Postprint: Experimental Calibration of High-Resolution Soft X-Ray Spectra of Astronomical Objects

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Abstract

Currently, utilizing atomic data generated by experimental facilities to analyze astrophysical X-ray observation spectra represents a novel research approach that has achieved significant progress in addressing challenges in astronomical observations. To measure high-resolution soft X-ray spectra of highly charged iron ions, an ultra-high vacuum flat-field spectrometer was designed and constructed on the EBIS-A platform at the National Astronomical Observatory. Operating in single-slit mode, this spectrometer employs a 1200 groove/mm variable-spacing diffraction grating, covering a wavelength range of 11.5-19.8 nm. Regarding the spectrometer' s measurement results, theoretical predictions were first conducted for the potentially observable radiation. Based on the working principle of electron beam ion traps and utilizing the Chianti database to analyze extreme ultraviolet spectral data from Heidelberg-EBIT (11.5-14.5 nm band), a linear regression model was initially established to calibrate shifts in line intensity peak positions caused by the experimental system. Subsequently, through collisional-radiative model simulations of soft X-ray spectra from iron ions at various ionization states, the line radiation of Fe VIII and Fe XIX-XXIII in the experimental measurements was identified, well reproducing the observed spectrum. Furthermore, blended lines of Fe XIX and Fe XX with relatively weak intensities compared to Fe XXIII transition lines were identified at 13.2925$±$0.10178 nm, though these weak lines were not resolved in the observed spectrum. Therefore, future experimental measurements can refer to these prediction results to evaluate the spectrometer' s performance.

Experimental Measurement and Calibration of High-Resolution Soft X-ray Spectra for Astrophysics

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Abstract

Current analysis of astrophysical X-ray observation spectra using atomic data generated by experimental facilities represents a novel research methodology that has made significant progress in addressing astronomical observational challenges. To measure high-resolution soft X-ray spectra of highly charged iron ions, an ultra-high vacuum flat-field spectrometer was designed and constructed on the NAOC EBIS-A platform. Operating in single-slit mode with a 1200 grooves/mm variable line-spacing diffraction grating, the spectrometer covers a wavelength range of 11.5–19.8 nm. For the spectrometer measurements, theoretical predictions of the detectable radiation were first performed. Based on the operating principle of electron beam ion traps and utilizing the Chianti database, we analyzed extreme ultraviolet spectroscopic data from Heidelberg-EBIT in the 11.5–14.5 nm band. A linear regression model was established to calibrate the peak position offsets of line intensities caused by the experimental system. Subsequently, soft X-ray spectra of iron ions in various ionization states simulated by a collisional-radiative model identified line radiation from Fe VIII and Fe XIX–XXIII in experimental measurements, satisfactorily reproducing the observed spectra. Additionally, blend lines of Fe XIX and Fe XX, weaker than the Fe XXIII transition line, were found at 13.2925 ± 0.10178 nm, though these weak lines were not resolved in the observed spectra. Therefore, future experimental measurements can reference these predictions to evaluate spectrometer performance.

Keywords: Soft X-ray spectra; NAOC EBIS-A; Ultra-high vacuum flat-field spectrometer; Line identification

0 Introduction

Soft X-ray spectroscopy provides crucial observational data for understanding the physical properties of hot, high-energy cosmic plasmas, containing K-shell and most L-shell transition radiation from abundant metals ranging from carbon to zinc. These transition lines enable diagnosis of high-temperature plasma temperature, density, radiative flux, astrophysical activity, and elemental composition and abundance. In exploring cosmic soft X-rays, the Chandra Low Energy Transmission Grating Spectrometer (LETGS, 6–176 Å) observation of the DA white dwarf GD 246 clearly identified highly ionized iron lines, revealing characteristic features of Fe VI, Fe VII, and Fe VIII ions in the 100–170 Å range. However, neither homogeneous composition models nor chemically stratified models developed by Adamczak et al. for atmospheric analysis adequately fitted the observed spectra, indicating missing physical mechanisms in current models. Targeted laboratory astrophysics measurements may resolve these soft X-ray astronomy challenges. Behar et al. demonstrated that precise atomic reference data are essential for high-resolution spectral analysis, while experimental measurements can generate substantial reliable atomic data including ionization and recombination cross-sections for charge balance calculations, as well as line lists, excitation cross-sections, and dielectronic recombination rates for X-ray interpretation.

Electron beam ion sources/traps (EBIS/T) serve as excellent laboratory soft X-ray sources and have made important contributions to astrophysical high-resolution spectroscopy. EBIS is frequently used as a benchmark for testing plasma spectral models because the electron density and temperature ranges of its produced plasma align completely with astrophysical plasma parameter space. Since the advent of EBIS, countries worldwide have established EBIT facilities for experimental measurements, including Livermore-EBIT studies of extreme ultraviolet spectra, Heidelberg-EBIT (FLASH-EBIT) measurements and diagnostics of Fe VI–XV in the 125–265 Å range, and Tokyo EBIT-CoBIT studies of electron density for highly charged iron ions in the EUV band. Domestically, the Shanghai EBIT facility developed by the Shanghai Institute of Applied Physics (Chinese Academy of Sciences) and Fudan University has achieved important scientific output regarding resonance radiation mechanisms of highly charged ions. This EBIS/EBIT-based spectroscopic measurement methodology has significantly improved precision and provided new experimental validation data for astrophysicists' fitting models. Building ultra-high vacuum flat-field spectrometers on EBIS platforms for experimental measurements of various ionization states of different elements not only provides reference line data for soft X-ray band measurements to improve line lists but also helps interpret unknown radiation sources and refine theoretical models.

Flat-field spectrometers with variable line-spacing diffraction gratings are exceptionally suitable for soft X-ray spectroscopy and represent commonly used measurement devices on most EBIT facilities. This work involves designing an ultra-high vacuum flat-field spectrometer for our laboratory. To maintain diffracted rays on the grating-defined plane, the incident angle must be carefully set to a specific default value. Consequently, spectrometer alignment and angular settings are critical for precise spectral focusing and wavelength determination. Furthermore, before the flat-field spectrometer installed on NAOC EBIS-A began measuring soft X-rays from highly charged iron ions, this paper processed experimental data from the Heidelberg-EBIT EUV spectrometer using SASAL analysis methods based on the Chianti database. Through linear regression modeling of the spectrometer' s dispersion equation and collisional-radiative modeling of iron ion soft X-ray spectra in the 11.5–14.5 nm range, we identified observable lines for future spectrometer operation, further evaluating its diagnostic capabilities and expected wavelength measurement accuracy.

1 Spectrometer Design

Electrons emitted from the cathode of the NAOC EBIS-A electron beam ion source are focused by a 0.6 T axisymmetric magnetic field to form an intense electron beam with current up to 200 mA. Colliding with atomic gas injected at the chamber center, the beam generates ions through impact ionization. The produced ions are confined in a 60 mm long ion trap formed by the radial potential from the electron beam and axial potential from external drift tubes. The electron beam within the trap progressively ionizes captured ions to higher charge states, creating a 60 mm × 500 m soft X-ray radiation source in the trap region. This radiation passes through a slit 10 mm long and 100 m wide, collimating the source onto the diffraction grating center while reducing CCD background radiation. The 1200 grooves/mm variable line-spacing diffraction grating reflects light of different energies onto a CCD detector (model PIXIS-XO 1024B) at the focal plane. The spectrometer primarily comprises a slit flange, six-way cross flange chamber, three-dimensional translation stage for movable grating positioning, rotation feedthrough for adjusting source incidence angle, vacuum pumps, and a two-dimensional adjustment mechanism for CCD positioning, as shown in Figure 1 [Figure 1: see original paper].

Since the electron beam focused by permanent magnets has a diameter of approximately several hundred micrometers, which limits imaging line resolution, an entrance slit adjacent to the NAOC EBIS-A trap region is necessary to effectively improve spectrometer resolution. However, slit dimensions affect both spectral resolution and signal-to-noise ratio: smaller slits yield higher resolution, but weaker light intensity results in poor CCD signal and extremely low data acquisition efficiency. The advantage of NAOC EBIS-A lies in its generation of intense radiation sources. With electron density of 10^{12} cm^{-3} and electron energy of several keV, the emissivity of a single iron ion is approximately 10^{-20} $\mathrm{erg} \cdot \mathrm{s}^{-1} \cdot \mathrm{cm}^{-2} \cdot \mathrm{ster}^{-1} \cdot \mathrm{Hz}^{-1}$. Ions extracted in pulsed mode along the beam direction and measured with a Faraday cup reveal ion numbers of 10^{3}-10^{9} for different charge states (e.g., H^{+} at 6\$×10$^{\{9\},Fe}$\{16+\}\$ at 1.9\$×10$^{\{9\},Fe}$\{26+\}\$ at 2.5\$×10$^{\{3\}),withevenhigherionnumbersinthetrapregion.Forexample,thestrongFe}$\{22+\}\$ emission line at 13.2906 nm has a radiant energy of 1.2566\$×10^\{-12\}\$ $\mathrm{erg} \cdot \mathrm{s}^{-1} \cdot \mathrm{Hz}^{-1}$ passing through the 10 mm × 100 m slit per unit time and frequency interval, corresponding to 0.0084 photons per second striking the grating. Considering grating X-ray reflectivity and beam reflection angle, 0.0019 photons per second are projected onto the CCD. Given the stability of NAOC EBIS-A sources, experiments typically collect signals continuously for several days. Based on these estimates, the CCD can accumulate 1666.2549 photons over 10 days, thereby balancing the CCD-slit relationship.

In the soft X-ray range, a 1200 grooves/mm variable line-spacing grating (model SHIMADZU 30-002) provides high reflectivity, with peak diffraction efficiency wavelength determined by groove depth. Grating X-ray reflectivity can be calculated through the Lawrence Berkeley National Laboratory (LBNL) Materials Sciences Division X-ray Optics Center [14] (https://henke.lbl.gov/optical_{constants}/), yielding 85%-90% reflectivity in the 10-20 nm band, as shown in Figure 2 [Figure 2: see original paper]. The aberration-corrected variable line-spacing grating combined with an array detector forms a spectrometer suitable for resolving soft X-ray spectra from radiation sources. The grating dimensions are 50$×30×10mm^{3}$ with gold coating, 87° incidence angle, 15 nm groove depth, and 25.3 mm detector length, fully covering the 1024$×$1024 imaging area of the CCD camera. The flat-field focusing wavelength range is 5-20 nm, though mechanical geometric constraints limit the actual measurable range to 11.5–19.8 nm.

The grating is mounted on the extension arm of a large-angle rotation feedthrough, which is installed on a three-dimensional translation stage. The stage extends the feedthrough into the center of the six-way cross flange chamber, allowing flexible grating position adjustment via XYZ orthogonal axes, as shown in Figure 1. The translation stage has 0.01 mm minimum scale, 0.002 mm sensitivity, and swing error less than 30 , providing excellent stability. The large-angle rotation feedthrough has 0.01° precision, with automated readout enabling precise grating rotation angle determination. This allows setting the distance from entrance slit to grating center at 237 mm, grazing incidence angle at 3°, and grating center to image plane distance at 235 mm—the optimal grating position. Opposite the 3D translation stage, a loose three-way flange is connected to another port of the six-way cross, with a vacuum gauge on top and a high-temperature-resistant glass window on the side for in-chamber grating adjustment monitoring, enabling observation of grating position and collimated beam incidence and reflection.

The CCD detector is a Princeton Instruments PIXIS-XO 1024B X-ray detector without AR coating (AR coating cannot detect X-rays below 500 eV), with measurement range 10 eV–20 keV. Readout mode provides microsecond resolution with thermoelectric air cooling to 203 K (-70°C), reducing dark current to 0.0004 electrons/pixel/second. Remaining noise primarily originates from system readout noise, typically ~3.1 electrons (rms) at 100 kHz digitization rate. This extremely low noise index permits longer exposure times for increased photon accumulation. The CCD camera mounts on a two-dimensional adjustment mechanism that positions it within the spectral region covered by the grating' s flat-field focal plane, as shown in Figure 1. Internal bearings prevent jamming, while guide mechanisms on the frame sides ensure the optical path follows the designated direction under vacuum load without deflection or sticking. The 2D adjustment frame top and bottom are equipped with two probes perpendicular and parallel to the optical path, respectively, connected to orthogonal displacement sensors (electronic rulers) measuring CCD relative movement in transverse and longitudinal directions with 0.02 mm precision. A pointer scale installed on one side of the 2D mechanism frame perpendicular to the optical path serves as a zero reference. Adding the relative distance to this zero reference yields the absolute CCD position after adjustment, facilitating fine-tuning from the current position to maximize photon collection.

Finally, the completed ultra-high vacuum flat-field spectrometer installed on the NAOC EBIS-A platform is shown in Figure 3 [Figure 3: see original paper], with overall dimensions of approximately 680\$×600×610$mm^{\{3\}.Theentiresystemoperatesunderultra-highvacuumconditions, achieving10}$\{-10\}\$ mbar vacuum after baking.

3.1 Wavelength Calibration

Before experiments, the spectrometer requires collimation adjustment [15] to ensure soft X-rays radiating from the NAOC EBIS-A electron beam ion source center successfully pass through the slit for CCD photon collection after dispersion. During collimation, a green laser from a monochromatic laser source serves as the alignment light, with adjustable spot size controlled below 3 mm diameter. First, grating horizontal placement is tested by directing laser light through an optical path (two mirrors) to the EBIS-A trap center and through the slit. The grating is rotated using the feedthrough until diffraction fringes appear on a distant vertical whiteboard at the same horizontal level as the slit, indicating the grating surface is parallel to the horizontal plane. The grating position and zero-order fringe position on the whiteboard are recorded. The grating is then rotated to form a 3° angle with the incident light, causing the reflected diffraction fringes to climb on the whiteboard. The zero-order fringe position is recorded again, and the vertical climbing distance H is measured, as shown in Figure 4 [Figure 4: see original paper]. Using the zero-order fringe position when the grating was horizontal as a reference point, the horizontal distance d from grating center to whiteboard is measured. When the grating tilts 3°, the theoretical zero-order fringe position on the whiteboard can be calculated, with vertical distance $h = d \times \tan(6°)$ from the reference point, where the 6° angle results from the 3° grating tilt.

By adjusting the 3D translation stage XYZ axes to change grating position and controlling the rotation feedthrough to tilt the grating, the measured vertical distance H in this experiment is approximately 12.85 cm, while the measured horizontal distance d = 122.4 cm. Based on these parameters, the theoretical h = 12.86 cm, demonstrating excellent agreement between measured H and theoretical h.

After obtaining spectral data, the primary task is calibrating the dispersion relation. Even for spectrometers on the same apparatus, slight instabilities before reuse (e.g., system vibration, adjustment uncertainties, grating aberrations, beam parameter variations) may cause minor offsets between measured radiation line intensity peak positions and corresponding theoretical line positions, necessitating recalibration. Here, we first calibrate the dispersion relation using data from the Heidelberg-EBIT EUV flat-field spectrometer (3.2°) [16]. Although this spectrometer differs from our NAOC laboratory design in component details, as shown in Table 1 —including entrance slit mode, grating incidence angle parameters, CCD camera type, and alignment methods–their construction, operating principles, and calibration methodology are fundamentally similar.

Table 1. Basic parameters of Heidelberg-EBIT EUV spectrometer and NAOC EBIS-A ultra-high vacuum flat-field spectrometer

Parameters	Heidelberg-EBIT EUV spectrometer	NAOC EBIS-A ultra-high vacuum flat-field spectrometer
Entrance slit mode	26 × 5/5.5/6 mm aperture slits	10 mm × 100 m single-slit
Diffraction grating	1200 grooves/mm	1200 grooves/mm
Incidence angle	3.2°	3°
Grating object distance	237 mm	237 mm
Grating image distance	235 mm	235 mm
CCD	$2048\times2048 pixels of 13.5\times13.5 \mu m^{2}$	$1024\times1024 pixels of 13\times13 \mu m^{2}$
Vacuum	Below 10^{-9} mbar	Up to 10^{-10} mbar

For Heidelberg-EBIT EUV flat-field spectrometer measurements of iron ions in various ionization states across 107–353 Å, Gaussian fitting yields precise CCD positions of emission line peaks for Fe VII–XXIV. For our wavelength range of interest, we selected Fe VIII and Fe XIX–XXII lines from the Chianti database [17] with identical radiative intensities in the 11.5–14.5 nm band for fitting, as shown in Figure 5 [Figure 5: see original paper], which provides eight fitted peak pixel values.

Although the calibration principle is identical, we employ a different method from that used by G. Y. Liang et al. in the Heidelberg-EBIT EUV spectroscopy experiments, where they obtained the wavelength-pixel dispersion equation through cubic polynomial fitting. Since diffracted lines on the CCD image plane approximate tangents to arcs with extremely small curvature, they can be treated as linear functions of wavelength. Consequently, the spectrometer dispersion equation can be analyzed using a linear regression model.

Based on the Chianti database, we similarly selected Fe VIII and Fe XIX–XXII reference lines corresponding to the eight fitted peaks in Figure 5 within this wavelength range to train the model. The Chianti database compiles extensive ion data for elements from H to Zn from published atomic data, representing the most accurate, comprehensive, and complete dataset currently available for analyzing spectral models of solar and stellar astrophysics in the 1-2000 Å wavelength range. Therefore, we selected the Chianti database as our baseline data. Due to the complexity of iron ion spectra making individual line selection difficult, calibration errors exist considering blend line effects. At identical peak positions, theoretical wavelengths of different iron ionization states and corresponding pixel values are fitted using equation (1), which expresses the linear relationship between wavelength (λ) and CCD pixel (x). The resulting regression model is shown in Figure 6 [Figure 6: see original paper], yielding model parameters: intercept a = 19.2844323 and coefficient b = -6.19978718 × 10^{-3}.

$$\lambda = a + bx \tag{1}$$

The coefficient of determination R^{2} [18] is typically used to evaluate regression models, representing the goodness-of-fit between observed values and the regression equation, with values closer to 1 indicating better fit. Testing yields R^{2} = 0.9955 for equation (1), demonstrating the model’ s suitability for wavelength calibration and its applicability for unknown data prediction. Figure 7 [Figure 7: see original paper] evaluates the calibration results through residual plots, showing residuals between observed and fitted values primarily distributed within or near 1 standard deviation (σ), with only one residual between 3σ, corresponding to the Fe XXI wavelength calibration error in Figure 6. In normal distributions, 99% of values fall within 3σ, indicating relatively high model accuracy. Therefore, the dispersion relation calibration using this linear regression model can calibrate observed spectra.

3.2 Soft X-ray Spectrum Simulation and Line Identification

Even comparing normalized measured values in the soft X-ray band with line radiative decay rates based on wavelength consistency makes line identification difficult. Due to spectral complexity in this band, not all lines can be identified, and some unidentified weak lines blended with stronger emission lines may affect wavelength and intensity measurements. Current spectrometers cannot yet resolve these issues.

Therefore, we prioritize estimating the iron ionization states contributing most significantly in the 11.5-14.5 nm range to identify their primary emission lines, such as the Fe XXIII transition at 13.2906 nm (1s\$^{2}\$2s2p ^{1}P$_{1}$-1s\$$^{\{2\}2s}$\{2\}\$ ^{1}S$_{0}$), Fe XXII transitions at 11.7144 nm (2s2p^{2} ^{2}P$_{1}$/$_{2}$-2s\$^{2}\$2p ^{2}P$_{1}$/$_{2}$) and 13.5812 nm (2s2p^{2} ^{2}D$_{3}$/$_{2}$-2s\$^{2}\$2p ^{2}P$_{1}$/$_{2}$), and Fe XXI transition at 12.8755 nm (2s2p^{3} ^{3}D$_{1}$-2s\$$^{\{2\}2p}$\{2\}\$ ^{3}P$_{0}$). Under optically thin conditions, the SASAL method [19] can analyze X-ray spectra and charge state distributions of various astrophysical and laboratory plasmas. The ECP_{EBIT} module in the SASAL spectral simulation package studies electron collision plasmas with monoenergetic electron beams, with fitting results that well reflect experimental measurements from electron beam ion traps. The ECP_{EBIT} module employs a collisional-radiative model to calculate optical emission from iron ions in different ionization states. Since excited state populations are extremely small, calculations of level populations show that higher transition levels have fewer particles in excited states. At electron temperatures of several keV, particles in ground states and quantum number 2 excited states are most abundant (~1-10^{-3}), while particles excited to quantum number 5 or higher levels are around 10^{-11} or fewer. Therefore, the model considers primary electron excitation and cascading, while electron ionization and recombination processes contribute minimally to level distribution and are neglected. Assuming electron collisional excitation/de-excitation and spontaneous decay rates between ion levels are the primary population mechanisms, solving equation (2) yields specific level populations:

$$\frac{dN_{q,j}}{dt} = \sum_{i<j} n_e C_{i\to j} N_{q,i} + \sum_{k>j} (n_e C_{k\to j} + A_{k\to j}) N_{q,k} - \sum_{i<j} (n_e C_{j\to i} + A_{j\to i}) N_{q,j} \tag{2}$$

where $N_{q,j}$ is the density distribution of ions with charge q in level j, n_e is electron density, $C_{i\to j}$ is excitation/de-excitation rate from level i to j, and $A_{k\to j}$ is spontaneous decay rate from level k to j. The first term represents excitation from lower level i to j, the first part of the second term represents de-excitation from higher level k to j, the second part represents spontaneous decay from k to j, and the third term represents de-excitation and spontaneous decay from level j to lower level i. Using the Chianti database and quasi-steady-state approximation to calculate excitation levels for each iron ion and setting $dN_{q,j}/dt = 0$ yields equilibrium level distributions, enabling calculation of line intensities:

$$I_{ij} = \nu_{ij} A_{ij} N_q \tag{3}$$

In actual measurements, line broadening means any emission or absorption line has finite width and profile rather than single frequency. Line intensity distribution across a frequency range can be fitted using Gaussian curves with full width at half maximum (FWHM) of 0.6 Å. Similar to the local thermodynamic equilibrium assumptions proposed by K. Schwarzschild and Milne to approximate stellar atmospheric physical states, the electron beams in NAOC EBIS-A and Heidelberg-EBIT are monoenergetic, and the soft X-ray radiation source generated by macroscopic collisions with gas atoms is in thermodynamic equilibrium, allowing experimental temperature determination. Heidelberg-EBIT experiments used electron energy $E_e = 5.64$ keV, current $I_e = 320$ mA, and electron density 1.0×10^{12} cm^{-3}. Using these parameters, theoretical spectra of iron ions in various ionization states calculated by the collisional-radiative model in the 11.5–14.5 nm band are compared with experimental measurements in Figure 8 [Figure 8: see original paper], where the yellow thin solid line represents the total simulated spectrum. Based on abundance fractions of various iron ions in Figure 8 and radiative flux from iron ion fitted peaks obtained through Gaussian fitting in Figure 5, dividing by line intensities calculated from the collisional-radiative model yields the iron ionization state fractions shown in Table 2 .

Table 2. Abundance ratios of Fe ions in various ionization stages

Ionic fraction	Ratio
Fe VIII/Fe XXIII	–
Fe XX/Fe XXIII	–
Fe XXI/Fe XXIII	–
Fe XXII/Fe XXIII	–

Note: Specific ratio values were not provided in the original text.

Figure 8 shows peak positions of iron ion lines from different ionization states (Fe VIII, Fe XIX–XXIII) in the experimental spectrum, consistent with G. Y. Liang et al.' s fitting results in the 11.5–14.5 nm band. Additionally, Figure 8 reveals that besides the dominant iron ion lines at peak positions, weaker lines from other ionization states are blended and difficult to resolve. Gaussian fitting of the highest peak near 13.2925 nm with FWHM = 0.10178 nm shows that besides the strong Fe XXIII line, weaker Fe XIX and Fe XX transition lines are present but unresolved in the measured spectrum. This demonstrates that spectrometer sensitivity and resolution are crucial for identifying blend lines and analyzing fine spectral structures.

Due to potential wavelength calibration errors, some offset exists between theoretical and observed spectra in Figure 8. However, with identical peak intensities, transition wavelengths can still be determined to assist experimental spectral line identification, as shown in Table 3 . Line identification is achieved by comparison with known radiative line sets. Various databases list extensive line tables differing in content, line numbers, and sources, with some using theoretical values and others experimental values. Currently, atomic spectral data from the National Institute of Standards and Technology (NIST) [20] serves as the reference standard, showing experimentally calibrated line positions. In Table 3, "(bl)" in the Ion column indicates that the ion' s line is blended with another line.

Table 3. Wavelength and transitions of identified lines by experiments

λ (nm)	Ion	Transition	Lower Level	Upper Level
–	Fe VIII	$1s^{2}2s^{2}2p^{6}3s^{2}3p^{6}3d\ {}^2D_{5/2} \rightarrow 1s^{2}2s^{2}2p^{6}3s^{2}3p^{6}4f\ {}^2F_{7/2}$	$1s^{2}2s^{2}2p^{6}3s^{2}3p^{6}3d\ {}^2D_{5/2}$	$1s^{2}2s^{2}2p^{6}3s^{2}3p^{6}4f\ {}^2F_{7/2}$

λ (nm)	Ion	Transition	Lower Level	Upper Level
–	Fe XIX (bl)	1s\$$^{\{2\}2s}$\{2\}2$p$^\{4\}\$ ^{3}P$_1$ → 1s\$$^{\{2\}2s2p}$\{5\}\$ ^{3}P$_2$	1s\$$^{\{2\}2s}$\{2\}2$p$^\{4\}\$ ^{3}P$_1$	1s\$$^{\{2\}2s2p}$\{5\}\$ ^{3}P$_2$
–	Fe XX	1s\$$^{\{2\}2s}$\{2\}2$p$^\{3\}\$ ^{4}S$_3/_2$ → 1s\$$^{\{2\}2s2p}$\{4\}\$ ^{4}P$_1/_2$	1s\$$^{\{2\}2s}$\{2\}2$p$^\{3\}\$ ^{4}S$_3/_2$	1s\$$^{\{2\}2s2p}$\{4\}\$ ^{4}P$_1/_2$
–	Fe XX	1s\$$^{\{2\}2s}$\{2\}2$p$^\{3\}\$ ^{4}S$_3/_2$ → 1s\$$^{\{2\}2s2p}$\{4\}\$ ^{4}P$_3/_2$	1s\$$^{\{2\}2s}$\{2\}2$p$^\{3\}\$ ^{4}S$_3/_2$	1s\$$^{\{2\}2s2p}$\{4\}\$ ^{4}P$_3/_2$
–	Fe XXI	1s\$$^{\{2\}2s}$\{2\}2$p$^\{2\}\$ ^{3}P$_0$ → 1s\$$^{\{2\}2s}$\{2\}2$p$^\{2\}\$ ^{3}P$_1$	1s\$$^{\{2\}2s}$\{2\}2$p$^\{2\}\$ ^{3}P$_0$	1s\$$^{\{2\}2s}$\{2\}2$p$^\{2\}\$ ^{3}P$_1$
–	Fe XXI	1s\$$^{\{2\}2s}$\{2\}2$p$^\{2\}\$ ^{3}P$_1$ → 1s\$$^{\{2\}2s2p}$\{3\}\$ ^{3}D$_1$	1s\$$^{\{2\}2s}$\{2\}2$p$^\{2\}\$ ^{3}P$_1$	1s\$$^{\{2\}2s2p}$\{3\}\$ ^{3}D$_1$
–	Fe XXII	1s\$$^{\{2\}2s}$\{2\}\$2p ^{2}P$_1/_2$ → 1s\$$^{\{2\}2s2p}$\{2\}\$ ^{2}P$_1/_2$	1s\$$^{\{2\}2s}$\{2\}\$2p ^{2}P$_1/_2$	1s\$$^{\{2\}2s2p}$\{2\}\$ ^{2}P$_1/_2$
–	Fe XXII	1s\$$^{\{2\}2s}$\{2\}\$2p ^{2}P$_1/_2$ → 1s\$$^{\{2\}2s2p}$\{2\}\$ ^{2}D$_3/_2$	1s\$$^{\{2\}2s}$\{2\}\$2p ^{2}P$_1/_2$	1s\$$^{\{2\}2s2p}$\{2\}\$ ^{2}D$_3/_2$
–	Fe XXIII (bl)	1s\$$^{\{2\}2s}$\{2\}\$ ^{1}S$_0$ → 1s\$^\{2\}\$2s2p ^{1}P$_1$	1s\$$^{\{2\}2s}$\{2\}\$ ^{1}S$_0$	1s\$^\{2\}\$2s2p ^{1}P$_1$

Note: Wavelength values were not fully specified in the original text.

Thus, analyzing Heidelberg-EBIT EUV spectrometer experimental data provides a reference template for future NAOC EBIS-A ultra-high vacuum flat-field spectrometer measurements of soft X-ray spectra from iron ions in various ionization states, while observations of iron ion transition lines in the 11.5–14.5 nm band can also test spectrometer performance.

4 Summary

This paper explored experimental measurement methods for studying high-resolution astrophysical soft X-ray spectra. An ultra-high vacuum flat-field spectrometer was designed for NAOC EBIS-A, leveraging the flexibility of 3D translation stages and rotation feedthroughs for grating positioning to employ either 1200 grooves/mm or 2400 grooves/mm gratings. By adjusting grating positions in three-dimensional space and rotation incidence angle directions using the translation stage and feedthrough, and adapting the CCD camera position using the 2D adjustment mechanism to match grating parameters, soft X-ray lines from heavier elements can be measured across different wavelength ranges: 5-20 nm for the former grating and 1-7 nm for the latter. In the 11.5-14.5 nm band, based on the positional properties of photons diffracted by the grating onto the CCD image plane, a linear regression model was established to calibrate minor perturbation-induced offsets between measured radiation line intensity peak wavelengths and theoretical positions. The coefficient of determination R^2 and residual plots demonstrate high calibration accuracy, enabling observed spectrum calibration. For metallic elements like iron, complex line radiation in the soft X-ray band was analyzed using a collisional-radiative model to calculate level distributions and line intensities for the dominant ionization states at intensity peaks. Due to line broadening effects, calculations were fitted with Gaussian profiles of FWHM = 0.6 Å. Comparison between theoretical calculations and experimental measurements reveals that intensity peaks in spectra contain not only lines from single ionization states but also blended weaker lines from other states. Even when lines can be identified with identical peak intensities, limited spectrometer resolution prevents observation of fine spectral structures. The designed flat-field spectrometer, capable of photon detection under ultra-high vacuum with its small entrance slit, high grating X-ray reflectivity, and high CCD signal-to-noise ratio, can effectively improve resolution and sensitivity, offering promise for observing blend lines and achieving precise wavelength calibration in upcoming soft X-ray spectroscopy experiments of iron elements.

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