Letter

Probing Cosmic Rays with Fe Kα Line Structures Generated by Multiple Ionization Process

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Abstract

Supernova remnants (SNRs) have been regarded as major acceleration sites of Galactic cosmic rays. Recent X-ray studies revealed neutral Fe Kα line emission from dense gas in the vicinity of some SNRs, which can be best interpreted as K-shell ionization of Fe atoms in the gas by sub-relativistic particles accelerated in the SNRs. In this Letter, we propose a novel method of constraining the composition of particles accelerated in SNRs, which is currently unknown. When energetic heavy ions collide with target atoms, their strong Coulomb field can easily cause simultaneous ejection of multiple inner-shell electrons of the target. This results in shifts in characteristic X-ray line energies, forming distinctive spectral structures. Detection of such structures in the neutral Fe Kα line strongly supports the particle ionization scenario, and furthermore provides direct evidence of heavy ions in the accelerated particles. We construct a model for the Fe Kα line structures by various projectile ions utilizing atomic-collision data.

Key words: atomic processes — radiation mechanisms: non-thermal — line: formation — cosmic rays — ISM: supernova remnants

1 Introduction

Supernova remnants (SNRs) have been regarded as major acceleration sites of Galactic cosmic rays (CRs). Radio, X-ray, and gamma-ray observations have been providing evidence that particles are indeed accelerated in expanding shells of SNRs via the diffusive shock acceleration mechanism (e.g., Koyama et al. 1995; Aharonian et al. 2007; Ackermann et al. 2013). However, the emission channels detected are all radiations from relativistic particles, and thus particles with lower energies were almost unexplored until recently.

Suzaku data recently revealed the presence of enhanced neutral Fe Kα (∼ 6.4 keV) line emission in some SNRs, where gamma rays are detected and thus particle acceleration is expected to be at work (e.g., W44: Nobukawa et al. 2018; W28: Okon et al. 2018; G323.7−1.0: Saji et al. 2018). In most cases, the line emission spatially coincides with dense gas in the vicinity of the SNRs. Based on these results, the authors interpreted that the Fe line emission is due to K-shell ionization of Fe atoms in the gas by particles accelerated in the SNRs. If the interpretation is the case,
sub-relativistic particles are mainly responsible for the Fe emission line since the production cross sections of the line emission peak at \( \sim 10 \text{ MeV} \) and \( \sim 20 \text{ keV} \) for protons and electrons, respectively (Dogiel et al. 2011).

Information on accelerated sub-relativistic particles can be exploited using the neutral Fe line emission. Dogiel et al. (2011) proposed an idea that species of radiating particles can be distinguished based on the equivalent width of the Fe line with respect to a non-thermal bremsstrahlung continuum from the same population of particles. Using the idea, Nobukawa et al. (2018), Nobukawa et al. (2019), and Saji et al. (2018) claimed that protons account for the majority of the Fe line emission in some SNRs. Makino et al. (2019) presented an analytical model in which they consider energy-dependent escape of CRs from an SNR shock into an interacting cloud, and calculated emission spectra from the cloud, i.e., Fe line emission from sub-relativistic protons and \( \pi^0 \)-decay emission from relativistic protons. Applying their model to W44 and W28, they successfully reproduced both the observed Fe line emission intensity and the gamma-ray spectra.

Fine structures of the Fe K\( \alpha \) line, if detected, can make another step forward in the study of sub-relativistic particles accelerated in astrophysical objects. Tatischeff et al. (2012) pointed out that charge exchange between fast heavy ions and ambient neutral atoms can produce broad line structures accompanying with narrower K-shell lines. Detection of such structures would allow us to prove the presence of heavy ions in accelerated particles and to constrain their composition. Apart from charge exchange, multiple ionization, which is the topic of this Letter, is another potentially important process caused by accelerated heavy ions, and thus can be a powerful diagnostic tool to probe accelerated particles.

In the present work, qualitatively estimate the effect of the multiple ionization process on the Fe K\( \alpha \) line emission. We calculate a model to predict line structures due to multiple ionization by using the knowledge from beam experiments. Based on our model, we show Fe K\( \alpha \) line structures expected to be detected in SNRs by high resolution X-ray spectroscopy with XRISM.

### 2 K\( \alpha \) line structures by impacts of mono-energetic ions

#### 2.1 K\( \alpha L^i \) peaks due to multiple ionization process

Ionization process of target atoms by projectile ions have been widely studied through both experimental and theoretical approaches. With studies by high-resolution crystal spectrometers, authors such as Burch et al. (1971) and Kauffman et al. (1973) found differences of line structures between proton- and ion-produced K\( \alpha \) spectra. Figure 1 shows spectra of Fe K\( \alpha \) line structures originally presented by Burch et al. (1971). The proton-produced spectrum has only the neutral Fe K\( \alpha_1 \) and Fe K\( \alpha_2 \) lines due to the K-L\(_1\) and K-L\(_2\) transitions, respectively. The O\(^{5+}\)-produced spectrum, on the other hand, has broad line-like structures in the 6350–6550 eV band. When projectile particles are heavy ions, their strong Coulomb field can easily cause simultaneous ejection of multiple inner-shell electrons of targets, resulting in the significant characteristic structures.

The multiple ionization structures consist of peaks called K\( \alpha L^i \) (\( i = 0–7 \)), each of which is superposition of the K-L\(_1\) and the K-L\(_2\) transition lines from ionized Fe atoms with \( i \) L-shell vacancies. The center energies of the K\( \alpha L^i \) peaks are higher by \( \sim i \times 20–30 \text{ eV} \) than those of the Fe K\( \alpha_1 \) and K\( \alpha_2 \) lines. This is because the K-L\(_1\) (K-L\(_2\)) transition lines shift upwards by \( \sim 20–30 \text{ eV} \) per L-shell electron ionization \( (= \Delta E_L) \) (e.g., Wang et al. 2012). The outer shell (M, N, ...) ionization is mainly manifested in broadenings of the K\( \alpha L^i \) peaks because the energy shift \( \Delta E_M \) (and \( \Delta E_N, \ldots \)) of the transition lines due to additional M-shell and outer shell vacancies are sufficiently smaller than \( \Delta E_L \), and is equal to or smaller than the natural widths of the transition lines.

#### 2.2 Modeling of K\( \alpha L^i \) peaks

The K\( \alpha L^i \) peaks are the sums of the K\( \alpha_1 L^i \) and K\( \alpha_2 L^i \) sub-peaks, which are superpositions of the K-L\(_1\) and K-L\(_2\) transition lines, respectively. The K\( \alpha_1 L^i \) (K\( \alpha_2 L^i \)) sub-peaks are expressed as superpositions of Lorentzians corresponding to transition lines. According to Horvat et al. (2006) and Horvat et al. (2009), K\( \alpha L^i \) spectra obtained in ion...
beam experiments can phenomenologically be reproduced by the sums of the Kα1L′ and Kα2L′ peaks described by Voigt functions, or a convolution of a Lorentzian and a Gaussian. Here, the Gaussian reflects broadening of the sub-peaks due to simultaneous ionization of electrons in outer shells. Taking the same approach, we modeled the Kα1L′ and Kα2L′ sub-peaks with the Voigt function.

We calculate the center energy of the sub-peaks with the scaling law given by Horvat et al. (2006). They expressed the energy shift $\Delta E'(eV)$ of each $Kα1L' (Kα2L')$ sub-peak with respect to the neutral $Kα2 (Kα2)$ line emission based on various data obtained by ion beam experiments. The energy shift $\Delta E'$ can be described as

$$\Delta E' = p_L^X [(i-1)(Z_2-a)+b]+i(c+dZ_2+ei+fZ_2) eV, \quad (1)$$

where $a = 9.11, b = 14.3, c = -11.6d, d = 1.493, e = 0.755, f = -0.0112$, and $Z_2$ is the atomic number of the target. The parameter $p_L^X$ is the ionization probability per L-shell electron in K-shell ionization. We calculate the ionization probability $p_L^X$ with the model by Horvat et al. (2006),

$$p_L^X = a'/[1 + (b'/X_2)'], \quad (2)$$

where $a' = 0.537, b' = 2.11$, and $c' = 2.02$. The parameter $X_2$ is a universal function derived by Sulik et al. (1987), and is described as

$$X_2 = 4V[G(V)]^{1/2}Z_1/(2v_1), \quad (3)$$

where $v_1, Z_1, V$, and $G(V)$ are the projectile velocity in atomic units, where is normalized to the Bohr velocity $2.18 \times 10^6$ m/s, the atomic number of the projectile, the ratio of $v_1$ to the average velocity of electrons in target atoms, and the Gryzinski Geometrical factor, respectively. We employ an analytical formula in McGuire & Richard (1973) for $G(V)$.

We then calculate the widths of the sub-peaks. The scaling law by Horvat et al. (2006) approximates the widths of the Gaussian of the Voigt function as

$$\sigma' = 4i(b-i)(Z_2-c) eV, \quad (4)$$

where $a = 0.0246, b = 9.86$, and $c = 10.40$. Following Horvat et al. (2006), we fix the line width of the Lorentzian component to the natural widths of the transition lines obtained by Campbell & Papp (2001).

The above scaling laws by Horvat et al. (2006) are derived from experimental data using a variety of solid targets with $Z_2 = 17–32$ and projectile ions with $Z_1 = 6–83$ at 2.5–25 MeV/amu. The data cover impacts by various ions with $\sim 10$ MeV/amu, where the cross sections for K-shell ionization of Fe atoms ($Z_2$) peak. We applied the scaling laws to the calculation of the Fe line structures generated by impacts of various ions in 0.5–1000 MeV/amu region, where collision nature is well-described by the perturbation theory and the scaling laws by Horvat et al. (2006) can be considered valid.

The intensity of each $Kα1L' (Kα2L')$ sub-peak can be expressed as a function of $p_L^X$. Under an assumption of independent L-shell electron ionization, a binomial distribution of

$$I_i = I_{tot} \sum_i^{8} p_L^{X_i}(1-p_L^{X_i})^{8-i}, \quad (5)$$

where

$$I_{tot} = \sum_i^{8} I_i, \quad (6)$$

gives a good description of the relative intensities of the KoL′ peaks (Kauffman et al. 1973).

According to Horvat et al. (2009), intensities of the KoL′ peaks are changed depending on the phase of the target, whether it is gas or solid. Compared to the solid target case, the Fe KoL′ peaks become dominant with gaseous targets. Horvat et al. (2009) derived the scaling law of $p_L^X$ similar to the equation (2) from atomic data of collisions between various ions at $\sim 10$ MeV/amu and monoatomic Ar gas. The scaling law for gas is the same as equation (2), but with $a' = 0.856, b' = 2.94$, and $c' = 1.71$.

### 2.3 Results

In Figure 2(a), we plot the models for the Ko line emitted by solid Fe bombarded by protons and fully ionized O and Fe ions. Figure 2(b) is the same but for gaseous Fe. The results clearly indicate that the intensities of the KoL′ peaks depends on the charge state and kinetic energy of the projectiles. The larger charge the projectile has, the more significant the KoL′ peaks become. This is naturally explained by a stronger Coulomb field of heavy ions. Regardless of the projectile species, the Fe KoL′ peaks are the most significant when the projectile kinetic energy is $\sim 1.6$ MeV/amu. Electrons generally are ejected most efficiently when the projectile ion velocity matches the average velocity of electrons in orbit of an atom (Bohr 1948). Since the kinetic energy of $\sim 1.6$ MeV/amu is translated into a projectile velocity close to that of Fe-L electrons, L-shell electrons are efficiently ionized around this energy.

Figure 3 shows a comparison between the computed models and experimental data by Horvat et al. (2006) and Horvat et al. (2009). In the experimental data, the KoL′ peaks ($i = 0–7$) are generated by impacts of projectile ions, while the Ko1 and Ko2 lines in Figure 3(a) are mainly induced by secondary electrons and X-rays. Our model reproduces the overall KoL′ peaks structures. However, we found some discrepancies of the line center energies...
Fig. 2. Fe Kα structures emitted from (a) solid and (b) gaseous Fe targets under bombardment by (i) protons, (ii) O^{8+}, and (iii) Fe^{26+} ions. The red and blue dashed curves denote the Fe Kα₁ and Fe Kα₂ structures, respectively.
The flux of the Fe KαL\textsuperscript{i} peak \( F_\text{i} \) by each ion species can be described as
\[
F_\text{i} \propto n_{\text{gas}} \int \sigma_{\text{KL}^i} v_{i\text{on}} \frac{dN_{i\text{on}}}{dE} \, dE, \tag{7}
\]
where \( n_{\text{gas}}, \sigma_{\text{KL}^i}, v_{i\text{on}}, \) and \( dN_{i\text{on}}/dE \) are the number density of Fe atoms in the dense gas, the production cross section of the Fe KαL\textsuperscript{i} peak, the velocity of the ions, and the differential spectrum of the ion, respectively. We applied the scaling laws for solid targets assuming that Fe is mainly in dust grains. Based on equations (5) and (6), the production cross section \( \sigma_{\text{KL}^i} \) can be calculated as
\[
\sigma_{\text{KL}^i} = \sigma_p \left( \sum_{i=p}^{8} X^i \right) \left( 1 - p_{L}^i \right)^{8-i}, \quad \sigma_p = \omega_K \times \sigma_{\text{ion}}, \tag{8}
\]
where \( \sigma_p, \sigma_{\text{ion}}, \) and \( \omega_K \) are the production cross section of the Fe Kα (\( \sum \) Fe KαL\textsuperscript{i} peaks) line, the K-shell ionization cross section, and the fluorescence yield (\( \approx 0.34 \)) (Krause 1979), respectively. We computed \( \sigma_{\text{ion}} \) with the program by Batić et al. (2013) based on the ECPSSR (Energy-Loss Coulomb-Repulsion Perturbed-Stationary-State Relativistic) theory (Brandt & Lapicki 1981).

3.2 Results and future observations

Figure 4 presents the result, where the models are folded with the response of the X-ray micro-calorimeter Resolve (Ishisaki et al. 2018) aboard XRISM (Tasbho et al. 2018). Accelerated ions have a power-law spectrum \( dN/dE \propto E^{-s} \) with \( s = 1 \) and \( s = 2 \) in the panels (a) and (b), respectively. The former is chosen, referring to the measurement of non-thermal bremsstrahlung in W49B by Tanaka et al. (2018). The latter is the index expected in diffuse shock acceleration at a strong shock. In both cases, the KαL\textsuperscript{i} (\( i = 1–7 \)) peaks appear in the 6420–6700 eV band. The intensities of each KαL\textsuperscript{i} peak strongly reflect the composition of the emitting particles. If particles accelerated in SNRs have a similar ion composition to CRs arriving at the solar system, the most significant peak is the KαL\textsuperscript{1} peak, which can be resolved into KαL\textsuperscript{1} and KαL\textsuperscript{2} with the Resolve. The intensities of the two sub-peaks are \( \approx 1/10 \) of those of Kα1 and Kα2. The Fe KαL\textsuperscript{1} and KαL\textsuperscript{2} sub-peaks are shifted by \( \approx 30 \) eV with respect to the Fe Kα1 and Kα2.

An \( \approx 30 \) eV energy resolution by X-ray micro-calorimeters would be necessary to resolve the structures. In addition to XRISM, future missions such as Athena (Barcons et al. 2017) and Super DIOS (Ohashi et al. 2018) with X-ray micro-calorimeters will able to detect the line structures. Such studies will play a complimentary role to CR-ionization rate estimates based on H\textsuperscript{+} absorption lines from H, He, ..., Fe, Co, and Ni ions in an energy range of 0.5–1000 MeV/amu.
(e.g., Indriolo et al. 2010). We finally note that potential targets would not be limited to SNRs, considering the recent claims of contribution of CR-ionization to the neutral Fe K line in the Arches cluster region (Tatischeff et al. 2012; Krivonos et al. 2017) and in the Galactic ridge (Nobukawa et al. 2015).

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References

Ackermann, M., et al. 2013, Science, 339, 807
Aharonian, F., et al. 2007, A&A, 464, 235
Barcons, X., et al. 2017, Astronomische Nachrichten, 338, 153
Batić, M., Pia, M. G., & Cipolla, S. J. 2013, Computer Physics Communications, 184, 2232
Bohr, N., 1948, Det Kgl. Danske Videnskabernes Selskab. Math.-fys. Medd. Xvii, No. 8.
Brandt, W., & Lapicki, G. 1981, Phys. Rev. A, 23, 1717
Burch, D., Richard, P., & Blake, R. L. 1971, Phys. Rev. Lett., 26, 1355
Campbell, J. L., & Papp, T. 2001, Atomic Data and Nuclear Data Tables, 77, 1
Dogiel, V., Chernyshov, D., Koyama, K., Nobukawa, M., & Cheng, K.-S. 2011, PASJ, 63, 535
Horvat, V., Watson, R. L., & Peng, Y. 2006, Phys. Rev. A, 74, 022718
Horvat, V., Watson, R. L., & Peng, Y. 2009, Phys. Rev. A, 79, 012708
Indriolo, N., et al. 2010, ApJ, 724, 1357
Ishisaki, Y., et al. 2018, Journal of Low Temperature Physics, 193, 991

Kauffmann, R. L., McGuire, J. H., Richard, P., Moore, C. F. 1973, Phys. Rev. A, 8, 1233
Kavčič, M., et al. 2000, Phys. Rev. A, 61, 052711
Krivonos, R., et al. 2017, MNRAS, 468, 2822
Koyama, K., Petre, R., Gotthelf, E. V., Hwang, U., Matsuura, M., Ozaki, M., & Holt, S. S. 1995, Nature, 378, 255
Krause, M. O. 1979, Journal of Physical and Chemical Reference Data, 8, 307
McGuire, J. H., & Richard, P. 1973, Phys. Rev. A, 8, 1374
Makino, K., Fujita, Y., Nobukawa, K. K., Matsumoto, H., & Ohira, Y. 2019, PASJ, 71, 78
Mewaldt, R. A. 1994, Advances in Space Research, 14, 737
Nobukawa, K. K., et al. 2015, ApJL, 807, L10
Nobukawa, K. K., et al. 2018, ApJ, 854, 87
Nobukawa, K. K., Hirayama, A., Shimaguchi, A., Fujita, Y., Nobukawa, M., & Yamauchi, S. 2019, PASJ, 71, 115
Ohashi, T., et al. 2018, SPIE Proc., 10699, 1069928
Okon, H., Uchida, H., Tanaka, T., Matsumura, H., & Tsuru, T. G. 2018, PASJ, 70, 35
Rymuza, P., Sujkowski, Z., Carlen, M., Dousse, J.-C., Gasser, M., Kern, J., Perny, B., & Rhéme, C. 1989, Zeitschrift fur Physik D Atoms Molecules Clusters, 14, 37
Saji, S., Matsumoto, H., Nobukawa, M., & Yamauchi, S. 2015, ApJL, 807, L10
Tashiro, M., et al. 2018, SPIE Proc., 10699, 1069922
Tatischeff, V., Decourchelle, A., & Maurin, G. 2012, A&A, 546, A88
Wang, X.-L., Dong, C.-Z., & Su, M.-G. 2012, Nuclear Instruments and Methods in Physics Research B, 280, 93