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X-ray spectroscopy of interstellar dust: from the laboratory to the Galaxy

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1 Introduction

1.1 Detecting dust in space

1.1.1 Discovering dust

The space between stars, also called the interstellar medium (ISM), is not a perfect vacuum. Between the stars, we can observe clouds of dust and gas of varying shapes, densities and sizes. These clouds can be observed, for instance, as dark patches in our own Galaxy contrasting with the light from the stars, as can be seen in Figure 1.1, panel a. In the 18th century the interest in these dark parts increased, due to the developments in the quality of telescopes, which made it possible to observe them in more detail. Caroline Herschel wrote to her nephew John Herschel encouraging him to observe a certain part of the sky, of which she said John's father, William Herschel, described it as a hole in the sky. However, in the early 20th century, these 'holes' were eventually discovered to be foreground clouds obscuring the stars behind them. In the 1890s Barnard started to photograph these clouds (eventually published in a catalogue, Barnard (1919)), which revealed many details of these clouds, invisible to the naked eye. Agnes Clerke described them in her book 'Problems in Astrophysics' as obscuring bodies (Clerke, 1903). Even in the case where no clouds are observed towards a star, it was found that extinction of light still takes place (Struve, 1847). It took until ~ 1930 to prove that the extinction, shown by the reddening of stars, is indeed caused by interstellar dust particles (independently described by Schalén (1929) and Trumpler (1930)). Since its discovery, the way dust has been perceived slowly changed. At first it was completely ignored, then it was considered to be a hindrance when trying to observe the stars and galaxies, but since the 1960s, dust has been more and more seen as an important component that drives many processes in the universe (Greenberg, 1963).

1.1.2 The life cycle of dust in the universe

The important role of dust in the universe is best shown by its role in every stage of the life cycle of stars. Of the normal matter in our Galaxy, about $5 - 10 \times 10^9 M_{\odot}$ (solar masses) resides in the ISM in the form of gas and dust, which is about 5-10% of the total mass of all the stars in the Galaxy (e.g., Tielens, 2010; McMillan, 2017). Only 1% of the mass of the ISM is in the form of dust (Boulanger et al., 2000). Although, looking at the big picture, dust may seem to contribute little to the total content of the universe, it is nevertheless a very important component, since it plays a defining role in every stage of the life cycle of stars.

The life cycle of stars is shown in its five different stages in Figure 1.2.

1. Sources of interstellar dust: Our starting point in this figure, is actually the last phase in

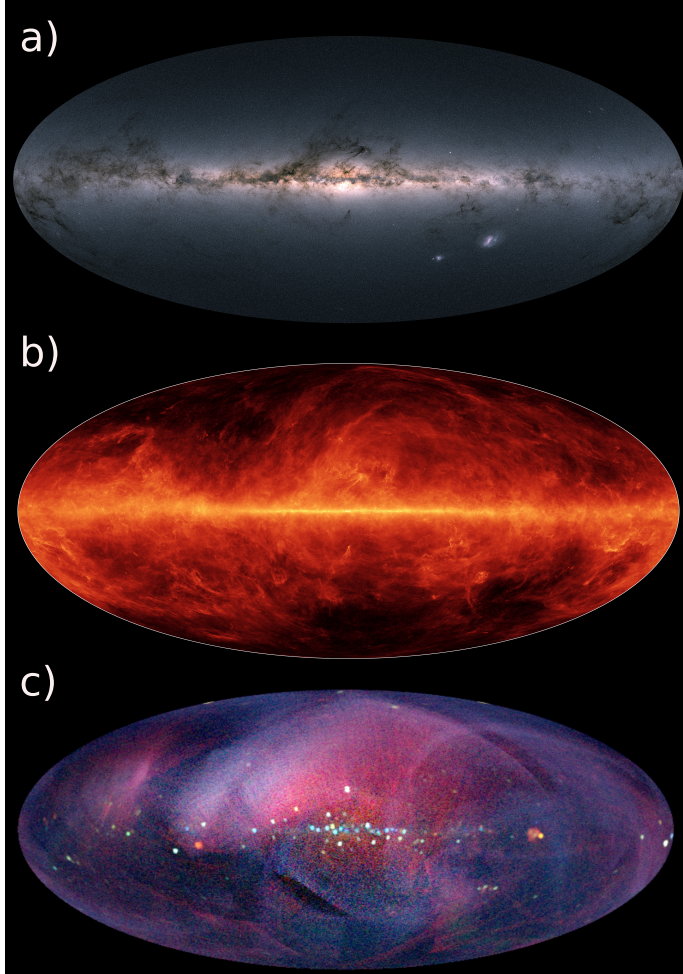


Figure 1.1: The Galaxy at three different wavelengths: a) The visible-near infrared: GAIA 330-1050 nm, image credit: ESA/Gaia/DPAC - b) infrared: Planck cold dust (20 K) map, image credits: ESA/NASA/JPL-Caltech - c) The X-rays: 0.5-16 keV MAXI all-sky survey, image credits: JAXA/RIKEN/MAXI team.

the life of a star. Stars enrich the universe with elements, produced during the nucleosynthesis process and in this way, provide the building blocks for the interstellar dust particles. Dust is thought to form as condensates in the atmospheres of evolved stars (mainly stars in the Asymptotic Giant Branch (AGB) phase) and consequently ejected in the ISM. Other potential sources of interstellar dust are supernovae (type Ia and type II), young stellar objects, red super giants and Wolf Rayet stars (Tielens, 2001). It is uncertain how much each of these sources contribute to the total dust budget. Especially the contribution of supernovae type II, is much debated (Cherchneff, 2013). Although

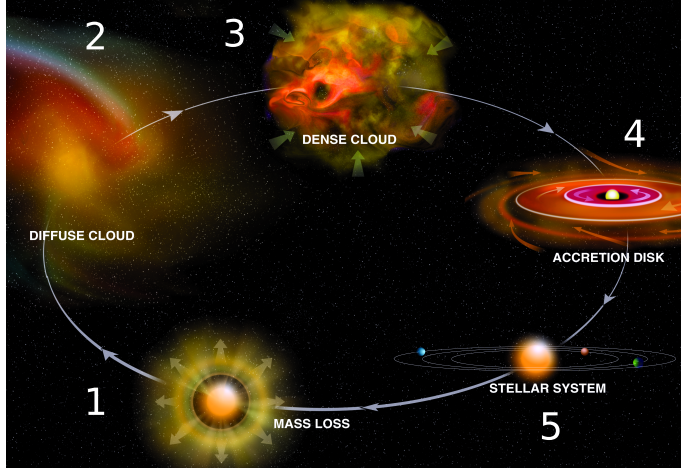


Figure 1.2: The life cycle of stars and interstellar dust in five stages: 1) evolved star, 2) diffuse cloud, 3) dense cloud, 4) protostellar disk phase and 5) evolved planetary system. At each stage in this cycle dust plays a crucial role. Image credit: Bill Saxton, NRAO/AUI/NSF.

recent observations by ALMA (Atacama Large Millimeter/submillimeter Array) show that more than $0.2 M_{\odot}$ of dust is produced in the central part of SN 1987a, the reverse shock, which arises after the shock wave of the supernova rams into the ISM, may (partly) destroy these dust particles again (Indebetouw et al., 2014).

2. Diffuse clouds: The next stage shows a diffuse cloud. The ISM is not a homogeneous medium, but is rather patchy, i.e., the gas and dust in the ISM can be found in clouds of various densities. Most of the volume of the ISM is filled with a low density intercloud medium ($n_{\text{H}} \approx 0.004 - 30 \text{ cm}^{-3}$, where n_{H} is the density of hydrogen). Diffuse clouds have slightly higher densities of $\sim n_{\text{H}} = 10^2 \text{ cm}^{-3}$ and extinction of $A_V < 1$ ¹. Once ejected in the ISM, dust is rapidly mixed with other dust and gas and will cycle many times between the cloud and intercloud phase on a very fast timescale ($\approx 3 \times 10^7 \text{ yr}$) (Tielens et al., 2005). Dust particles in diffuse clouds and in the intercloud medium find themselves in a violent environment. Collisions with cosmic rays may destroy the internal crystalline structure of the grains. Dust can be destroyed by supernovae shocks through sputtering and shattering (e.g., Guillet et al., 2007, 2009; Jones and Nuth, 2011). This destruction process is in fact predicted to be so successful, that it is still not clear why not all of the dust has been destroyed, since the formation timescale of the

¹Extinction due to dust (A_{λ}) varies with wavelength λ and depends on the composition and size distribution of ID particles. It can be connected to reddening of starlight by the extinction factor $R_V = A_V / (A_B - A_V) \equiv A_V / (E(B - V))$, where A_B and A_V are the extinctions measured at the B (4405 Å) and the V (5470 Å) photometric bands. Their difference is equal to the color excess or “reddening” $E(B - V)$, i.e., the difference between the observed color of the star and the color it would have when unaffected by extinction. In the Galaxy $R_V = 3.1$ in the diffuse ISM. Since gas and dust are well mixed in the ISM, A_V , commonly used to indicate the extinction along the line of sight, is a measure for the column density of hydrogen N_{H} : $N_{\text{H}}/A_V = 1.9 \times 10^{21} \text{ cm}^{-2} \text{ mag}^{-1}$, for $R_V = 3.1$ (Bohlin et al., 1978).

dust (~ 2000 Myr) is assumed to be much longer than the destruction timescale (~ 500 Myr) (Jones et al., 1994, 1996; Jones and Nuth, 2011). A solution to the problem of the formation of grains may be found in (re-)forming dust in the ISM itself (Dwek, 1998; Zhukovska et al., 2008; Draine, 2009; Zhukovska et al., 2018). In diffuse environments, dust is also exposed to stellar radiation (UV photons and X-rays) and cosmic rays. The grains absorb UV radiation and re-emit in the infrared. When observing the galaxy in the mid infrared, most of the observed radiation is emitted by dust particles, as can be seen in Figure 1.1 (panel b). Due to the grain heating by UV radiation, dust in diffuse clouds plays an important role in H_2 formation on the surface of grains (Gould and Salpeter, 1963; Cazaux and Tielens, 2004; Wakelam et al., 2017). The same supernovae shocks that may destroy the dust particles, as well as stellar winds, collisions between clouds and turbulence, can also cause a disturbance in the diffuse cloud which may lead to compression of the cloud into a denser, translucent, cloud. Translucent clouds can be found within diffuse clouds, with $1 < A_V < 2.5$ and densities of $n_{\text{H}} \approx 10^3 \text{ cm}^{-3}$. At this stage, the cloud becomes dense enough for dust grains to shield the interior of the cloud from optical and UV radiation, allowing molecules to form (Ciolek, 1995; van Dishoeck, 2014). Dust may act as a coolant for the gas in the case where the surrounding gas has a higher temperature than the dust grains, causing the cloud to cool down further and compress (Falgarone and Puget, 1985; Galli et al., 2002; Li et al., 2003).

3. Dense clouds: From the diffuse and translucent clouds, we now go to the next stage, namely a dense cloud. Dense clouds are defined as clouds with $A_V > 3$ and densities of $n_{\text{H}} = 10^3 - 10^6 \text{ cm}^{-3}$. Most of the gas is now in the form of molecules. In these dense clouds, dust grains can catalyze chemical reactions on their surfaces by bringing atoms and molecules together (van Dishoeck, 2014, and references therein). They may grow in size due to coagulation (Ossenkopf, 1993) and layers of ice can form around the dust particles, of which water ice is observed to be the main constituent (Whittet et al., 1997; Pontoppidan, 2004). A dust particle may go through multiple cycles in and out of the dense cloud into the diffuse ISM and back. However, when the cloud becomes so massive that the gas pressure no longer support it, the cloud can become gravitationally unstable and will eventually collapse (Shu et al., 1993).
4. Consequently, a star forms at the center of the cloud. The nebula has now flattened into a disk. Again, dust plays an important role as the building blocks in the formation of planets inside the disk. When the gas has been dissipated from the disk, a dusty debris disk remains (Wyatt, 2008). The star will start to blow the smallest dust particles out of the disk, depending on strength of the solar wind and the radiation pressure of the star.
5. When the star has cleared its surroundings, a planetary system emerges. As the star ages, it will start to return matter into the ISM and the whole process can start again.

Cosmic dust can be observed virtually everywhere: in our solar system, around young stars, in giant clouds, the Galaxy, but also in distant galaxies (Hughes et al., 1998) and it is already present in the earliest eras of the universe (Watson et al., 2015). Interestingly these galaxies are the dustiest of them all, suggesting that dust is rapidly and effectively formed in the early universe. Hence, studying dust can help us to understand how the universe evolved. Besides

the arguments in favor of dust studies already given, there is of course another important reason to study dust, because we and everything around us all consists of cosmic dust. Therefore, if we want to understand the origin of life, it is necessary to understand the origin, formation and composition of cosmic dust.

1.2 Observational constraints on dust properties

After establishing that dust was actually present in the universe, it became necessary to model the interstellar dust. In the first place to take the extinction into account, in order to obtain accurate distance estimates of stars. However, since dust plays a role in many processes in the universe, it has become an essential component in many astronomical models. In order to develop accurate interstellar dust models, is important to understand the properties of dust: what interstellar dust exactly consists of, how it interacts with radiation, what the grain size distribution is, what shape and internal structure of the grains is and whether these properties change in different environments. Most of the properties of dust that are derived so far, have been obtained from observations of dust in the Galaxy. We list the main properties and findings in this paragraph.

1.2.1 Composition of interstellar dust

To understand interstellar dust (ID), a key parameter in this research field is to determine its composition. An important constraint on the composition of dust is given by the abundance of elements. We assume that the abundance is similar to the solar environment. Since the solar system abundances (in this thesis we will use the abundance set of Lodders and Palme (2009)) are well known, it is possible to predict the abundances in the ISM. In the upper panel of Figure 1.3 the abundance of elements versus the ionization energy of the corresponding atom can be seen. However, not all elements are abundant in the gas phase of the ISM. Some of the most abundant elements are missing in the gas phase (also referred to as depleted from the gas phase) and are thought to be instead included in dust particles. The depletion of elements from O to Zn is given in the middle panel Figure 1.3 (Jenkins, 2009).

The combination of abundance and depletion, indicates that dust should mainly consist of C, O, Mg, Si, Fe and possibly S. Besides these elements, less abundant, but highly depleted elements, such as Ti, Ca, Ni and Al can also be present in dust. The abundant elements He (not shown in Figure 1.3) and Ne are chemically inert and therefore do not contribute to the composition of dust. N is not a large constituent of dust either, but this is explained by its inclusion in the highly stable gas form of N_2 (Gail and Sedlmayr, 1986).

Besides depletion studies, the composition of interstellar dust can be identified using more direct methods, such as identification through IR spectroscopy of circumstellar or interstellar dust and through studies of pre-solar interstellar dust grains recovered from meteorites or interplanetary dust particles. An overview of detected dust species is given in Table 1.1 (Tielens et al., 2005). There is a wide variety of dust species, reflecting the wide range of stellar sources of interstellar dust with different physical conditions (temperature, pressure, elemental abundances).

The way dust is produced is also an important factor in the composition of dust. However,

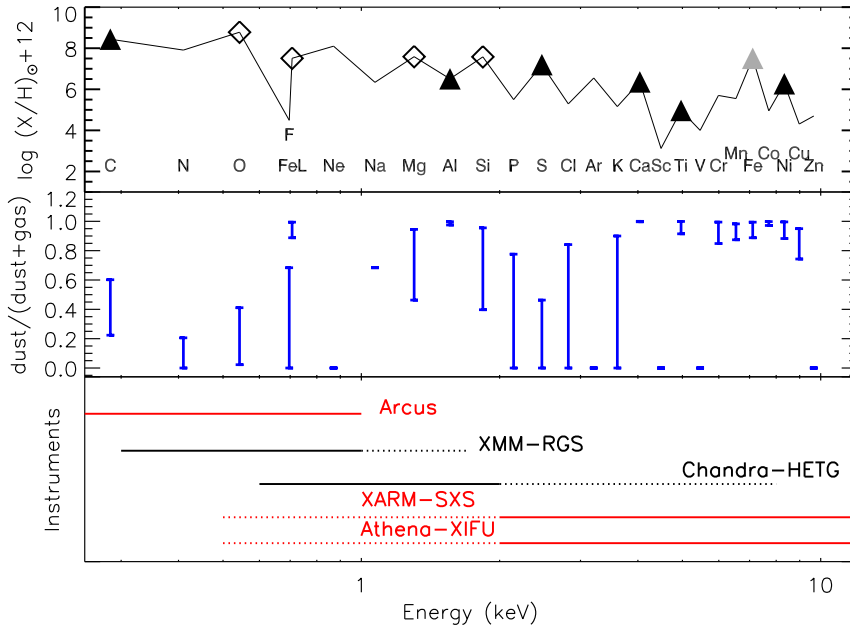


Figure 1.3: Figure taken from Chapter 4. Upper panel: abundance pattern as a function of energy for the absorbing elements in the X-ray band. Abundances of elements versus their K- or L-shell ionization energies. Abundances follow Lodders and Palme (2009) and they are expressed in terms of $\log(X/H)+12$. In this framework, the abundance of hydrogen is 12. The open diamonds mark the elements that are accessible by current X-ray instruments. The triangles are the relevant elements that will be accessible by future instruments to study dust. Middle panel: range of depletions. Lower panel: energy range covered by present (black) and future (red) missions. The solid line highlights the energy range where the capabilities of the instruments are optimal for observing absorption by dust.

there is much uncertainty in how much each of the dust producing sources contribute to the total dust budget. The most studied and understood dust producing sources in the Galaxy are AGB stars. AGB stars are either oxygen rich or carbon rich. One of the first molecules to form in the atmospheres of these stars is CO. Depending on the surplus of either carbon or oxygen, AGB stars are thought to produce carbonaceous or silicate dust grains (Andersen, 2007).

Combining abundance and depletion studies, theory and observations, dust in the ISM can be roughly divided into two main groups, namely silicates (e.g., pyroxene and olivine types) and carbonaceous dust, with the addition of oxides (e.g., MgO, SiO, SiO₂), carbides (mainly SiC) and metallic iron (Draine, 2011).

Since the main building blocks of silicates, the elements Si, O, Mg and Fe, are found to be depleted in dust, interstellar silicates are assumed to be a major constituent of dust. This is indeed supported by observations. Silicates are detected in the ISM in infrared spectra by their characteristic 10 μm (stretching of the Si-O bond) and 20 μm (bending of the O-Si-O structure) features (e.g., Knacke and Thomson, 1973). These features indeed show that silicates are abundant in the interstellar medium and give the opportunity to investigate which species of silicates may be present. It is of great advantage that a wide variety of silicates are also

present on earth and can be characterized in laboratories through standard mineralogical and chemical techniques (Jaeger et al., 1994). The infrared spectra of interstellar silicate analogues offer the possibility for comparison with observations. The main contributions to the silicate infrared features are pyroxenes ($\text{Mg}_x\text{Fe}_{(1-x)}\text{SiO}_3$) and olivines ($\text{Mg}_{2x}\text{Fe}_{(2-2x)}\text{SiO}_4$) with $0 < x < 1$, although the ratio in which they occur in space is uncertain, as well as their Mg/Fe ratio (Kemper et al., 2004; Chiar and Tielens, 2006; Min et al., 2007). From the infrared features, it was also determined that $<2\%$ of dust in the Galaxy is in crystalline grains (Kemper et al., 2004). Therefore, most of the dust, as observed in the infrared, is amorphous, meaning the crystalline structure in these grains is negligible.

Carbon is often mainly modelled by graphite (e.g., Mathis et al., 1977), but given that silicates are mostly amorphous, it is suspected that carbon dust particles also underwent amorphization and also exist in the ISM in the form of (hydrogenated) amorphous carbon (Compiègne et al., 2011). Furthermore, smaller amounts of carbon can be locked up in nano-diamond particles (Tielens et al., 1987; Lewis et al., 1987) and Polycyclic Aromatic Hydrocarbons (PAHs, e.g., Tielens, 2013). Figure 1.4 shows two grains, a) SiC and b) and c) graphite, from interstellar origin, retrieved from the Murchison meteorite (Zinner, 2007). The grains show both a crystalline and amorphous structure, indicating the wide variation in the shape of dust grains.

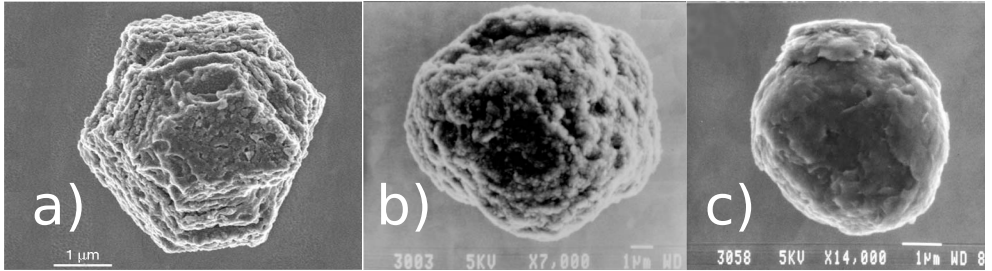


Figure 1.4: Presolar carbon grains from the Murchison meteorite: a) silicon carbide, b) and c) graphite adapted from Zinner (2007), image credit: Sachiko Amari and Scott Messenger.

1.2.2 Grain sizes and size distributions

The sizes of dust grains are an important modelling parameter, since they are connected with their origin and evolution. Grain size distributions are used many in interstellar dust models. There are many different size distribution models, with different input parameters for the grain composition and particle size range. All these size distributions seem to agree that most of the dust mass is in the large grains, while the surface area is dominated by the smaller grains. The extinction curve, which is shown in the right panel of Fig 1.5, can be used to determine the sizes of interstellar dust grains (Greenberg, 1968). Specifically, the extinction at a certain wavelength depends on a typical grains size, since the extinction cross section $C_{\text{ext}} \propto \pi a^2$ and the grain size extinction is consequently dominated by particles of size $a = \lambda/\pi^2$, where λ is the wavelength. Small grains ($\sim 0.01 \mu\text{m}$) dominate the extinction in the UV, while large grains

($\sim 0.3 \mu\text{m}$) are responsible for the extinction in the near infrared. In this way, a size distribution can be tested by fitting them to the interstellar extinction curve. Mathis et al. (1977) developed a size distribution model (MRN, Mathis-Rumpl-Nordsieck) for average diffuse clouds that consists of two separate dust grain components, namely bare spherical silicate and graphite grains. Due to its simplicity, MRN can be easily implemented in numerical programs and is therefore still used in many interstellar dust models. The MRN distribution is given by: $n(a)da = A \cdot a^{-3.5}da$, where a is the particle size, $n(a)$ is the number of grains, and A is the normalisation constant which depends on the type of dust (e.g., silicates or graphite). Particle sizes range between $0.005 < a < 0.25 \mu\text{m}$. The left panel of Figure 1.5 shows interstellar grain size distributions derived from the extinction curve (as shown in the right panel). The size distributions are plotted as mass fractions, where $m(a)$ the differential mass, instead of the more commonly used number of grains $n(a)$ (Kim et al., 1994). The mass distribution derived from the extinction curve is shown by the histogram with the contributions of graphite and silicate displaced by a factor of 10, for clarity. The MRN distribution is shown by the solid lines. This simple exponential function fits the extinction well, but at larger wavelengths the size distribution departs from an exponential. It also shows a sharp cut off at particles sizes beyond $0.25 \mu\text{m}$. The dashed line in Figure 1.5 (right panel) (Kim et al., 1994), for example, shows a size distribution with a smooth cut-off at large particle sizes. More elaborate size distributions may include more complex grain composition and non-spherical grains (e.g., Weingartner and Draine, 2001; Zubko et al., 2004; Draine and Li, 2007; Shen et al., 2008; Draine and Fraisse, 2009; Hoffman and Draine, 2016). In this thesis, we will mainly use MRN size distributions, but also discuss alternative distributions and their implications.

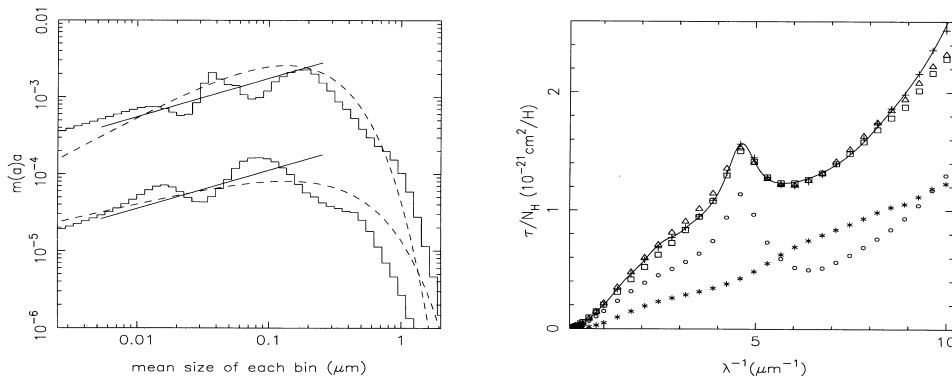


Figure 1.5: Left: interstellar grain size distributions - plotted as mass fractions - derived from the extinction curve (as shown in the right panel). The top histogram shows the mass fractions per particle size bin of silicates and the lower histogram shows graphite, displaced downward by a factor of 10. The solid line shows the MRN size distribution. The dashed curves are size distributions derived by Kim et al. (1994). Right: the corresponding extinction curve normalized to the hydrogen column density. The calculated extinction curve is compared to the observations in the right panel. The contributions due to graphite (o) and silicates (*) are shown separately. Figure taken from Kim et al. (1994).

1.2.3 Open questions on interstellar dust

In the past decades, our understanding of ID has hugely improved. However, there are still significant gaps in our knowledge. Here we list the main open questions on ID that will be considered in this thesis.

- We do not yet completely understand the composition of dust. For instance, we do not know which types of silicates are most abundant in the ISM and consequently what the ratio is between olivine and pyroxene. Furthermore, there are large uncertainties about how Fe, S, O and C are incorporated into dust (e.g., Mathis, 1996; Dwek, 1997; Wakelam and Herbst, 2008; Wang et al., 2015; Dwek, 2016). Iron bearing silicates cannot account for all the iron locked up in dust. Sulfur is only found to be depleted along some lines of sight, but it has surprisingly been detected in grains of interstellar origin retrieved from meteorites and interplanetary dust particles (e.g., Bernatowicz, 1997; Zinner and Amari, 1999; Westphal et al., 2014). A possible solution to both of these problems can be found in the form of metallic iron and/or iron sulfate inclusions in silicates, also referred to as GEMS (glass with embedded metal and sulfides, Bradley, 1994; Floss et al., 2006; Keller and Messenger, 2013). The depletion of oxygen cannot be explained solely through silicates, leaving still an amount of oxygen unaccounted for. In the case of carbon, we encounter the opposite problem, since traditional ID models require twice as much carbon in dust than is actually observed from depletion studies.
- We do not yet understand how dust is produced and how it is processed in the ISM. For instance, there are uncertainties about the amorphization processes of dust. Since most of the silicate dust appears to be amorphous, this may suggest either strong amorphization in the ISM, perhaps due to cosmic rays, or grain growth in the ISM itself. However, considering that 5-15% of the stardust formed around oxygen rich stars is in the form of crystalline magnesium rich silicates (Kemper et al., 2001; Molster et al., 2002; Waters, 2004) and that crystalline interstellar grains have been retrieved from meteorites and interplanetary dust particles, the amount of crystalline grains observed in the ISM is surprisingly low.
- We do not precisely understand if the properties of dust change with different environments. The chemical composition of dust may change with environment since we observe an increase in abundances of elements toward the central part of the Galaxy (Pedicelli et al., 2009; Rolleston et al., 2000; Davies et al., 2009). Furthermore, the wide range in depletion of some elements like Mg, Si and S seems to suggest a difference in composition of dust along varying sight lines. However, we do not yet know how the composition of interstellar dust changes with the environment. In dense environments, dust grains may have the opportunity to grow and therefore we might expect larger grains in denser environments. However, although this works well in modelling of dust grains, observations seem to indicate that dust in the Galaxy is well mixed.

In the remainder of the introduction we will discuss how the X-ray band can help to solve these issues.

1.3 Using the X-rays to study dust

Astronomy has always benefitted from observations at wavelengths that are beyond the range of sensitivity of our own eyes. The X-rays provide interesting advantages when studying interstellar dust with respect to other wavelengths:

- X-rays are sensitive to a wide range of column densities ($N_{\text{H}} \sim 10^{(20-23)} \text{ cm}^{-2}$); this makes it possible to analyze the dust content in various regions of the Galaxy.
- Scattering and absorption of dust can be simultaneously studied.
- Absorption of both gas and dust can as well be measured simultaneously for elements with absorption features in the X-ray band. For these elements, depletion is easy to determine, because the dust abundance does not have to be inferred from a reference solar abundance.

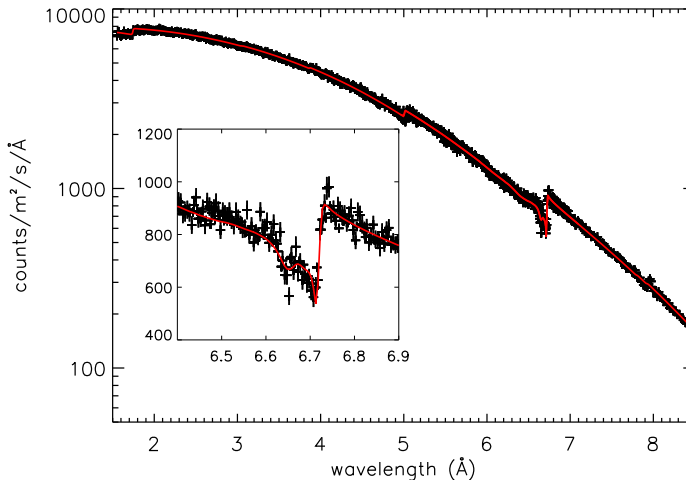


Figure 1.6: Spectrum of the low mass X-ray binary GX 5-1 with Si K-edge at 6.7Å. The source is observed by *Chandra* using the HETGS instrument. The red line shows a fit to the spectrum using our silicate dust extinctions models described in Chapter 2 and 3. The inset shows the details of the area around the Si K-edge, where the XAFS are visible.

The launch of the X-ray satellites *XMM-Newton* and *Chandra* marked the start of a new era in the study of interstellar dust using X-ray spectroscopy. These telescopes have a spectral resolution which is suitable to study the details in the spectra of X-ray sources which arise due to absorption and scattering by dust particles along the line of sight (LOS). The X-ray spectra of X-ray binaries can be used to study the intervening gas and dust along their lines of sight, simply using them as a lantern shining through the ISM. These sources consist of two components, a neutron star or a black hole which accretes material from a companion star, usually a normal star (viz., a non-giant star). These systems are very bright in X-rays, because the accreted material from the companion star forms a disk around the accretor, which emits

in the X-rays due to the gravitational potential energy of the in-falling matter. X-ray binaries are divided in two groups, Low Mass X-ray binaries (LMXB) and high mass X-ray binaries, depending on the mass of the companion star (Lewin et al., 1997). The bright LMXBs are particularly useful in dust studies due to their high flux and simple spectra. Most LMXB do not show sharp intrinsic absorption features in the soft and intermediate X-rays (i.e., photon energies lower than 10 keV), but are rich with absorption from the ISM. Most of the X-ray binaries can be found in the plane of the Galaxy. The X-ray sky can be observed in Figure 1.1 panel c), where the many of the point sources are bright X-ray binaries. An example of a spectrum is given in Figure 1.6. Around $6.74 \text{ \AA}$ we can observe a discontinuity in the spectrum, which is called an ‘edge’. An edge occurs at wavelength where the energy of the incoming X-ray photons equals the binding energy of a core electron. The X-ray photon can be effectively absorbed and ionizes the core electron, causing a steep increase in absorption. The edge is usually indicated by the element and the electron shell, for instance in the case of Figure 1.6 we observe the Si K-edge. Depending on the brightness of the source, the column density along the LOS, and the characteristics of the telescope, we can observe the edges of different elements. Figure 1.3 shows the ionization energies of the elements C to Zn. The extinction features of O, Mg, Si and Fe in the X-ray band, fall within the range of the range of XMM-Newton and Chandra. These elements are also the main building blocks of silicates, making the X-ray band especially suitable for the study of silicon based dust. As can be observed in Figure 1.6, the edge is not smooth, but contains features. These features, X-ray Absorption Fine Structures (XAFS), can be used as a fingerprint for the type dust we are observing, since each different dust composition results in a unique pattern (Rehr and Albers, 2000). The extinction models that can be derived from laboratory studies can be used to characterize ID (e.g., Martin, 1970; Martin and Sciama, 1970; Evans, 1986; Woo, 1995; Forrey et al., 1998; Draine, 2003; Lee and Ravel, 2005; Lee et al., 2009; Costantini et al., 2012).

1.3.1 X-ray Absorption Fine Structures

XAFS arise from the wavelike nature of electrons and the fact that an atom in a dust grain is surrounded by neighboring atoms (Meurant, 1983). When an incoming X-ray photon encounters a dust grain, it can be absorbed by an atom in the grain, as shown in Figure 1.7. Consequently, an electron in one of the inner shells of the atom is expelled to the continuum. The ejected photoelectron has a kinetic energy which is equal to the difference between the excitation energy of the atom and the energy of the incoming photon. The electron now behaves like a wave, also indicated as a photoelectron. This can be seen in the panel a) of Figure 1.7, where the photoelectron is depicted as a wave emanating from the site of the absorbing atom. If there are no neighboring atoms, we obtain an absorption feature as shown on the right in panel a). However, in panel b), the absorbing atom is surrounded by neighboring atoms, as is the case in dust grains, and the photoelectron is now scattered by these atoms. New waves emanate from the site of the neighboring atoms. These waves are superimposed on the initial wave and cause alternating constructive or destructive interference at the site of the absorbing atom, depending on the kinetic energy of the photoelectron. In this way, the probability of the photoelectric effect to occur is changed at the site of the absorbing atom. The XAFS pattern depends on the type of element and the position of the neighboring atoms. Each different dust composition will give a different and unique XAFS pattern. Even when

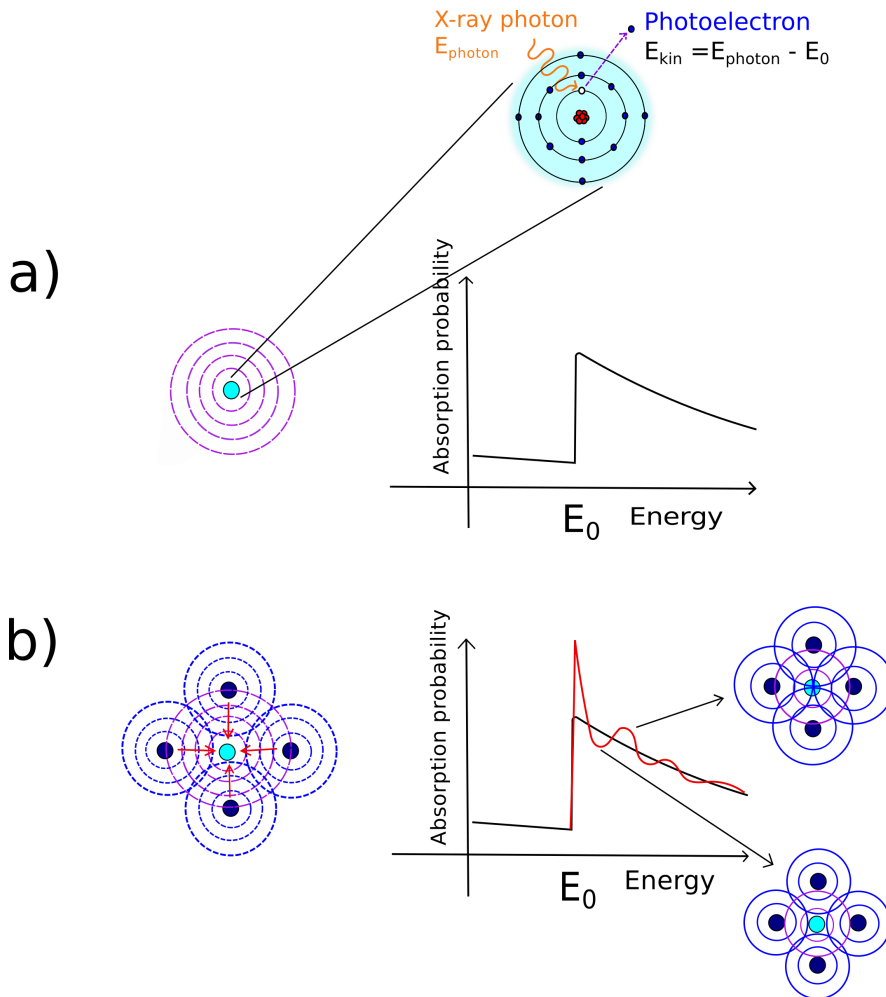


Figure 1.7: X-ray absorption fine structures (XAFS) are features observed in X-ray absorption spectra. Above panel a) we show the photoelectric effect. An X-ray photon is absorbed and a core-level electron is promoted out of the atom. The electron has a kinetic energy which is equal to the difference of the photon energy E_{photon} and the binding energy E_0 of the electron. Panel a): The resulting photoelectron can be considered as a wave emanating from the site of the atom, indicated by the purple circles. On the right the resulting absorption probability versus the energy is shown. The probability increases at the energy of the binding energy and then gradually decays with increasing energy. Panel b): Here we show the same situation, but now the absorbing atom is surrounded by neighboring atoms. The initial wave is scattered by these atoms and new waves emanate from these sites, indicated by blue circles. On the right we show again the resulting absorption probability, where the black line indicates the situation of panel a) and the red line shows the modified absorption (i.e., XAFS) when the neighboring atoms are present. The scattered blue waves are superimposed on the initial purple wave and cause alternating constructive or destructive interference at the site of the absorbing atom, depending on the kinetic energy of the photoelectron. This process is shown by the two insets on the right.

the composition of the material is kept the same, differences will occur when the lattice structure in which the atoms find themselves changes, because the distance between the atoms changes. XAFS are therefore suitable to study the level of crystallinity. Figure 1.8 shows a set of six absorption measurements of silicates with different crystalline structures and different compositions (Zeegers et al., 2017). When a sample is amorphous (i.e., the regular crystalline lattice structure has been destroyed) it loses its clearly peaked crystalline structure, as can be observed by the difference between amorphous and crystalline pyroxene, indicated by sample 2 and 3. A difference can be observed between two types of silicates as demonstrated here by the difference between olivine ($[\text{Mg}, \text{Fe}]_2\text{SiO}_4$) and pyroxene ($[\text{Mg}, \text{Fe}]\text{SiO}_3$).

1.3.2 From X-ray laboratory studies of interstellar dust to extinction models

In order to derive the properties of ID from the X-ray spectra, it is necessary to have a set of detailed extinction cross section models to analyze the edges in the spectra. The composition of these models should reflect the dust present in the ISM. Since we know from observations that interstellar dust mainly consists of silicates and carbonaceous particles, we can measure the properties of similar types of dust in the laboratory. Many of these analogues have been developed, but their spectra are mostly measured at longer wavelength, with a focus on infrared studies. On the other hand, literature data of XAFS in edges interesting for astronomy, does not contain measurements tailored to use in the ID studies, since these edges are often measured for commercial and industrial purposes. When available in literature, these materials are mostly crystalline, while dust in the ISM appears to be mostly amorphous (Kemper et al., 2004). This lack of available models led to the start of laboratory measurement campaigns to create a database for edges of interstellar dust analogues (Lee et al., 2009; Costantini and de Vries, 2013).

In 2010 we started a large campaign at SRON Utrecht in the Netherlands (Costantini and de Vries, 2013). The aim is to measure XAFS of all the available edges in the X-ray band for a wide range of dust analogues, in order to avoid uncertainties in the interpretation of the X-ray spectra and to provide extinction models over a broad wavelength range. Since the X-ray band, with the edges of O, Si, Fe and Mg that can be observed with the available telescopes, is currently particularly suitable for silicates, we focused on these dust species. Each wavelength or energy range has its own dedicated laboratory instrumentation to measure the XAFS. For edges in the soft X-rays (<1 keV) scanning electron microscope, with a free electron laser, can be used to measure the edges of, for instance, O K and Fe L. At higher energies (1 - 10 keV) a dedicated beamline at a synchrotron facility can be used to measure the edges of e.g., Mg K-, Si K-, S K- and Fe K-edges. As an example, Figure 1.8 shows the resulting laboratory measurements of the Si K-edge.

From the resulting laboratory absorption measurements, the refractive index can be obtained. The complex refractive index is given by: $m = n + ik$, where the optical constants n and k are the respective real and imaginary part. The refractive index is an important property of materials, because when n and k are known, we can model how a material interacts with light. The two are related to each other through the Kramers-Kronig relations (see, Bohren, 2010, for an extensive review of the Kramers-Kronig relations). From the laboratory measurements, k can be obtained, and using the Kramers-Kronig equation n can be derived (described in detail in Chapter 2). The optical constants can consequently be used to derive extinction, which

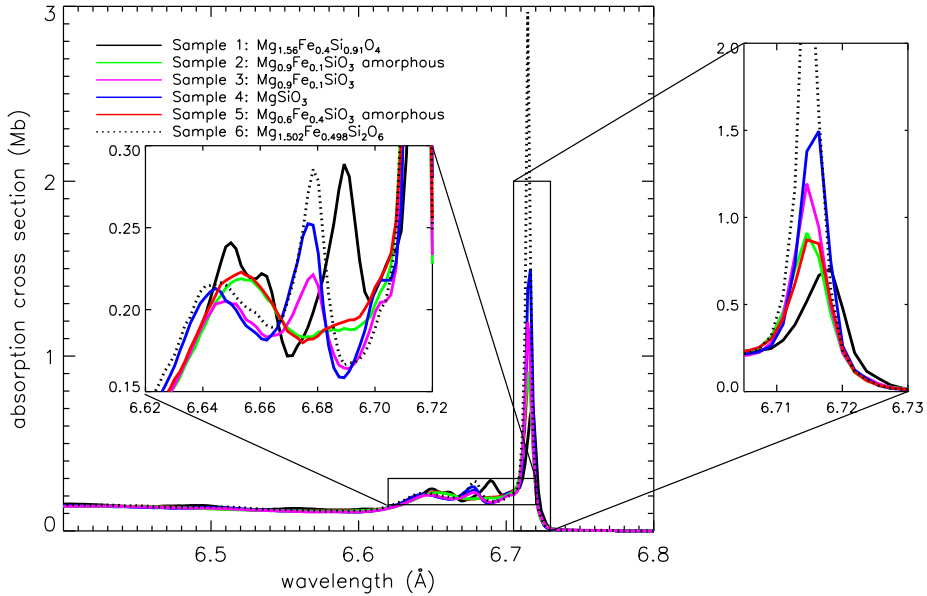


Figure 1.8: Figure taken from Chapter 2, showing the absorption cross sections of the Si K-edge of six silicate samples. The inset shows the XAFS, where the differences between the crystalline structures of olivines and pyroxenes can be observed by comparison of e.g., sample 1 and 4. The effect of amorphization can be observed by comparing e.g., sample 2 and 3, where some of the XAFS features are absent in the amorphous sample.

consists of absorption and scattering. There are several approximations to obtain the extinction efficiency (Q_{ext}). They all require energy, the optical constants and a particle size as input parameters. Figure 1.9 lists the different approximation methods of extinction. The most used approximations in the X-rays are Rayleigh-Gans, Mie Theory (Mie, 1908), which can only be used for spherical grains, and Anomalous Diffraction Theory (ADT, van de Hulst, 1957). It depends on the parameter space of interest (i.e., particle size and energy) which of these methods is preferred. These methods return Q_{ext} , per wavelength or per energy unit, particle size and, if required, per scattering angle. To obtain the total cross sections per energy or wavelength unit ($C_{\text{ext}} = \pi a^2 Q_{\text{ext}}$), we need to integrate over the particle size distribution. The size distribution has an important effect on the resulting extinction models, which is shown in Figure 1.10 and Chapter 2.

The extinction cross section models can be implemented in a spectral fitting code and the spectra of an X-ray source can consequently be fitted with the dust models (Figure 1.6). From these fits, we can obtain information on the composition, crystallinity and size distribution of the grains.

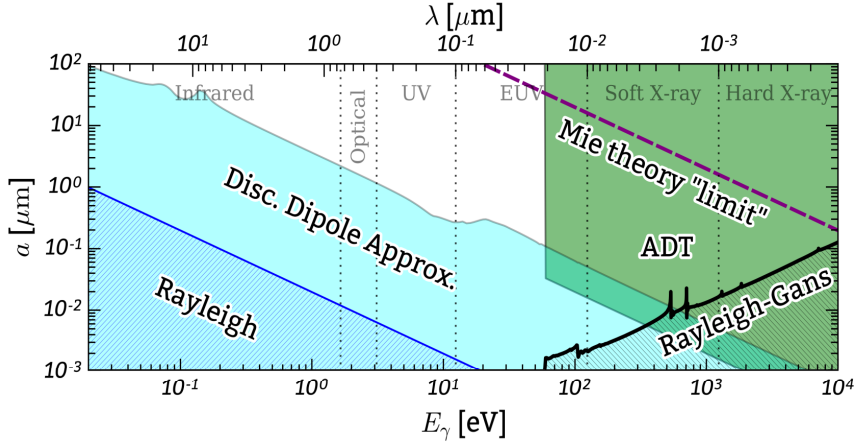


Figure 1.9: Validity regions for approximation schemes to calculate scattering and absorption by nonspherical dust grains. The Mie Theory is only valid for models with spherical grains. At X-ray energies Mie Theory, discrete dipole approximation (DDA), anomalous diffraction theory (ADT) and Rayleigh-Gans approximation can be used, depending on the energy range and the particle sizes involved. Adapted from Hoffman and Draine (2016).

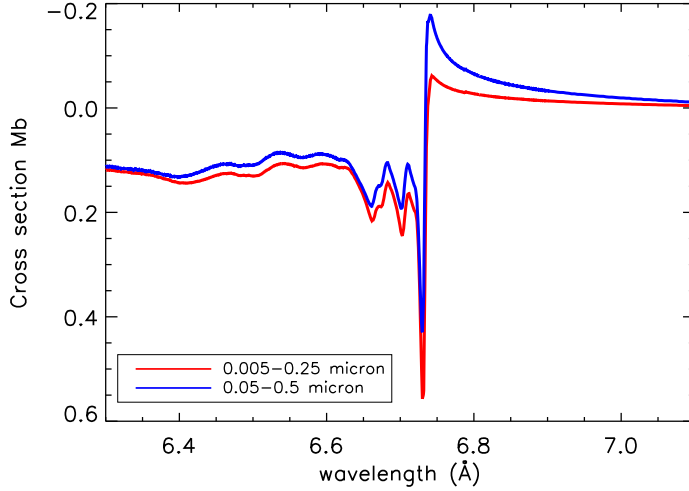


Figure 1.10: Two different size distributions that demonstrate the effects of scattering on the Si K-edge. The red line corresponds to an MRN size distribution. A size distribution with large particles is shown by the blue line. The difference can mainly be observed just before the edge, around $6.75\text{\AA}$, where the scattering feature near the edge is enhanced in the model that includes large particles, Chapter 2.

1.3.3 Mapping the dust in the Galaxy

For accurate modelling of interstellar dust, it is important to know whether the properties of dust change when the environment in which they are located changes. We can map the dust in different environments of the Galaxy by studying the extinction features of X-ray binaries along a variety of sight lines, since these sources are naturally distributed over the Galactic plane. The study profits from the large amount of archival data of these observatories, built up in the past 19 years. The spectra of many X-ray binaries have been observed and are currently publicly available in the corresponding databases, namely *Chandra* TGCat and the XMM-*Newton* Science archive. Not all the absorption edges can be accessed at the same time. When the column density increases, the soft energy X-rays will become more and more absorbed by the ISM. This allows to observe edges at higher energies for denser sightlines, provided that the source is bright enough at the wavelength of the edge and not all the X-rays are absorbed.

The diffuse sightlines have been studied using the O K-edge and Fe L-edge (Lee et al., 2009; Costantini et al., 2012; Pinto et al., 2013). A column density of $2 \times 10^{21} \text{ cm}^{-2}$ along the line of sight is necessary to observe the edges and study these environments.

From these observations, it was found that in these diffuse environments, 15-20% of the oxygen and 65-90% of the iron is depleted in dust (Costantini et al., 2012; Pinto et al., 2013). Along the line of sight of LMXB 4U 1820-30 Costantini et al. (2012) found that Mg-rich silicates and metallic iron fitted the edges of O K and Fe L, respectively. Therefore, they suggest that the dust may consist of iron-poor silicates with metallic iron inclusion, supporting the presence of GEMS in the ISM. After analyzing the spectra of 9 X-ray binaries, Pinto et al. (2013) find that the ISM appears chemically homogeneous on large scales, showing similar gas ionization ratios and dust mixtures. A limiting factor at that time was the sparse availability of models of the dust edges. Upcoming studies will be more elaborate on the dust content at these diffuse lines of sight (Psaradaki et al., in prep.). The X-rays also provide the opportunity to measure abundances of the elements of observable edges. For many elements, a gradient in the abundance can be observed, indicating that the abundance gradually increases toward the Galactic center (e.g., Rolleston et al., 2000; Pedicelli et al., 2009; Davies et al., 2009; Pinto et al., 2013). This gradient depends on the stellar elemental yields. In the X-rays, this increase in abundances is observed in the diffuse ISM for the elements O, Ne, Fe and Mg. However, most of these abundance gradients are not well defined in the central Galactic environment.

In this thesis, we study the most central part of the Galaxy, with high column-density sight lines. The dense ISM can be explored using the edges of Mg K (Rogantini et al., in prep.), Si K (Chapter 2 and 3), S K (Chapter 4) and Fe K (Rogantini et al., 2018). The Si K-edge is currently particularly suitable for this study, since it lies in the optimal point of the *Chandra* HETGS grating's effective area and resolution. In order to observe this edge, we need a line of sight column density of $1 - 10 \times 10^{22} \text{ cm}^{-2}$. Along these sight lines the X-rays will pass many dense areas, namely several spiral arms and the Galactic Bulge, depending on the distance of the source, as can be seen in Figure 1.11. This is ideal to study the dense areas of the Galaxy and investigate whether this environment is significantly different from the diffuse environments.

1.3.4 X-ray scattering haloes

X-rays are efficiently scattered at small angles by interstellar dust grains, producing a halo of diffuse emission around the source. This was first predicted by Overbeck (1965) and detected for the first time by Rolf (1983). The haloes are very narrow, usually of arcminute scale angular size, because X-rays are strongly forward scattered. The halo is very faint in comparison to the source, since it contains at most 20% of the brightness of the source (Predehl and Schmitt, 1995). In order to observe the halo, it is necessary to use sensitive instruments with sub arcminute angular resolution, which is provided by *XMM-Newton* and (especially) *Chandra*. The intensity and shape of the halo depend on the source flux from which the scattered X-rays originate, but also the particle size distribution, the chemical composition of the dust and the location of the dust grain along the line of sight (e.g., Mauche and Gorenstein, 1986; Predehl and Schmitt, 1995; Predehl and Klose, 1996; Costantini et al., 2005). The scattering haloes can therefore be used to constrain and test dust models (e.g., Smith et al., 2006). In order to derive the properties of the dust from the observations, the halo can be modelled. However, in the modelling, the position of the dust along the line of sight is degenerate with the dust size distribution and this degeneracy can only be broken in some special cases. For example, observations of expanding X-ray dust scattering rings around variable X-ray sources provide an opportunity to investigate the location of dust clouds along the line of sight (Tiengo et al., 2010). In Chapter 5 of this thesis, we explore the possibilities of observing a scattering halo produced by a debris disk. In this special case, the degeneracy is broken as well, since the position of the dust along the line of sight is known.

1.4 Thesis outline

High resolution X-ray spectroscopy is an important tool in interstellar dust studies. By studying dust features in X-ray spectra and scattering haloes around X-ray sources, we may be able to answer fundamental questions about interstellar dust, such as the composition of interstellar dust, the processing of dust in the ISM and the possible differences of the dust properties in different environments of the Galaxy. In this thesis, we mainly use the Si K-edge to study the properties of silicate dust, one of the main constituents of ID. The study profits from new laboratory data of interstellar dust analogues. Observing the Si K-edge requires high column densities and we therefore observe sources whose radiation passes through the dense environment of the central Galactic region.

Chapter 2

In this chapter, we present a pilot study of the Si K-edge in the observations of the X-ray binary GX 5-1. This bright X-ray binary is located near the Galactic center and the spectrum contains a prominent Si K-edge feature, as can be seen in Figure 1.11. We present laboratory measurements of silicate compounds that we took in 2012 at the Soleil synchrotron facility in Paris using the Lucia beamline. The sample set consisted of pyroxenes with varying Fe/Mg ratios and an olivine. Among the pyroxene silicates there were two amorphous samples present. Using the extinction models obtained from the laboratory data, we derived the properties of the interstellar silicate dust along the line of sight by fitting the Si K-edge seen in absorption

in the spectrum of GX 5-1. The impact of the presence of large particles along the line of sight is studied by modelling the edge with two different particle size distributions.

Chapter 3

In this chapter we used high-quality grating spectra of nine LMXBs to study the ISM in the central part of the Galaxy. The location of the sources can be observed in Figure 1.11. The sources are located in or near the Galactic Bulge. This is an old and probably well mixed environment of the Galaxy, which may be reflected by the composition of the dust we observe. The previous set of 6 samples present in Chapter 2 has been expanded to 15, including, i.a., amorphous olivine, and quartz samples. We use the Si K-edge in the high-quality spectra of the X-ray binaries provided by the *Chandra* observatory to study the properties of the dust along different sightlines. Moreover, we are able to study the abundance and depletion of silicon in detail in an area where it is otherwise difficult to obtain constraints on these parameters.

Chapter 4

In Chapter 4 we present an outlook for edge studies with future telescopes, as listed in Figure 1.3. We focus on the K-edges of C, S, Al, Ni, Ti and Ca. We make use of literature data for all the edges, with the exception of the Al K-edge, which was measured by us at Soleil with the Lucia beamline. We model the edges of these elements using the techniques developed in Chapter 2 and apply them to simulations of spectra produced by future X-ray telescopes taking into account the expected performance of the detectors concerning resolution and sensitivity. In the case of carbon and sulfur, the characterization of the chemistry of the absorbing dust can be determined. Observations of the sulfur edge may give more insight in the presence of sulfur in dust and in GEMS in particular. Since iron sulfates are thought to be an important constituent of GEMS, we use these compounds in our modelling. This characterization of the chemistry, will be more difficult for the other elements. The cosmic abundance of both Ni and Ti does not allow a detailed study of the features in the edge. Despite the high abundance, the modest changes in the shape of the edges of Al and Ca may not be significant do not show much variation. However, the observation of these edges will provide the opportunity to directly measure the depletions of these elements.

Chapter 5

In Chapter 5 we explore the theory of X-ray scattering for a new parameter space, where the small angle approach is no longer valid and where the size distribution of the dust includes large ($> 1 \mu\text{m}$) particles. We apply this theory, for the first time, to the environment of stellar debris disks where such conditions apply. We use as a best test case the debris disk around the star AU Microscopii. This star is a flaring M star, which is bright in the X-rays. A debris disk is a circumstellar belt of dust and debris. The sizes of the particles in the disk range from small dust particles up to large unobservable planetesimals (e.g., Lagrange et al., 2000; Wyatt and Dent, 2002). The system is well studied and we can make use of the known geometry of the disk. Since we know where the dust is located, we can model the predicted scattering halo using different dust composition. We find that models with a steeper slope, moderately strong

stellar wind model and a composition of silicates and graphite are the ones that would enhance a theoretical halo. After comparing the models with observations of the system, we find that the models do not produce a significant scattering halo, using the current spatial resolution. Future X-ray mission may enable us to observe the X-ray halo of debris disks. Such a X-ray telescope would require a PSF which has a FWHM < 0.5 arcsec, i.e., smaller than the FWHM of Chandra.

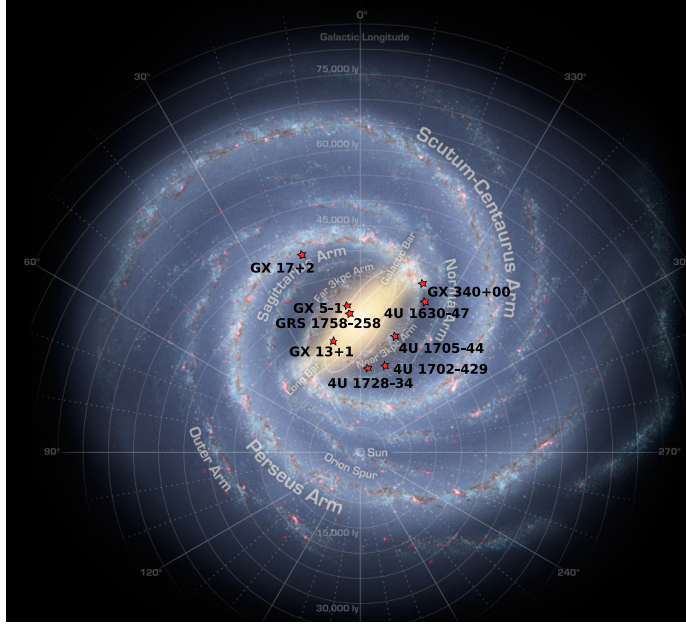


Figure 1.11: Artist's conception of a top-down view of the Milky Way, based on infrared images from NASA's Spitzer Space Telescope. The red stars indicate the position of the LMXBs studied in this thesis. Image credit: NASA/JPL-Caltech/R. Hurt

1.5 Future dust studies in the X-rays

There is a bright future for X-rays and interstellar dust. There are currently three upcoming X-ray observatories suitable for dust studies, which are currently at different stages of development. In chronological order this will be: XARM (expected to launch in 2021), Arcus (final selection in 2019, expected launch in 2023) and *Athena* (expected to launch in the early 2030s). These observatories will explore different parts of the energy spectrum, as is shown in Figure 1.3, allowing to study previously unavailable edges in detail. In the near future, there will be the XARM observatory, that will allow us to study the S and Fe K-edge. XARM is the successor of the lost Hitomi observatory and will have the same calorimeter detector characteristics on board (Mitsuda et al., 2014). The C K-edge will become available with the Arcus observatory around 2023 (Smith et al., 2017), if the mission is selected for the next phase in

2019. Around 2030, the *Athena* observatory containing the calorimeter X-IFU will provide us with unprecedented spectral resolution (Barret et al., 2016). It will be suitable to study the Fe K-edge in detail. Both the chemistry and the size distribution of the grains can be studied in detail (Rogantini et al., 2018). Using *Athena* and XARM, we will be able to discriminate between different dust species in the case of both Fe and S. Together these edges will be useful in the possible detection of GEMS in the ISM. Furthermore, *Athena* will allow to investigate the contribution of dust from less abundant elements, such as Al, Ni, and Ca. X-ray halo studies will profit from improvements in the spatial resolution. LYNX (also known as the X-ray Surveyor) and/or AXIS, may provide a spatial resolution that makes it possible to better constrain the dust size distribution and composition of the dust in for instance a debris disk system such as AU Mic.

Besides these new upcoming observatories, *Chandra* and *XMM-Newton* will still be available. Initially, these observatories would have a mission duration for 5 and 10 years respectively, but the missions have been extended several times. In 2016, following a very positive outcome from engineering studies, the *Chandra* team announced that it is planning and looking forward at least ten more years of operations. This will make it possible to observe more X-ray binaries and to re-observe other X-ray binaries in order to refine the quality of the observations.

Other advances will be obtained from laboratory studies. The aim for X-ray dust studies is to combine the measured edges of interstellar dust analogues in global extinction models over a broad wavelength range. Our campaign to measure all the relevant edges is currently ongoing, but by the time these new observatories will be put into operation, we will be ready to observe the extinction features of dust in detail.

Table 1.1: An inventory of circumstellar dust

material	AGB	Post-AGB	PN	Nova	T Tauri	Herbig AeBe	RSG	Wolf Rayet	LBV	SN Type II	Massive YSO
amorphous silicates	1, 2	1	1	1	1	1	1		1	1	1
crystalline forsterite	1, 2	1	1		1	1	1		1		
crystalline enstatite	1, 2	1	1		1	1	1		1		
aluminum oxide	1 (?), 2									2	
spinel	1 (?), 2									2	
TiO ₂	2										
hibonite	2										
MgO	1										
Fe	1 (?)									1	
PAHs	1, 2	1	1	1		1	1	(1)	1		
Amorphous carbon	2	1	1	1				1			
Graphite	2			2						2	
Diamond		1				1				2	
SiC	1,2		1	2						2	
other carbides	2	1 (?)								2	
Si ₃ N ₄										2	
MgS	1	1	1						1		
carbonate			1 (?)		1 (?)	1 (?)					
ice	1	1	1		1	1	1				1

1 - Astronomical data; 2 - Meteoritic data; AGB: Low mass ($< 8 M_{\odot}$) stars on the Asymptotic Giant Branch. Post-AGB: Low mass ($< 8 M_{\odot}$) stars in transition from the AGB phase to the planetary nebula phase. PN: The white dwarf remaining after the phase of prodigious mass loss on the AGB ionizes the ejecta forming a glowing nebula called a planetary nebula. Nova: The cataclysmic nuclear explosion caused by the accretion of hydrogen onto the surface of a white dwarf star. T Tauri: A low mass ($\sim 1 M_{\odot}$) protostar. Herbig AeBe: Intermediate-mass ($1.5 < M < 10 M_{\odot}$) pre main-sequence stars with spectral types A or B. RSG (Red supergiant): Late and cool ($T \sim 3000 K$) stage in the evolution of massive stars ($M > 8 M_{\odot}$). Wolf Rayet: Hot stars characterized by massive stellar winds; some condense carbon dust in their ejecta. LBV (Luminous blue variable): The most massive, brightest and bluest stars are variable and may experience periods of eruptive mass loss. SN type II: The explosion of a massive ($M > 8 M_{\odot}$) star at the end of its lifetime. Massive YSO: Luminous and massive protostar characterized by vast amounts of cold dust and gas. Astronomical identifications which are particularly ambiguous are labelled with (?) in this table. Table taken from Tielens et al. (2005).

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