Compton Shoulder Diagnostics in Active Galactic Nuclei for Probing the Metallicity of the Obscuring Compton-thick Tori

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Abstract

We analyzed the spectral shape of the Compton shoulder around the neutral Fe–Kα line of the Compton-thick type II Seyfert nucleus of the Circinus galaxy. The characteristics of this Compton shoulder with respect to the reflected continuum and Fe–Kα line core intensity are powerful diagnostics tools for analyzing the structure of the molecular tori, which obscures the central engine. We applied our Monte-Carlo-based X-ray reflection spectral model to the Chandra High Energy Transmission Grating data and successfully constrained the various spectral parameters independently, using only the spectral data on the Fe–Kα emission line. The obtained column density and inclination angle are consistent with previous observations and the Compton-thick type II Seyfert picture. In addition, we determined the metal abundance of the molecular torus for the case of the smooth and clumpy torus to be $1.75^{+0.19}_{-0.17}$ and $1.74 \pm 0.16$ solar abundance, respectively. Such slightly over-solar abundance can be useful information for discussing the star formation rate in the molecular tori of active galactic nuclei.

Key words: galaxies: active – galaxies: individual (Circinus) – galaxies: nuclei – galaxies: Seyfert – techniques: spectroscopic

1. Introduction

The large amount of luminosity of active galactic nuclei (AGNs) is sustained by gas accretion onto supermassive black holes (BHs) at the center of each galaxy. The accretion disk and the BH are surrounded by an optically thick, dusty torus (e.g., Telesco et al. 1984; Antonucci & Miller 1985). A large geometrical thickness of the torus (Lawrence 1991; Antonucci 1993) indicates that numerous dusty clumps, rather than a smooth mixture of gas and dust, constitute the torus with a large clump-to-clump velocity dispersion (Krolik & Begelman 1988).

The torus is illuminated by the central accretion disk (e.g., Glass 2004; Suganuma et al. 2004). Since the disk illumination is weak toward its mid-plane, the innermost edge of the torus can connect with the outermost edge of the accretion disk continuously (Kawaguchi & Mor 2010). Specifically, the torus potentially acts as the role of a reservoir for the gas inflow to the accretion disk, with mutual influences. Although various clumpy torus models for the infrared emission of AGNs have been developed (e.g., Nenkova et al. 2002, 2008; Hönig et al. 2006), the observed near-infrared emission is not explained by these models in many cases (e.g., Mor & Netzer 2012; Leipski et al. 2014). Accordingly, fitting for the observed mid-infrared emission is not enough for solving the degeneracy among various parameters (the clump size, the metallicity, the viewing angle, etc.).

The Compton shoulder (e.g., Matt et al. 2004). The flux ratio of the Compton shoulder with respect to the line core depends on both the column density of the reflection material $N_{\text{H}}$ and the Fe abundance (Matt 2002; Furui et al. 2016). For example, although the metallicity of the Circinus galaxy is estimated to be $1.2$–$1.7$ solar via the depth of the Fe–Kα edge (Molendi et al. 2003), the depth, in principle, also depends on $N_{\text{H}}$ (Yaqoob et al. 2015). The Fe–Kα flux and the continuum shape also depend on these parameters, and hence X-ray spectroscopic data of binaries and AGNs around the Fe–Kα line enables us to constrain various parameters (Furui et al. 2016; Odaka et al. 2016).

In this paper, we applied a developed X-ray reflection spectral model for the two types of density structures (smooth and clumpy) of the torus of the AGN to constrain these parameters independently, focusing on the structure of the Compton shoulder. In the next section, the data we used is briefly introduced. Then, we present the spectral modeling (Section 3) and the results (Section 4). Finally, we carry out discussions, followed by the conclusion of this study.

2. Observations and Data Reduction

Shu et al. (2011) reported the analysis result of 10 Compton-thick type II Seyfert galaxies observed by the Chandra High Energy Transmission Grating (HETG) and their detailed analysis for the Fe–Kα line width constrained the line-emitting region. Because of the excellent energy resolution of the Chandra HETG, some of their samples show a hint of the spectral structure due to the Compton shoulder in the foot region of the Fe–Kα line emission, such as the galaxies NGC1068, Centaurus A, NGC4388, and the Circinus galaxy. The Fe–Kα line intensity of the Circinus galaxy is the highest among the samples of Shu et al. (2011) and the structure of the Compton shoulder was the most distinctive. Therefore, we selected the Circinus galaxy for our analysis.
The Circinus galaxy was observed by the *Chandra* HETG four times from 2000 June to 2004 November, with a net total exposure of about 185 ks. Table 1 gives a summary of these observations. We utilized the archival *Chandra* data and reduced the data with the software package *Chandra* Interactive Analysis of Observations (CIAO) v4.10 with the calibration data base (CALDB) version of 4.7.3, followed by standard analysis procedures described in the CIAO analysis thread for the HETG/ACIS-S Grating Spectra. The *chandra_repro* task has been applied for the standard data distribution to extract grating spectra and detector responses. Although higher orders of the grating data provide a higher energy resolution, we used only the first orders of the grating data because only the first orders of the data allow for the investigation of the feature of the Compton shoulder for its better photon statistics. We combined the positive and negative arms with the *combine_grating_spectra* script provided by CIAO. The background spectrum was extracted from the original combined data format using the *tg_bkg* script so that we could deal with the *Chandra* HETG spectra using the XSPEC. Finally, we combined all of the spectra and detector responses of the four observations into one file with the *mathpha* and *addrmf* tools in the standard *FTOOLS*. The reduced spectrum was analyzed using the spectral fitting tool XSPEC (Arnaud 1996). We utilized the C-statistics for the minimization without any energy-binning procedures. All the quoted errors in the following sections were of a 90% confidence level. The spectral fitting was employed in the 4–8 keV energy band to avoid any contamination of the complicated spectral features, which are often reported for the type II Seyferts in the soft X-ray energy band (Bianchi et al. 2006).

The *Chandra* HETG grating spectroscopy is performed by analyzing the dispersion image, which is accumulated by the X-ray telescope. By extracting dispersion spectra following the standard *chandra_repro* processes, the extracted zeroth-order, nondispersed image extends up to at least the 5′ scale, which is larger than the point-spread function (PSF) of the *Chandra* HRMA. Therefore, our analyzed spectrum could include not only the central torus region but also a more extended outer region. The central torus region, whose radius of ∼30 pc (<(1 − 1.5)⁰), based on the ALMA observation (Izumi et al. 2018), is considered the main contributor of the Fe–Kα line for Circinus (Marinucci et al. 2013), and thus we fit the extracted X-ray data with our torus model.

### 3. Spectral Modeling and Analysis

The observed X-ray emission from obscured AGNs consists of several continuum components and complicated emission line profiles. A Comptonized emission by the hot corona around the central black hole can be observed as the simple power-law shape up to the hard X-ray regime. However such a direct component cannot be observed below 10 keV for the Compton-thick object, due to the strong absorption by the surrounding torus. Instead, various reflected and scattered emissions are observed in this energy range. The reflection component from the Compton-thick tori consists of a Compton scattered hard spectrum with various line emissions, including a prominent Fe–Kα line and its Compton shoulder. For analyzing the characteristics of this Compton shoulder from the reflection component, which is the main goal of this study, an accurate modeling of the reflected and scattered continuum is essential. We consider other additional spectral components: the scattered continuum from a distant region such as the narrow-line region and various ionized lines that are not included in our current reflection model. Figure 1 shows a schematic picture of our baseline model used for this analysis. The details of the modeling for each component are given below.

#### 3.1. Reflection Component from the Compton-thick Torus

Odaka et al. (2011) developed a Monte Carlo simulation framework to calculate the radiation transfer in the astronomical object (MONACO) and we have already succeeded in reproducing the reflection component from the AGN by applying this framework (Furui et al. 2016). This model has many parameters, including metal abundance, absorption column density, density distribution inside the torus (smooth or clumpy), etc. Furui et al. (2016) found that these parameters influence the strength and the shape of the Compton shoulder, indicating that the Compton shoulder can solve the degeneracy among various parameters using data with high enough energy resolution. Odaka et al. (2016) demonstrated that a degeneracy between the metallicity and the column density of a reflection material (for a slab or spherical geometries) is solved by utilizing the *Chandra* HETG data of a high-mass X-ray binary GX 301-2. We apply the torus model to the Compton shoulder of the AGN to comprehend the extent to which the degeneracies of these parameters are solved. In this analysis, we free three parameters for our torus model: hydrogen column density at the torus mid-plane N_H, metal abundance, and the inclination angle for the observer (θ_in) as well as the normalization. We changed the abundance of all metals heavier than beryllium, keeping the same ratio as that from the solar abundance table of Anders & Grevesse (1989). The important parameter of this analysis is the normalization ratio between the Fe–K emission line and its Compton shoulder. Therefore, we can say that if we change only the iron abundance, our results would not be changed so much. We fixed other several parameters: the opening angle of the torus, the innermost radius of the torus, and the turbulent velocity of the torus element, set to 60°, 2 × 10⁶ cm, and 0 km s⁻¹, respectively. In the clumpy model, the volume-filling factor of the clump and the scale factor of each clump (the ratio of radii between each clump and the torus) are set to 0.05 and 0.005, respectively. According to Furui et al. (2016), the parameters related to the clumpy torus...
(the volume-filling factor and scale factor of clumps) do not affect to the shape and ratio with respect to the continuum of the Compton shoulder which are important features to determine the three parameters that we focused on here, and other parameters related to the torus geometry could affect to the normalization of the reflection but would not change the features around the Compton shoulder.

In addition, we set the absorption column density of the direct (transmitted) component (Section 3.2) to \( N_{\text{H}} \), in order to take into account the fact that our simulation model assumes the donut-shaped material distribution of the torus. The spectral shape of emission lines, including Fe–K\(\alpha\), and their Compton shoulder are calculated based on the Monte Carlo simulation. We examined both the smooth and clumpy torus models to constrain the density structure of the torus with the characteristics of the Compton shoulder. Then, we discuss how and to what extent the derived parameters differ from each other.

### 3.2. Direct Continuum from the Nucleus

We introduce the direct emission component, albeit contributing little for Compton-thick objects, since it affects to the estimation of the intensity of the scattered continuum component as described below. The spectral model of this component is the simple power-law model with a fixed photon index value of 1.9, which is a typical value for the type-I AGNs whose direct component is observed. It is difficult to constrain the normalization of this direct component by the Chandra HETG data due to the limited energy band. In the spectral fitting, the normalization is scaled so that the Compton reflection component (Section 3.1) and this direct component have similar number counts around 7.0 keV for \( N_{\text{H}} = 10^{24} \text{ cm}^{-2} \), which is found in our Monte Carlo simulation for an inclination angle of \( \cos \theta \sim 0.3 \) and \( N_{\text{H}} \sim 10^{24} \text{ cm}^{-2} \).

### 3.3. Scattered Continuum from the Distant Region

Sometimes, a power-law component is required in addition to the reflection component, even for the Compton-thick object at a softer energy band. The spectrum of this additional power law, with the photon index identical to the primary power law (1.9 in this analysis), is much softer than the reflection. This additional component is believed to come from the scattering of the direct component by less dense material located at the distant region compared with the Compton-thick torus, for instance the narrow-line region (Awaki et al. 2000, 2008; Matt et al. 2009). The fitted structure of the Compton shoulder should be sensitive to the reflected continuum, and fitting for the reflected continuum is also affected by such an additional power-law component. Therefore, we added this component to our model. We set the constraint on the normalization parameter as the ratio with respect to the direct component (before attenuation by the torus). This flux ratio is estimated to be between 0.001–0.05 (Bland-Hawthorn et al. 1991; Bland-Hawthorn & Voit 1993; Matsumoto et al. 2004). We found that the value of 0.001 gives the best fit to our data. Thus we apply this ratio in the following analysis.

### 3.4. Ionized Emission Lines

In the X-ray spectrum from the AGN, not only a neutral Fe–K\(\alpha\) emission but also other emission lines from highly ionized materials are often observed (Iwasawa et al. 1997; Matt et al. 2004). We found that the Chandra HETG spectrum of the

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**Figure 1.** Schematic image of our baseline model. The solid, dotted, and dotted–dashed arrow lines represent the direct, reflection, and scattered component, respectively, which are mainly introduced in this analysis. An example of the simulated spectrum is also shown, where the contribution of each component to the overall spectrum can be seen.
Figure 2. Spectral fitting result using our baseline model. The green dashed, orange dashed–dotted, red dotted, magenta dashed–dotted–dotted, and black solid lines represent the reflection, scattered, direct, emission line component, and their combination, respectively. The left and right panels show the results obtained by the smooth and clumpy torus structures as the reflection component, respectively.

Table 2
Summary of the Obtained Spectral Parameter in Our Analysis

| Smooth Torus Model | Reflection Component | Direct Component | Scattered Component |
|--------------------|----------------------|-------------------|---------------------|
| $N_H$ [$10^{22}$ cm$^{-2}$] | incl. ($\cos^2\theta_{ia}$) | MA$^a$ | $N_H$ [$10^{22}$ cm$^{-2}$]$^b$ | $\Gamma$ | $\Gamma$ | Scale Factor$^c$ | $\chi^2$(d.o.f) |
| 355±50.8 | 0.24$^{+0.17}_{-0.08}$ | 1.98$^{+0.20}_{-0.19}$ | 1.9 (fixed) | 1.9 (fixed) | 0.003 | 1.47 (580) |
| 406±56.7 | 0.26$^{+0.12}_{-0.10}$ | 1.75$^{+0.19}_{-0.17}$ | 348 | 0.001 | 1.43 (580) |
| 410±53.2 | 0.27$^{+0.12}_{-0.09}$ | 1.71$^{+0.21}_{-0.19}$ | 340 | 0.0003 | 1.41 (580) |
| 411±52.4 | 0.28$^{+0.11}_{-0.09}$ | 1.70$^{+0.21}_{-0.19}$ | 339 | 0.0002 | 1.43 (580) |

| Clumpy Torus Model | Reflection Component | Direct Component | Scattered Component |
|--------------------|----------------------|-------------------|---------------------|
| $N_H$ [$10^{22}$ cm$^{-2}$] | incl. ($\cos^2\theta_{ia}$) | MA$^a$ | $N_H$ [$10^{22}$ cm$^{-2}$]$^b$ | $\Gamma$ | $\Gamma$ | Scale Factor$^c$ | $\chi^2$(d.o.f) |
| 404±40.7 | 0.34$^{+0.04}_{-0.09}$ | 1.98$^{+0.17}_{-0.18}$ | 296 | 1.9 (fixed) | 1.9 (fixed) | 0.003 | 1.46 (580) |
| 465±54.3 | 0.35$^{+0.08}_{-0.09}$ | 1.74$^{+0.16}_{-0.16}$ | 326 | 0.0001 | 1.44 (580) |
| 494±61.8 | 0.30$^{+0.08}_{-0.07}$ | 1.66$^{+0.16}_{-0.16}$ | 338 | 0.0003 | 1.43 (580) |
| 499±63.3 | 0.37$^{+0.07}_{-0.07}$ | 1.65$^{+0.16}_{-0.16}$ | 338 | 0.0002 | 1.44 (580) |

Notes. $^a$MA stands for the metal abundance, which is scaled to the solar value. 
$^b$The column density for the direct component is related to that of the reflection component as a function of $N_{H,\text{direct}} = N_{H,\text{refl}} \times \sqrt{1 - 4 \cos \theta_{ia}}$, see the text for details.
$^c$Normalization of the scattered component is scaled from that of the direct component by this factor.

Circinus galaxy also show complicated line structures around the $6.5 \sim 7.0$ keV energy band. First, we added multiple Gaussian functions to represent all of the emission and absorption features, but we found that it was difficult to identify the origin of most of the fitted lines and it did not affect the structure of the Compton shoulder. Although the $\Delta \chi^2$ value is not negligible ($\Delta \chi^2 \sim 50$ for the 580 to 575 change of the degree of freedom), we just left two of the most prominent and easily understandable emission lines and one absorption line, which come from He- and H-like iron (6.70 keV and 6.97 keV for emission lines and around 6.79 keV for the absorption line), respectively.

We also considered a galactic absorption and line broadening due to the random motion of the emitting/reflecting gas by the Gaussian convolution with the $gsmooth$ model in XSPEC. Since our reflection model calculated the spectrum in only a source frame, we introduce the redshift effect using the $zshift$ model. Therefore, our baseline model consists of the formula $gsmooth \times zwabs \times (PL_{scat} + zwabs \times PL_{direct} + zshift \times Reflection + emission\_lines)$.

4. Results

Figure 2 shows the Chandra HETG spectrum and fitting result of our baseline model, together with each spectral component, as we described in Section 3. We examined two torus models, the smooth and clumpy torus. As shown in the Figure 2, both torus models fit the observed data well and significant differences did not appear in this analysis. The summary of the obtained spectral parameters is given in the
Table 2. We obtained the column density of $4.1^{+1.9}_{-0.6}$ and $4.7^{+1.1}_{-0.5} \times 10^{24}$ cm$^{-2}$ for both torus models and they are consistent within the statistical errors. These values are consistent with the previous picture that this object is in the Compton-thick state and similar to the value that was reported based on the broadband spectroscopy by Suzaku ($4.6^{+0.47}_{-0.23} \times 10^{24}$ cm$^{-2}$; Yang et al. 2009) and NuSTAR ($6 - 10 \times 10^{23}$ cm$^{-2}$; Arévalo et al. 2014). We successfully constrain the inclination angle to be $\cos \theta_{\text{ini}}$ with the values of $0.26^{+0.08}_{-0.10}$ and $0.35^{+0.08}_{-0.09}$ for the smooth and clumpy torus models, respectively, even if we free this parameter. Since the torus mid-plane and our line of sight are parallel for $\cos \theta_{\text{ini}} = 0$, the obtained inclination angle means a nearly edge-on view of the torus. Interestingly, we also constrain the metal abundance for both the smooth and clumpy torus models to $1.75^{+0.12}_{-0.17}$ and $1.74^{+0.16}_{-0.16}$ solar, respectively. Our baseline model successfully constrains not only the absorption column density but also inclination angle and even metal abundance, despite only analyzing a limited energy band from 4 to 8 keV. As we discussed above, the Compton shoulder diagnostics with our reflection model give this great constraint.

We try to find any differences between our smooth and clumpy torus models to discuss whether Compton shoulder diagnostics are also useful in constraining the intra-torus structure. Figure 3 shows the comparison of the confidence contours between the smooth and clumpy torus models for these three parameters. We cannot see any clear differences between the smooth and clumpy torus models (other than a trend that the clumpy model tends to show a slightly larger $\cos \theta_{\text{ini}}$) even in these parameter spaces and we cannot conclude by our analysis which torus model is better. Furui et al. (2016) suggested that different behaviors can be observed based on the simulated spectra of the Hitomi SXS. Therefore, higher-resolution spectroscopy with a much better signal-to-noise ratio will show the difference of such parameter correlations with respect to not only column density but also metal abundance, and it could be very useful in constraining the torus structure.

5. Discussion

Since several torus parameters such as the inclination angle, metal abundance, and column density are degenerate, many X-ray studies for modeling the torus structure have assumed fixed parameter sets, e.g., solar abundance (Massaro et al. 2006; Arévalo et al. 2014). We have successfully constrained these three parameters without any restrictions utilizing the combination of the Chandra HETG high-resolution spectroscopic data and spectral modeling of the Compton shoulder based on the detailed Monte Carlo simulation, even when we used data only around the Fe–K$_\alpha$ emission line. This means that the Compton shoulder could be a strong diagnostics tool for analyzing the torus structure. Furui et al. (2016) have already suggested this possibility by showing the dependence of the structure of the Compton shoulder and other parameters based on the detailed studies of the simulated reflection spectral model. For example, the ratio of the intensity between the Fe–K$_\alpha$ line core and the Compton shoulder depends on the metal abundance in a manner different from the $N_{\text{H}}$ dependency of the Fe–K$_\alpha$ flux. In this study, we have proved this concept by applying this reflection model to the actual observational data. Our analysis showed that the metal abundance of the Circinus galaxy is slightly higher than that of the solar abundance (e.g., $1.75^{+0.19}_{-0.17}$ for the smooth torus case). This over-solar abundance we obtained through this analysis is consistent with the metallicity in narrow-line regions (over 100 pc–1 kpc scales in general) of other AGNs ((1-4) solar; Groves et al. 2006; Du et al. 2014). In this study, we estimate the metallicity of the torus on much smaller scale (tens of parsecs).

Star formation in clumpy tori may play a major role in angular momentum transport in tori (e.g., Vollmer & Beckert 2003; Vollmer et al. 2008). Wutschik et al. (2013) developed such a model to explain nearby AGNs, obtaining a star formation rate of $\sim 1 M_\odot$ yr$^{-1}$ in tori. Our measurement implies that the star formation in the torus should not be at an enormous rate if the star formation governs the gas inflow within the torus.

Another important challenge of this study is the investigation of the detailed torus structure by applying the different torus modeling, the smooth and clumpy models, to the observational data. Unfortunately, we cannot obtain a significant discrimination of these two torus models with this analysis. Broadband spectroscopy up to the hard X-ray energy band to detect the direct component could bring a further constraint on the column density of the torus independently. Therefore, the simultaneous combination of the high-resolution spectroscopy around the Fe–K$_\alpha$ line and the hard X-ray observation are important. It is encouraging to perform deep Chandra HETG observations for the type II Seyfert galaxy and the simultaneous observations by NuSTAR and it is also interesting to compare the parameters that are determined by such broadband continuum and our Compton shoulder diagnostics, or further high-resolution spectroscopy by the future missions of XARM (Tashiro et al. 2018) and ATHENA could provide a finer
spectral modeling of both the Compton shoulder and the continuum.

6. Conclusion

In this study, we have demonstrated that various torus parameters, including the hydrogen column density at the midplane, $N_\text{H}$, the inclination angle, and metal abundance, can be constrained independently with the Chandra HETG high-resolution spectroscopy of the Compton shoulder using only the limited energy band around the Fe–K$\alpha$ emission line. We applied the developed Monte-Carlo-based X-ray reflection spectral model to the Circinus galaxy, and obtained the hydrogen column density of the molecular torus as $\sim 4 \times 10^{24}$ cm$^{-2}$, which is consistent with that reported based on the broadband spectroscopy. In addition, the inclination angle and the metal abundance were successfully determined without fixing other parameters. The obtained inclination angle means that this object is viewed at nearly an edge-on geometry. The important result of this study is that we constrained the metal abundance of the molecular torus to be slightly over-solar abundance ($\sim$1.75 solar), which could give information about the evolution of an environment around the supermassive black hole, such as the star formation history around the molecular torus. Further higher-resolution and spatially resolved spectroscopy, which would be brought by future missions such as XARM and ATHENA, can measure not only these parameters from many other type II Seyferts, but also can give a discrimination of the detailed torus geometry such as smooth and clumpy density profiles.

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