberated by the incident electron beam (Garvie 2010). This is identified as the \(1s - \pi^*\) transition of \(O_2\), whose energy is relatively well known. Most recent results report this feature at 530.92±0.06 eV (Leutenegger et al. 2020). However, for consistency with our oxygen analysis of the same experiment, (Psaradaki et al. 2020), we used the value 530.5 eV (Garvie 2010, Jiang & Spence 2006) as a reference to refine the absolute energy scale of the iron profiles.

3.2.4 Cross sections

Once the raw data have been post-processed taking into account the specifics of the experiment, the procedure that leads to the extinction cross section follows closely what already presented for the other measurements of this campaign (Zeegers et al. 2017, Rogantini et al. 2018, Rogantini et al. 2019, Psaradaki et al. 2020). The raw data have been simply transformed into a transmission profile \((T, \text{Fig. 3.2, top panel})\) and the pre- and post-edge were normalized to the profiles prescribed by the calculations in Henke et al. (1993). The depth of the transmission edges \(x\) has been chosen in order to mimic an optically thin ISM \((x = 0.01 \mu m)\). The goal is to obtain both the imaginary and real part of the refractive index index \(m = n + ik\) (Fig. 3.2, bottom panel). The \(\Im m(m)\) is provided by the above calculated transmittance via \(\alpha = 4\pi k/\lambda = \ln(T)/x\). Here \(\alpha\) is the attenuation coefficient, \(\lambda\) is the wavelength

\(^1\)https://hyperspy.org/
3.2 Laboratory data

**Figure 3.2:** *Top panel:* normalization of the experimental transmission (black line) to the pre- and post-edge calculated from the Henke tables (red line) for amorphous olivine. *Bottom panel:* calculation of the real ($n$, black solid line) and imaginary ($k$, red dashed line) part of the refractive index for amorphous olivine. The $k$ term has been multiplied x2 for a clearer visualization.
considered and $T$ is the transmittance (for a complete description, see Zeegers et al. 2017). The $\Re(e(m))$ term, representing the scattering part of the refractive index, can be obtained via the Kramers-Kronig relations (Kramers 1927; Kronig 1926) using the procedure presented in Watts (2014).

In order to calculate the cross sections for each compound, we used the Anomalous Diffraction Theory (ADT, Van de Hulst & Twersky 1957), which calculates the extinction of light that interacts with a material. This method is valid over the X-ray band (0.1–10 keV) and for grain sizes $\gtrsim 3 \times 10^{-3} \mu m$ at $\sim 700$ eV, where the Fe L edges are (Hoffman & Draine 2016). The size distribution of dust was chosen to follow the Mathis et al. (1977) prescription (hereafter MRN distribution). In this distribution the number of grains of a certain size $n(a)$, follow a powerlaw distribution

$$n = A \int_{a_-}^{a_+} a^{-\gamma} d(a),$$

where $a_+ = 0.25 \mu m$ and $a_- = 0.005 \mu m$ are the maximum and minimum grain size over which the integral is calculated and $\gamma = 3.5$.

The resulting cross sections are presented in Fig. 3.3. The profiles do not display sharp features, nor indication of substructures (van Aken et al. 1998). Their distinctive features are given by the edge energy (calibrated as described in Sec. 3.2.3) and the $L_3$ to $L_2$ ratio. For metallic iron, the only material for which we did not perform an experimental measurement, we calculated the extinction cross section starting from the iron-L profiles presented in L09.

Finally, these cross sections were implemented in the already existing SPEX (Kaastra et al. 1996) model (AMOL, Pinto et al. 2010). The extinction profiles are smoothly connected to the absorption cross section as a function of energy defined in (Verner et al. 1996) and already implemented in the program. The Fe L edges presented here complete the set of experimentally measured edges for a given compound. Therefore, if say the Fe L cross section of olivine is implemented in the AMOL model, the experimental edges of Mg K (Rogantini et al. 2019), Si K (Zeegers et al. 2017, 2019), O K (Psaradaki et al. 2020) and Fe K (Rogantini et al. 2018) of the same specimen are already in place allowing for a global modeling.

### 3.3 The astronomical data

Cyg X-1 has been extensively observed by both XMM-Newton and Chandra. As explained in Sect 3.1, this source is both exceptionally bright in every spectral state ($F_{(0.5-2keV)} \sim 0.6 - 1.8 \times 10^{-8}$ erg cm$^{-2}$ s$^{-1}$, this study) and inconstant in its spectral characteristics. It may change in flux, continuum shape and absorption. The measured neutral column density may vary of orders of magnitude (Grinberg et al. 2015) and an intrinsic ionized absorber may appear in the spectrum, depending on the epoch. It is therefore crucial to choose the observations when two basic requirements are met: (i) the source must be in a high/soft state, to ensure high signal-to-noise ratio in the absorption features. For this source in particular, it has been observed
that when in flaring state, the spectral modulations of absorption are no longer significantly correlated with orbital phase (Sect. 3.1 and Grinberg et al. 2015). (ii) The spectral characteristics should be optimized for the study of ISM. This means that the neutral column density must be consistent with the H\textsc{i} measurements along the Cyg X-1 line of sight ($N_{\text{H}} = 7.05 \times 10^{21}$ cm$^{-2}$ HI4PI Collaboration et al. 2016). We note that the intrinsic ionized absorber displays a high ionization parameter ($\xi > 3$, this study)$^2$, therefore its absorption lines will be mostly placed above 1 keV and they do not interfere with the ISM absorption features.

### 3.3.1 XMM-\textit{Newton} data reduction

Cyg X-1 has been extensively observed by XMM-\textit{Newton}-RGS (den Herder et al. 2001). All observations in the archive were first analysed, using the standard data reduction SAS tools (SAS ver. 19), in order to select for the above mentioned requirements. Then, all observations with high-instrumental background were discarded. In the remaining observations, short background flares intervals were also discarded. Cyg X-1 is a bright source in all spectral states, therefore the spectra may be affected by pileup. Pileup in grating spectra has the effect of transferring events from bright

\footnote{$\xi = L/nr^2$ is an indicator of how ionized a gas is. Here $L$ is the luminosity of the ionizing source, $n$ is the gas density and $r$ is the distance of the gas from the source.}
### Table 3.2: Observation log for the data used in this paper.

<table>
<thead>
<tr>
<th>ObsID</th>
<th>time</th>
<th>net exp. time</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>yyyy-mm-dd</td>
<td>ks</td>
</tr>
<tr>
<td>XMM1</td>
<td>0202401101</td>
<td>2004-10-06</td>
</tr>
<tr>
<td></td>
<td>0202401201</td>
<td>2004-10-08</td>
</tr>
<tr>
<td>XMM2</td>
<td>0202760301</td>
<td>2004-11-20</td>
</tr>
<tr>
<td></td>
<td>0202760401</td>
<td>2004-11-26</td>
</tr>
<tr>
<td></td>
<td>0202760501</td>
<td>2004-12-02</td>
</tr>
<tr>
<td>MEG</td>
<td>2741</td>
<td>2003-02-04</td>
</tr>
<tr>
<td></td>
<td>2742</td>
<td>2003-02-08</td>
</tr>
<tr>
<td></td>
<td>2743</td>
<td>2003-04-25</td>
</tr>
</tbody>
</table>

region of the lower order spectrum to higher orders. A way to recognize pile up is therefore to inspect when the ratio of the 1st and the 2nd order deviates from unity (Costantini et al. 2012). The second order starting energy is located at double the energy of the 1st order, therefore not all the RGS energy range can be covered. As pile up can severely distort the continuum, we did not include those energies that could hamper the fit. After this selection, we consider for the analysis only two sets of data, combining the RGS1 (which contain the oxygen region) data of observations taken close in time, which we label XMM1 and XMM2 in Table 3.2 respectively. In this Table we list the observation ID, the time of the observation and the net exposure time after background filtering. The energy ranges considered, restricted due to pile up, were 21–36 Å and 18–36 Å for XMM1 and XMM2 respectively.

#### 3.3.2 Chandra data reduction

We used the *Chandra*-HETG (Canizares et al. 2005, ObsID 2741–2743; Table 3.2), observed in timed exposure (TE) mode, with a subarray of 512 rows in the ACIS-S detector, in order to mitigate pileup. The three observations were obtained close in time (labeled MEG in the table). This ensures a relatively stable continuum shape and absorption properties. We used the data reduction software CIAO (ver 4.13, Fruscione et al. 2006) to create response matrices, effective areas and to combine the data. We use in this analysis the MEG data only because of its higher sensitivity with respect to HEG in the iron L edges region. We restricted the fit to the wavelength region 15–21 Å. At longer wavelength the signal-to-noise was too low to allow a meaningful modeling. Extending the band towards shorter wavelength would also emphasize the effect of broad band pileup, hampering the continuum modeling.
3.4 Modeling of the data

We used the spectral fitting package SPEX (ver 3.06.01) for the spectral modeling. The goodness of fit was decided using the C statistics (first formulated in Cash 1979) for Poisson distributed data. In the limit of a large number of counts per spectral bin, this distribution tends to a \( \chi^2 \) distribution (Baker & Cousins 1984). The errors are quoted for 68% (1\( \sigma \) significance) confidence level, unless otherwise stated. We linked the data sets presented in Sect. 3.3 via the sector option in SPEX. This allows to simultaneously fit some parameters, while leaving parameters specific of each data set to vary. In particular, each data set was locally fitted with a phenomenological powerlaw continuum, while the parameters of the absorbers in our Galaxy were tied to be the same for all data sets. The spectrum displays evident photoelectric edges due to neutral oxygen and iron (Fig. 3.4), typical for this value of hydrogen column density, as well as narrow features, likely due to gas at different temperatures.

3.4.1 The gas phase

In Fig. 3.4 we show the model parameters of the best fit of the absorption components. The abundances adopted are the proto-solar values described in (Lodders & Palme 2009). We fit the coldest gas phase with a HOT model in SPEX, fixing the temperature at \( 8 \times 10^{-3} \) eV, ensuring that the model displays only neutral species for the gas. Note that in previous works on the subject using SPEX (ver <3.05), the temperature for which all ions are in the neutral state was 0.5 eV. These values should not therefore be compared\(^3\). This component displays a prominent 1s-2p O\( ^{\text{i}} \) absorption line at 23.5 Å. However, other less prominent lines are also visible in the spectrum. We fit the component responsible for the 1s-2p O\( ^{\text{ii}} \) line with a second HOT component. This gas component (\( T \sim 3 \) eV) fits predominantly O\( ^{\text{ii}} \), and O\( ^{\text{iii}} \) in the oxygen band. Additional components include an \( \sim 11 \) eV gas and a higher ionization gas (\( T \sim 70 \) eV). These gas phases produce discrete features in the oxygen band, while in the iron L band, they rather produce blends of multiple iron ions, that would be difficult to identify without a global fit. In particular, Fe\( ^{\text{iii}} \)–Fe\( ^{\text{iv}} \), Fe\( ^{\text{v}} \)–Fe\( ^{\text{vii}} \) and Fe\( ^{\text{xv}} \)–Fe\( ^{\text{xvii}} \) are the ions with larger column densities for the 3, 11, 70 eV phases, respectively. We tested the presence of ionized gas intrinsic to the source using the XABS model, however the spectra do not display any evidence of it, at least in the energy band considered here.

3.4.2 The dust phase

In order to fit the contribution of dust to the oxygen and iron edges, we systematically included all dust components (Table 3.1) in the modeling, together with the gas

\(^3\)https://spex-xray.github.io/spex-help/changelog.html#version-3-06-01
Figure 3.4: Detail of the iron (top panel) and oxygen (bottom panel) spectral region as seen by *Chandra*-MEG and *XMM-Newton*-RGS (only XMM1, for clarity) respectively. The best fit model is shown in red and the data as black crosses. The spectrum and the model have been normalized by the continuum, in order to emphasize the transmission. The individual transmission models are shown at the top of the plot and explained in the legend.
### Table 3.3: Parameters for the modeling of the absorption components.

<table>
<thead>
<tr>
<th>comp</th>
<th>$N_H$</th>
<th>$T_{cold}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>comp 1</td>
<td>70.7 ± 0.7</td>
<td>0.08 fix.</td>
</tr>
<tr>
<td>comp 2</td>
<td>1.8 ± 0.2</td>
<td>2.7 ± 0.7</td>
</tr>
<tr>
<td>comp 3</td>
<td>1.4 ± 0.1</td>
<td>10.7 ± 0.4</td>
</tr>
<tr>
<td>comp 4</td>
<td>0.2 ± 0.1</td>
<td>70 ± 20</td>
</tr>
<tr>
<td>comp 5</td>
<td>8.1 ± 0.4 × 10$^{-3}$</td>
<td>3.2 × 10$^{-4}$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>2.0 × 10$^{-4}$</td>
</tr>
<tr>
<td></td>
<td>8.9 ± 0.6 × 10$^{-4}$</td>
<td></td>
</tr>
</tbody>
</table>
\[ C-stat/dof \] 1871/1152

Notes:
Units are $10^{20}$ cm$^{-2}$ for column densities ($N_H$), eV for temperatures ($T$). The line broadening ($\sigma_v$) has been kept fixed at the default value of 100 km s$^{-1}$.

For Mg and Si we report the values predicted by the model.

Components (Sect. 3.5.1). We used the AMOL model in SPEX. This model can fit four dust components at the time. Following Costantini et al. (2012), the unique combinations to be fitted are given by: $n = n_d! / 4!(n_d - 4)!$, where $n_d$ is the number of dust profiles. In this case it resulted in 715 fits. In Fig. 3.4 we display the absorption spectrum, normalized for the continuum emission, for the iron and oxygen spectral region. The red continuous line indicate the best fit (Tab. 3.3). The contribution of the single dust and gas components are also highlighted.

To evaluate the better fits among all the combinations, we use the Akaike Information Criterion ($AIC$), valid for non-nested models (Akaike 1974) as in this case. The $AIC$ for a single fit is given by $AIC = 2k - 2ln(L_{max})$, where $k$ is the number of degrees of freedom and $C_{stat} = -2ln(L_{max})$. In our case, $k = 0$, as all fits have the same degrees of freedom. It has been demonstrated (Burnham & Anderson 2002) that fits with a difference of $AIC$, $\Delta AIC$, less than 4 can be considered undistinguishable from a statistical point of view, and therefore acceptable. On the contrary, fits with $\Delta AIC > 10$ can be disregarded. In Fig. 3.5, the fractional contribution of the models to the fit are shown both for $\Delta AIC < 4$ and $\Delta AIC < 10$ (less significant fits). We see that the results are tightly clustered around two compounds in particular: forsterite and olivine. The uncertainty associated to their contribution to the total dust (58% for forsterite) is about 6%, taking into account the range of values within $\Delta AIC < 4$. 

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3 Iron in interstellar dust along the line of sight of Cyg X-1: an X-ray view

Figure 3.5: Bar chart of the relative contribution of the fitted compound to the total amount of dust. The bars indicate fits that obey the condition $\Delta AIC < 4$ (red) and $\Delta AIC < 10$ (grey). The error bars are an indication of the minimum and maximum percentage of a given compound. The values for the least significant compounds should be considered as upper limits.

The summed contribution of any other material, within the acceptable range, is not more than 3% of the total.

3.5 Discussion

We have performed a systematic fit of the O K- and Fe L-edges, using all possible combination of 13 dust compounds (Table 3.1 and Fig. 3.3). As noted in the figure, the $L_3$ and $L_2$ features do not display sharp distinctive peaks, but they are rather smooth. The best fit is therefore determined by both the edge energy shift and the $L_3$-to-$L_2$ ratio. As demonstrated in Psaradaki et al. (2020), the oxygen cross section profiles are similarly smooth. It is therefore of crucial importance to fit both edges to reduce degeneracies in the fit. The energy resolution of the laboratory data ($\Delta E = 0.25\text{eV}$) is adequate to the astronomical data, as the resolution of Chandra-MEG and XMM-Newton-RGS is $\sim 0.9$ and $\sim 1\text{eV}$ at the FeL and OK edges, respectively. Another important factor is the inclusion of all gas components in the fit. Thanks to our global fit, the elusive contribution of the iron gas-transitions (Sect. 3.5.1) could be determined.
3.5.1 The multi-temperature gas in the ISM

The total hydrogen column density for the cold phase in the X-rays is determined by the shape and depth of the low energy cut off, that in XMM-Newton-RGS data extends down to 36Å. We found a value \(N_H \sim 7.07 \times 10^{21} \text{ cm}^{-2}\) fully consistent with recent H i measurements (HI4PI Collaboration et al. 2016). Previous estimates (e.g. Kalberla et al. 2005) reported a H i column density about 3% smaller than what reported here. Previous Chandra results reported smaller values \(N_H \sim 5.4 – 6.21 \times 10^{21} \text{ cm}^{-2}\) (Schulz et al. 2002; Juett 2004; Hanke et al. 2009), probably due to the shorter long wavelength coverage with respect to RGS.

Specific elements in the colder phase (namely O, Fe, Mg and Si), are depleted from the gas phase. The simultaneous fit of gas and dust allows a robust determination of the gas-to-dust ratios for the elements best represented in the energy band studied here. For example the oxygen 1s-2p strong transition is located at 23.5Å, distinct both from other gas features and from the dust absorption, whose range of action is in roughly in the (22.7–23.5)Å range (Fig. 3.4). Evidence of a multi-temperature gas is given by the presence of O ii and other, weaker, features belonging to O iii–O v. Thanks to the global fitting provided by the HOT model, where line equivalent widths are linked by a common temperature, also the amount of ionized iron in the crowded Fe L-edges region could be determined. The ratio of the ionized oxygen and ionized iron to the total gas budget of these elements is \(3.8 \pm 0.4\%\) and \(38 \pm 7\%\) for oxygen and iron, respectively. The apparently large fraction of ionized iron is solely due to the small portion of iron in the neutral gas phase.

3.5.2 The iron inclusion in dust

ID towards lines of sight with a higher-column density, pointing mainly at sources in and around the Galactic bulge, show a remarkable homogeneity in terms of silicate content, that have been secured to be in the form of amorphous olivine, for the most part (Zeegers et al. 2019; Rogantini et al. 2020). However, more diffuse lines of sight seem to show more diversity in their chemical composition, as the fitting of the oxygen and iron region show (Chapter 4 and Costantini et al. 2012). In particular, a preference for Mg-rich silicates is shown, while the compound with more important iron inclusion have a smaller contribution. In this study we show how the best fit is reached for a mixture of forsterite (Mg2SiO4), and amorphous olivine (FeMgSiO4), where the first constitutes 58 ± 6% of the dust. The Mg-to-Fe ratio is 3.7 ± 0.2 (Mg/(Mg+Fe)=0.78±0.03) pointing to a relatively iron poor content along the diffuse sight lines. In our fits, iron rich silicates (e.g. Fe2SiO4), for the models that obey the condition \(\Delta AIC < 4\), never reach a significant amount \((N_{Fe}^{fayalite} < 2 \times 10^{15} \text{ cm}^{-2})\). Silicates are therefore present in a mixture in this diffuse sightline (Mattsson et al. 2019), but skewed towards Mg-rich silicates (Poteet et al. 2015). For diffuse sight lines,
a magnesium rich inclusion of oxygen is in agreement also with the ratio of oxygen to
the other silicate-forming elements, as observed in the UV band (Jenkins 2009). We
cannot draw conclusions on crystallinity, as for one of our best fit component, only
the crystalline compound was available for the measurements. However, as shown
in Psaradaki et al. (2020), the oxygen profiles are in general smooth and, in some
cases, the amorphous counterpart of a material does not differ significantly from
the crystalline one. Future measurements on amorphous forsterite might clarify this
uncertainty.

3.5.3 The iron inclusion in metal, oxides and sulphides

Our best fit, based on our experiments, showed a prevalence of amorphous olivine
in the iron edge fitting. Amorphous olivine is believed to be abundant in the ISM,
as far-infra-red and X-ray analysis of the Mg and Si K-edges in spectra towards the
galactic center show (e.g. Kemper et al. 2004; Zeegers et al. 2019; Rogantini et al.
2020). However, other works, based on the analysis of diffuse ISM lines of sight, point
to a prominent role of metallic iron (e.g. Costantini et al. 2012, W19). In our set of
samples (Tab. 3.1) we adopted the metallic iron profile as measured by Kortright &
Kim (2000) and used in L09. As pointed out above (Sect. 3.5), one of the distinctive
characteristics of the different compounds is the energy of the edge onset, that needs
to be determined with accuracy. However, for metallic iron the literature values do
not converge to a common energy edge (see Appendix B). The energy range covered by
the onset of the edge corresponds to \( \Delta \lambda \sim 0.041 \text{ Å} \), to be compared to the Chandra-
MEG resolution (\( \sim 0.023 \text{ Å} \)). Determining the amount of metallic iron along the line
of sight is therefore bound to provide uncertain results.

We further tested the parameter space covered by the metallic iron displacement
(Fig. B.1), repeating the fitting (with forsterite and olivine, see above), adding this
time a separate AMOL component containing metallic iron and with a shift in wave-
length space following a grid of values. This grid covers the different values in the
literature and also extend towards shorter wavelengths. The column densities of dust
and gas components were free to vary in the fit. The result is shown in Fig. 3.6, where
the total iron column density (squares) is the sum of the individual contribution of
cold gas (diamonds), iron in olivine (triangles) and metallic iron (asterisks). The
vertical lines show the edge energy of L09 at which \( \Delta \lambda = 0 \), as it is the default value
used in this study, and W19, respectively. The plot shows that the column density
of metallic iron increases as the shift increases, but it is always a small fraction of
the total column density. Because of this small contribution, even large shifts are
accepted by the fit.

Further we also tested the case where olivine is set to zero in the fit and only metallic
iron, (with a free shift) is allowed to fit the iron edges. The best fit is found for a
displacement \( \Delta \lambda = 0.049 \pm 0.005 \) (see X-axis in Fig. 3.6 for a comparison). The fit is
3.5 Discussion

Figure 3.6: Iron column density as a function of the shift, measured in Å, adopted for the metallic iron L-edges during the fit. The resolution of Chandra-MEG is 0.023 Å. The iron L complex is approximately 0.3 Å wide. The vertical lines indicate the position of the L09 and W19 measurements.

Table 3.4: Relative abundances and depletion values from the present analysis.

<table>
<thead>
<tr>
<th>elem.</th>
<th>$N^{\text{gas}}$</th>
<th>$N^{\text{dust}}$</th>
<th>$A_Z/A_Z^\odot$</th>
<th>dust/ISM</th>
</tr>
</thead>
<tbody>
<tr>
<td>O</td>
<td>420 ± 25</td>
<td>81 ± 4</td>
<td>1.17 ± 0.05</td>
<td>0.16 ± 0.01</td>
</tr>
<tr>
<td>Fe</td>
<td>1.4 ± 0.5</td>
<td>8.6 ± 0.5</td>
<td>0.44 ± 0.03</td>
<td>0.86 ± 0.05</td>
</tr>
</tbody>
</table>

Notes: Abundances are referred to Lodders & Palme (2009)
Column densities are in units of $10^{16}$ cm$^{-2}$.

However worse than the best fit presented in Sect. 3.4.2, with $\Delta C/\Delta d.o.f. = 24/1$. Our study does not find evidence of iron locked in oxides ($N_{Fe}^{\text{magnetite}} < 2 \times 10^{15}$ cm$^{-2}$). Iron oxide in the form of magnetite should be the end product of iron transformation in a silicon and oxygen rich circumstellar environment (Field & Cameron 1975; Jones et al. 1990) and therefore a likely component of the fraction of iron not included in the silicates (Mattsson et al. 2019). We find similarly low values for sulphides (FeS and Fe$_2$S), which have been also hypothesized to constitute a non-negligible fraction of iron in dust (Westphal et al. 2014; Costantini et al. 2019, and references therein).
3.5.4 Abundances and depletions

In Table 3.4 we report the values of abundances and depletions with the associated statistical error for oxygen and iron, which are the elements covered by our Chandra and XMM-Newton analysis. Oxygen has been found to be slightly overabundant (∼1.17 with respect to solar). This value is in line with previous results on diffuse sight lines (Costantini et al. 2012; Psaradaki et al. 2020). The depletion of oxygen is consistent with the moderate values observed in the UV band (Savage & Sembach 1996; Jenkins 2009) and in the X-ray band (e.g. Pinto et al. 2013). As detailed in Chapter 4, along diffuse lines of sights we do not expect to register the anomalies in the oxygen abundances as for dense sight lines (Whittet 2010).

The depletion of iron is severe (0.86 ± 0.05), in agreement with previous X-ray studies (see also Chapter 4). Such a high depletion has been always recognized as problematic, as the iron produced by stellar processes should produce a maximum depletion of about 35%, in contradiction to what observed (Dwek 2016). Zhukovska et al. (2018) also theorise that a large fraction of dust should be newly created, out of gas condensation, in the ISM. This would result in more than 70% depletion for iron.

The abundance of iron in this study is instead not in line with previous X-ray studies of this spectral region, as for diffuse sightlines the iron amount was consistent with solare values, within the errors (Costantini et al. 2012; Pinto et al. 2013). This value could however be increased, as we observe that the fit in the iron region is still missing the contribution of large grains in the model. This issue will be addressed in a future study.

3.5.5 A popular line of sight: comparison with previous works

Cyg X-1 has been targeted not only for its extraordinary intrinsic spectral and timing properties (Sect. 3.1.1), but also to study the intervening ISM, in particular the cold gas and dust phase. Here we compare our results with previous works. Numerous works used the Chandra-gratings data to study both the iron and oxygen region. For the latter, the excellent view that Chandra-MEG offered in the beginning of the mission, allowed to study the O i-iii transitions in great detail. These studies did not yet formally include the dust component (Juett 2004; Schulz et al. 2002; Hanke et al. 2009). The iron L-edges were soon noticed to be shifted with respect to the gas photoelectric edge (Juett et al. 2006; Hanke et al. 2009). The amount of cold iron has been shown to vary slightly, possibly as a function of the absolute luminosity of the source, hinting at an ionization taking place near the source, when it is burtsing (Hanke et al. 2009; Juett et al. 2006). The value of iron in a cold phase (dust and gas) is in this study ∼ 1 × 10^{17} cm^{-2} (Tab. 3.4), an intermediate value between the two extreme values of ∼ 2.52 × 10^{17} cm^{-2}, when the source is in low-state (see Tab. 3 in Hanke et al. 2009, for additional literature values), and ∼ 0.96 × 10^{17} cm^{-2} when
the source is in flaring state (Juett et al. 2006). It has to be noted however that this
value is based on the fitting of the L\textsubscript{3} and L\textsubscript{2} edges, which has been conducted with
different methods and assumptions in those works.
Studies using dedicated dust laboratory measurements of the iron L-edges, formally
included in the fit, were first carried out in L09 and more recently in W19 using
archival Chandra data. Both works focused only on the iron L-edges region. In the
earlier case the contribution of the warm phase was recognized, but deemed not sig-
nificant in the fit whereas in the most recent work, it was not included. Between both
works, as well as in the present one, there is little overlap in the dust measurements.
In all three, metallic iron was used (Sect. 3.5.3), and in both our and W19 work both
an amorphous olivine and FeS were included. In the earlier work, five the samples
used were iron rich oxides and fayalite. The most recent work was instead focussed
on GEMS (Glass with Embedded Metals and Sulphides) materials. In both our work
and in W19, the correct extinction (rather than only absorption) profiles were used.
Here we used a fixed dust size distribution, while in W19, the upper limit on the
dust distribution (\(a^+\) in MRN) was a free parameter. Therefore a straightforward
comparison is difficult. We discuss in Sect. 3.5.3 how the inclusion of metallic iron, a
major component in W19 modeling, should be taken with caution.

### 3.6 Conclusions

In this paper we presented the 12 materials that we characterized at the iron L spectral
region at the electron microscope facility Titan in Cadiz (Spain). One additional
material (metallic iron), was taken from the literature. These models of the iron L-
edges were used, together with the O K edge measurements (Psaradaki et al. 2020),
to test the chemical composition of the interstellar dust along the line of sight of
Cyg X-1. Our results can be summarized as follows:

Both iron and oxygen are significantly depleted. The dust/(gas+dust) ratio is
0.86 and 0.16 for iron and oxygen respectively. This is in line with previous results
both at longer wavelengths and in the X-ray band.

While the oxygen abundance has been found to be supersolar (\(A_Z/A_{\odot} \sim 1.17\)),
the abundance of iron is significantly subsolar (\(\sim 0.44\)). This value may be mitigated
when the contribution of large grains, likely needed in the fit, is considered.

The chemistry of interstellar grains along the line of sight is shared between the
Mg-rich end of olivine (forsterite, MgSiO\textsubscript{4}), and amorphous olivine (FeMgSiO\textsubscript{4}, which
constitutes about 42% of the amount of dust).

We discuss the role of iron in the modeling and we point out how the uncertainties
in the measurements of metallic iron (not present in our batch of materials), can
greatly influence the outcome of the fit of this and previous works on this subject.
Determining the amount of metallic iron in the ISM is an important information to
solve the puzzle of the ‘missing iron’.

Along the line of sight of Cyg X-1 coexist gas components with different temperatures. A cold component, whose column density is consistent with the H\textsubscript{i} radio measurements, and at least other three components, with temperatures in the range \(\sim 3-70\) eV, that explain the presence of transitions from ionized ions in the spectrum.

Acknowledgements

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