X-ray impact on the protoplanetary disks around T Tauri stars

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ABSTRACT

Context. T Tauri stars have X-ray luminosities in the range $L_X = 10^{28} - 10^{32}$ erg s$^{-1}$. These luminosities are similar to their UV luminosities ($L_{UV} \sim 10^{30} - 10^{31}$ erg s$^{-1}$) and therefore X-rays are expected to affect the physics and chemistry of the upper layers of their surrounding protoplanetary disks.

Aims. The effects and importance of X-rays on the chemical and hydrostatic structure of protoplanetary disks are investigated, species tracing X-ray irradiation (for $L_X \geq 10^{30}$ erg s$^{-1}$) are identified and predictions for [O i], [C i], and [N ii] fine structure line fluxes are provided.

Methods. We implemented X-ray physics and chemistry into the chemo-physical disk code ProDiMo. We include Coulomb heating and H$_2$ ionization as heating processes and both primary and secondary ionization due to X-rays in the chemistry.

Results. X-rays heat the gas causing it to expand in the optically thin surface layers. Neutral molecular species are not significantly affected in terms of their abundance and spatial distribution, but charged species such as N$^+$, OH$^+$, H$_2$O$^+$, and H$_2$O$^+$ display enhanced abundances in the disk surface.

Conclusions. Coulomb heating by X-rays changes the vertical structure of the disk, yielding temperatures of ~8000 K out to distances of 50 AU. The chemical structure is altered by the high electron abundance of the gas at the disk surface, causing an efficient ion-molecule chemistry. The products of this, OH$^+$, H$_2$O$^+$ and H$_2$O$^+$, are of great interest for observations of low-mass young stellar objects with the Herschel Space Observatory. Both [O i] (at 63 and 145 μm) and [C ii] (at 158 μm) fine structure emission are affected only for $L_X > 10^{30}$ erg s$^{-1}$.

Key words. protoplanetary disks – methods: numerical

1. Introduction

Young stellar objects emit X-ray radiation (Koyama et al. 1994), which is associated with magnetic coronal processes (Flaccomio et al. 2005; Wolk et al. 2005; Imanishi et al. 2001), jets (Pravdo et al. 2001) mostly producing soft X-rays (Güdel et al. 2007), or outflows launched in the region between the star and the disk as predicted by the X-wind model (Shu et al. 2000). Non-accreting weak-line T Tauri stars (WTTS) are found to be more X-ray luminous than classical accreting T Tauri stars (CTTS) (Stelzer & Ertel 2001) mostly producing soft X-rays (Güdel et al. 2007), or GTTS (Güdel et al. 2007) found X-rays to be important in heating the surface layers of the disk. Gorti & Hollenbach (2004, 2008) include X-rays to predict [Ar II], [Ne II], [Fe I], [S I], [Fe II], and [Si II] as good indicators of gas physics in the disk. Woods & Willacy (2009) studied carbon isotope fractionation using the same method as Gorti & Hollenbach (2004) to calculate the X-ray ionization rates. Henning et al. (2010) studied the role of UV and X-rays on C$_2$H column densities and the excitation conditions in disks around T Tauri stars.

The scope of this paper is to take a step back and first perform a study of the impact of X-rays on the 2D disk structure, on molecular ionized species, and on observational diagnostics such as [O I], [C II], and [N II]. These molecular species were not studied in the above listed previous papers, but are of fundamental interest in the light of their detections with the Herschel satellites (Benz et al. 2010; Bruderer et al. 2010). We undertake an exploratory study of the relative effects of UV and X-rays on the protoplanetary disks hydrostatic, thermal, and chemical structure using a series of X-ray models with different $L_X$ (X-ray luminosity).

2. Model

The chemo-physical disk modeling code ProDiMo (Woitke et al. 2009; Kamp et al. 2010) has been updated with X-ray physics and chemistry.
Table 1. Examples of molecular dissociation and cross-section calculation.

<table>
<thead>
<tr>
<th>Molecule</th>
<th>Product 1</th>
<th>Product 2</th>
<th>Cross-section</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO</td>
<td>C 2⁺</td>
<td>O</td>
<td>σ_{CO} = 1/3σ_C +</td>
</tr>
<tr>
<td>C</td>
<td>O ²⁻</td>
<td>1/3(0.5σ_C + 0.5σ_O) +</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>O ³⁻</td>
<td>1/3σ_O</td>
<td></td>
</tr>
<tr>
<td>CH</td>
<td>C 2⁺</td>
<td>H</td>
<td>σ_{CH} = σ_C</td>
</tr>
</tbody>
</table>

Notes. CO dissociation can end up in three different channels, which are summed to give the total CO cross-section. CH is only assumed to follow one path. Molecules included: H₂, CH, NH, OH, CN, CO, N₂, SiH, NO, O₂, SiO, CH₂, NH₂, H₂O, HCN, CO₂.

2.1. Input spectrum

The incident stellar spectrum used in Woitke et al. (2009) is composed of a solar model with Teff = 5800 K and the chromospheric fluxes of HD 129333 (Dorren & Guinan 1994). The UV luminosity between 91.2 and 205 nm is L_{UV} ~ 4 \times 10^{31} \text{ erg s}^{-1}. Different models for the X-ray input spectrum are adopted in the literature: Nomura et al. (2007) use a two-temperature thin thermal-plasma model to fit the observed TW Hydrae spectrum; Ercolano et al. (2008) compiled synthetic coronal spectra using line and continuum emissivities from the CHIANTI compilation of atomic data; Gorti & Hollenbach (2008) use a thermal blackbody. We place the X-ray source on the star and follow Glassgold et al. (1997) and Igea & Glassgold (1999) in using an analytic input spectrum to describe the bremsstrahlung emission from an isothermal plasma \( F(E) \propto 1/E \cdot \exp(-E/kT_x) \) where \( E \) is the photon energy between 0.1 and 100 keV, \( kT_x = 1 \text{ keV} \), and \( T_x \) is the plasma temperature. The X-ray input spectrum is added to the input spectrum shown in Fig. 2 in Woitke et al. (2009).

2.2. X-ray chemistry

The following paragraphs describe the implementation of primary and secondary ionization in the code. Forty-one primary ionization reactions and 16 secondary ionization reactions were added to the chemical network.

Primary ionization

The primary rates for X-ray absorption are calculated following Meijerink & Spaans (2005) (Appendix D.3.1). The cross-sections are taken from Verner & Yakovlev (1995). Since X-rays are likely to be absorbed in the K-shells, we assume that every X-ray absorption leads to a single ionization for H, He, Si, and Cl and a double ionization for C, N, O, S, and Fe (Meijerink & Spaans 2005). We take into account molecular X-ray absorption, which always leads to dissociation, of the species. Table 1 lists two examples of how the total dissociation rates are calculated. When the difference in weight of the elements that form the molecule is large (e.g. CH, OH, H₂O etc.), we use the cross-section of the heavier element, when the weight is comparable (e.g. CO, CN, NO etc.) we combine the cross-sections of the single elements.

Secondary ionization

The fast electrons generated by the X-ray absorption can further ionize the gas. The rates are computed as shown in Meijerink & Spaans (2005, Appendix D.3.2) using experimental data from Lennon et al. (1988). The volumetric rates are a function of the local chemistry, i.e. they depend on the species densities \( n_H, n_H^0, n(\text{ion}) \), and \( n_e \) (where \( n_H \) is the hydrogen atom density and \( n(\text{ion}) \) is the hydrogen nuclei density). This has to be taken into account when solving the chemical equilibrium. The additional entries in the chemical Jacobian that come from the X-ray secondary ionization reactions are implemented following Sect. 5.6 in Woitke et al. (2009).

2.3. X-ray heating

We added Coulomb heating (Dalgarino et al. 1999) and H₂ ionization heating (Meijerink & Spaans 2005, Appendix B.1) to the heating processes listed in Woitke et al. (2009). The Maloney et al. (1996) heating rate holds only for gas with low \( x_e \), while Dalgarino et al. (1999) present the more general case for different high and low ionization gases (atomic/molecular). The heating efficiency increases by a factor of 7–8 in a highly ionized gas and a factor of 2 in a highly ionized molecular gas (Shull & van Steenberg 1985).

2.4. Parameter space

We computed five different models with increasing \( L_X \) to compare the results with the UV only case (model 1) for a disk surrounding a T Tauri star (Table 2). In model 1, X-rays are switched off. This is the model presented in Woitke et al. (2009). For more details, we refer to the original paper. X-ray models (model 2–5) have the same parameters as model 1, but include stellar X-rays (\( L_X = 10^{29} \to 10^{32} \text{ erg s}^{-1} \)). We added Cl, Cl⁺, and double ionized species (C²⁺, N²⁺, O²⁺, S²⁺, Fe²⁺) to the chemical network. The X-ray emission is treated as a point source at the location of the star.

3. Results

We analyze the results obtained from the five models described above. We first present the thermal and hydrostatic structure of the various models. We then describe the impact of X-rays on the chemistry and fine-structure line emission, focusing on the main differences between the UV-only model and the combined UV+X-ray models.
Temperature and density structure

The low density ($n_{\text{H}1} < 10^8 \text{cm}^{-3}$) surface layers directly exposed to X-ray radiation are heated efficiently by means of Coulomb heating; in all X-ray models, temperatures reach ~8000 K (Fig. 1). The extension of this high temperature region increases with $L_X$: it reaches 2 AU in model 2 and 100 AU in model 3 and 4. In model 5, the temperature is slightly lower for $r > 50$ AU but the whole disk is warmer (Fig. 1). X-rays dominate the thermal balance only in the upper layers down to $(X/\text{UV})_{\text{heat}} = 1$. Beyond $(X/\text{UV})_{\text{heat}} = 1$, UV heating takes over and becomes the main heating process. Deeper within the mid-plane, both X-ray and UV heating are negligible, but their ratio is again inverted and harder X-rays ($E > 10$ keV) deposit more energy than UV radiation (Fig. 2).

The inner wall of the disk is always directly illuminated by the stellar radiation causing the inner rim (0.5 AU < $r < 0.7$ AU) to have a large scale-height and hence vertical extent. In the UV model, the shadowed disk atmosphere beyond the inner rim has a lower vertical scale-height since radiation cannot penetrate efficiently and sustain high gas temperatures. Only radiation that impinges the disk at higher angles ($z/r > 0.6$) and scattered radiation reach the outer disk causing the temperature to increase and consequently the production of a second bump at ~9 AU. When X-rays are switched on, the temperature increase in the surface layers directly affects the vertical density distribution there since we keep the radial surface density profile fixed. The inner rim of the disk ($r < 1$ AU and $z/r > 0.1$) is more puffed up (Fig. 2). The second bump at ~9 AU is also more vertically extended; in model 5, it even “merges” with the inner rim and flares as a whole (Fig. 2, third panel).

Chemistry

The abundances of neutral molecules such as CO, OH, and H$_2$O generally change by less than an order of magnitude over the entire modeling space. On the other hand, the ion chemistry in the disk surface strongly changes: the electron abundance in the upper layers increases by a factor of $10^3$. This leads to an enhancement in the OH$^+$, H$_2$O$^+$, H$_2$O$^+$, and N$^+$ abundances. Secondary ionization of H$_2$ increases the H$_2$$^+$ abundances. H$_2$$^+$ collisions with H$_2$ produce H$_3$$. Subsequent collisions of H$_3$ + with O, OH, and H$_2$O lead to the production of OH$^+$, H$_2$O$^+$, and H$_3$O$^+$, respectively. Figure 4 shows how the vertical column densities of these species change with $L_X$ for three different disk radii: 3, 10, and 100 AU. Both OH$^+$ and H$_2$O$^+$ respond more efficiently than H$_2$O$^+$ to the X-ray radiation as the total mass ratio $M(\text{OH}^+)/M(\text{H}_2\text{O}^+)$ only doubles from model 1 to model 5, while $M(\text{OH}^+)/M(\text{H}_3\text{O}^+)$ increases by more than a factor of 5.

OH$^+$: OH$^+$ formation is enhanced approximately proportionally to the X-ray luminosity. Its total mass increases from $8 \times 10^{-15}$ $M_\odot$ in model 1 by a factor of 3.6 in model 3 to about a factor of 500 in model 5 (Table 4).
As the X-ray luminosity increases, OH\(^+\) formation is enhanced and pushed outwards, where the disk is colder. The column density of OH\(^+\) increases substantially beyond \(r > 10\ \text{AU}\) in all models. It reaches ~100 times its initial value (model 1) in model 3 at 100 AU (Fig. 4).

**H\(_2\)O\(^+\):** The \(\text{H}_2\text{O}\)^+ mass increases by a factor of 3 (a factor of 100) between model 1 and model 3 (and Model 5). The column density again increases toward the outer part of the disk. Model 3 has ~10 times higher column density than Model 1 at both 10 and 100 AU. As for OH\(^+\), \(\text{H}_2\text{O}\)^+ appears to move toward the outer part of the disk with increasing X-ray luminosity.

**H\(_3\)O\(^+\):** The \(\text{H}_3\text{O}\)^+ mass is slightly less affected by X-rays: it is two times higher than in the UV case in model 1 and ten times in model 4. In model 3, model 4, and model 5, the region of high \(\text{H}_3\text{O}\)^+ abundances is also clearly pushed to larger radii and hence the species mass averaged temperature becomes lower.

**N\(^+\):** We find the most extreme mass increase for N\(^+\) in all X-ray models (Table 4) and at all radii: in model 3, it is 1000 times higher than in the UV-only case.

In models 4 and 5, the N\(^+\) mass increases proportionally in the outer part of the disk (Fig. 4, right lower panel). Figure 5 shows the column density ratio of the X-ray dominated N\(^+\) to the UV dominated C\(^+\). With increasing \(L_X\), the N\(^+\) column density is enhanced by two (outer disk) to six (inner disk) orders of magnitude.

**Line predictions**

In Table 3, we list the flux prediction of [O\(\iota\)] 63 \(\mu\)m, [O\(\iota\)] 145 \(\mu\)m, [C\(\iota\)] 157 \(\mu\)m, and [N\(\iota\)] 205 \(\mu\)m for all the models. Figure 3 shows their values as a function of the X-ray luminosity. The [N\(\iota\)] line flux shows the strongest correlation with the X-ray flux, increasing by five orders of magnitude from model 1 to model 3. The oxygen fine-structure line fluxes and the [C\(\iota\)] line flux are constant from model 1 to 3 (Fig. 3), because they originate in the UV-heated layer. Only in models 4 and 5 do the line fluxes increase with \(L_X\).

**4. Discussions and conclusions**

We have found that X-rays mainly impact the surface layers of protoplanetary disks. The hydrostatic structure of these layers is changed significantly: X-ray radiation is mostly absorbed in the tenuous layers (\(c/r \geq 0.2 \text{ cm}^{-2}\)) increasing the temperature to \(\sim 8000\ \text{K}\); at those temperatures, cooling by [O\(\iota\)], Fe II, and Ly\(\alpha\) balance the X-ray heating. This causes the density structure to flare more strongly than in the UV-only case (Fig. 2).

The general results of Nomura et al. (2007) and Glassgold et al. (2004) are qualitatively confirmed, showing that the inner rim and the surface layers are dominated by X-rays. In addition, we have found that the more distant parts, out to 100 AU, are also affected (Fig. 4). We find that the size of the high temperature X-ray driven region increases with \(L_X\). This is because our model uses the Dalgarno et al. (1999) prescription for X-ray heating and of our choice of the input spectrum. The heating efficiencies of Dalgarno et al. (1999) lead to \(\approx 7\)–8 times higher rates in regions with high electron fraction, than Maloney et al. (1996). Furthermore, our input spectrum has higher photon flux in the range 0.1–0.3 keV than, e.g., Gorti & Hollenbach (2008) and Nomura et al. (2007). These soft X-ray photons are absorbed at low vertical column-densities causing high e\(^-\) densities there and are thus more efficient in heating the upper layers. This was also noted in Gorti et al. (2009).

Gorti & Hollenbach (2008) found X-rays to be the dominant heating process in slightly deeper layers than we do. This is most likely because we include UV scattering from dust, which leads to a more substantial vertical penetration of FUV radiation into the disk. Nomura et al. (2007) also show that FUV penetrates deeper than X-rays, because FUV scattering is more efficient than X-ray Compton scattering at 1 keV, which is not included in our model. Gorti & Hollenbach (2008) also consider a less steep
of OH and H$_2$O are a characteristic signature of an X-ray dominated region as discussed by van der Werf et al. (2010) after the detection with Herschel/SPIRE in the ultra-luminous galaxy Mrk 231. Furthermore, this is extremely interesting in the context of the detection of these species in a massive YSO by Herschel (Benz et al. 2010). The column densities that we find from our X-ray irradiated disks are of the same order of magnitude as those derived in Benz et al. (2010). This suggests that a disk could in principle provide a substantial contribution to the line fluxes emitted from these molecules, making our result extremely relevant to future Herschel studies of low-mass YSOs.

The abundance of these ions increases especially at larger radii ($r > 10$ AU), while the N$^+$ abundance rises considerably at all radii. The latter is not observed in the UV model because of the high ionization potential of N(I)+ = 14.5 eV. We have found that the N$^+$ flux emitted at 205 $\mu$m in model 3 is $\sim 5 \times 10^{-22}$ W/m$^2$, coming for 90% from the upper layers beyond 10 AU. This is much smaller than the current Herschel sensitivity limit of $5 \times 10^{-18}$ W/m$^2$ (HIFI, 5$\sigma$ in 1 h) and even below current sensitivity estimates for SPICA/SAFARI ($10^{-19}$ W/m$^2$, 5$\sigma$ in 1 h). We have only considered X-ray ionization, but the flux is unlikely to change if EUV is present. Additional ionization occurs only at smaller radii, because of the low penetration depth of EUV radiation (Hollenbach & Gorti 2009). The formation of molecular ionized species moves toward the outer disk as $L_X$ increases.

5. Outlook

Our predicted N$^+$ line fluxes are too low to be observed with current instruments. In contrast, the [OI] 63 $\mu$m and [CII] 157 $\mu$m lines are observable in the presence of UV luminosities of $\sim 10^{31}$ erg s$^{-1}$ and/or strong X-rays ($L_X > 10^{30}$ erg s$^{-1}$). In the context of the Herschel observatory, the OH$^+$, H$_2$O$^+$, and H$_2$O$^+$ lines are extremely interesting as they are likely to be observable with the HIFI, PACS, and SPIRE instruments. These hydride ions and the already observed [Ne II] and [Ar II] line fluxes, will be addressed in a future paper (Aresu et al., in prep.). We will also investigate a larger parameter space and the effect of the change in disk structure – especially of a higher inner rim and greater flaring – on the overall SED. Future work will also include the creation of a grid of X-ray models following the Woitke et al. (2010) approach.

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