Revisiting the Fe XVII Line Emission Problem: Laboratory Measurements of the 3s–2p and 3d–2p Line-formation Channels

Chintan Shah1, José R. Crespo López-Urrutia1, Ming Feng Gu2, Thomas Pfeifer1, José Marques3,4, Filipe Grilo4, José Paulo Santos4, and Pedro Amaro4

1 Max-Planck-Institut für Kernphysik, D-69117 Heidelberg, Germany; chtian@mpi-hd.mpg.de
2 Space Science Laboratory, University of California, Berkeley, CA 94720, USA
3 University of Lisboa, Faculty of Sciences, BioISI, Lisbon, Portugal
4 Laboratório de Instrumentação, Engenharia Biomédica e Física da Radiação (LIBPhys-UNL), Departamento de Física, Faculdade de Ciências e Tecnologia, FCT, Universidade Nova de Lisboa, 2829-516 Caparica, Portugal; pdamaro@fct.unl.pt

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Abstract

We determined relative X-ray photon emission cross sections in Fe XVII ions that were mono-energetically excited through dielectronic recombination (DR), direct electron-impact excitation (DE), resonant excitation (RE), and radiative cascades. By reducing the electron-energy spread to a sixth of that of previous works and increasing counting statistics by three orders of magnitude, we account for hitherto unresolved contributions from DR and the little-studied RE process to the 3d transitions, and also for cascade population of the 3s line manifold through forbidden states. We found good agreement with state-of-the-art many-body perturbation theory (MBPT) and the distorted-wave (DW) method for the 3s transition, while in the 3d transitions known discrepancies were confirmed. Our results show that DW calculations overestimate the 3d line emission due to DE by ~20%. Inclusion of electron-electron correlation effects through the MBPT method in the DE cross-section calculations reduces this disagreement by ~11%. The remaining ~9% in 3d and ~11% in 3s/3d discrepancies are consistent with those found in previous laboratory measurements, solar, and astrophysical observations. Meanwhile, spectral models of opacity, temperature, and turbulence velocity should be adjusted to these experimental cross sections to optimize the accuracy of plasma diagnostics based on these bright soft X-ray lines of Fe XVII.

Key words: atomic data – atomic processes – line: formation – methods: laboratory; atomic – plasmas – X-rays: general

Supporting material: data behind figure

1. Introduction

X-rays from astrophysical hot plasmas at a few MK are recorded by grating spectrometers on board the Chandra and XMM-Newton X-ray observatories. They are dominated by the L-shell 3d–2p and 3s–2p transitions in the 15–17 Å range from Fe XVII (Ne-like ions) (Canizares et al. 2000; Paerels & Kahn 2003) that are used for electron temperature, density (Behar et al. 2001; Mewe et al. 2001; Xu et al. 2002; Beiersdorfer et al. 2018), velocity turbulence, and X-ray opacity diagnostics (Brickhouse & Schmelz 2005; Werner et al. 2009; Sanders et al. 2011; de Plaa et al. 2012; Kallman et al. 2014). Decay from the states [2p5 3d1/2J=1], [2p5 3d3/2J=1], and [2p5 3d3/2J=1] to the [2p6]1S0 ground state produces the 3d–2p transitions called 3C, 3D, and 3E, respectively. The 3s–2p decays known as 3F, 3G, and M2 lines proceed from [2p5 3s1/2J=1], [2p5 3s1/2J=1], and [2p5 3s1/2J=1], also to [2p6]1S0.

Since the optically thick line 3C and the intercombination line 3D both have low contributions from cascades (Mewe et al. 2001), their intensity ratio mainly depends on direct electron-impact excitation (DE) and dielectronic recombination (DR) processes. The diagnostic utility of this ratio is strongly hampered by discrepancies between observations and various predictions of their oscillator and collision strengths, which can lead to overestimating opacity effects (Parkinson 1973; Brown et al. 1998, 2006; Laming et al. 2000; Beiersdorfer et al. 2002, 2004; Chen 2007, 2008a; Liang & Badnell 2010). Although laboratory measurements shown to be in agreement with each other (Brown et al. 2006; Gillaspie et al. 2011), they disagree with state-of-the-art predictions of the 3C/3D collision-strength ratio (see Brown & Beiersdorfer 2012). So far, only one theoretical work (Chen 2008b) predicted a low 3C/3D ratio in agreement with experimental data (Brown et al. 2006; Gillaspie et al. 2011). However, a later calculation performed by the same author (Chen 2011) produced a high 3C/3D ratio, in consensus with the most-advanced theoretical predictions (Safronova et al. 2001; Gu 2009; Bernitt et al. 2012). Furthermore, a comprehensive comparison of the 3C/3D ratio in the Ne-like isoelectronic sequence from Ar IX to Kr XXVII exhibited discrepancies between measurements and predictions (Santana et al. 2015). Particularly, theories deviate by 10%–35% from experiments in the case of Fe XVII. A novel X-ray laser spectroscopy measurement at the LCLS free-electron laser facility measured 3C/3D oscillator-strength ratio, which is also proportional to the collision-strength ratio under Bethe approximation, also produced a low 3C/3D ratio in agreement with previous measurements and observations (see Bernitt et al. 2012 and its supplementary material). Nonlinear effects in X-ray lasers could reduce the 3C/3D ratio (Oreshkina et al. 2014; Loch et al. 2015). While a recent semi-empirical calculation has predicted a value close to that experimental result (Mendoza & Bautista 2017), this theoretical approach was quickly disputed (Wang et al. 2017). In short, in spite of forty years of efforts, the 3C/3D intensity-ratio discrepancy remains essentially unsolved to this date.
Alternative approaches use the forbidden $M_2$ line or the $3G+M_2$ line blend for opacity and turbulence-velocity diagnostics, as the $M_2$ line is optically thinner than the $3D$ line (Werner et al. 2009; de Plaa et al. 2012). However, astrophysical observations of the $(3G+M_2)/3C$ ratio and $3s/3d$ or $(3F+3G+M_2)/(3C+3D+3E)$ ratio also depart from theories and spectral models (de Plaa et al. 2012), and laboratory ratios are consistently larger than the calculated ones (Beiersdorfer et al. 2002, 2004). This could be explained if $M_2$ is mainly fed by complex cascades following DE, with contributions from the resonant excitation (RE) (Beiersdorfer et al. 1990; Doron & Behar 2002; Gu 2003; Tsuda et al. 2017) process. Another argument points to the same cause as the $3C/3D$ discrepancy.

Understanding whether $3C/3D$ and $3s/3d$ discrepancies are caused by DR, RE, or cascade contributions to $3s$ and $3d$ line manifolds is highly critical given the wide-reaching diagnostic applications of these lines. Most previous laboratory works mainly focused on DE cross-section measurements at discrete electron beam energies. However, comprehensive laboratory validations of the DR, DE, and RE contributions to these transitions are essential to construct reliable spectral models, and are urgently needed in view of the upcoming high-resolution space missions XRISM Resolve (Tashiro et al. 2018), Arcus (Smith et al. 2016), and Athena (Barret et al. 2016).

Here we perform laboratory measurements of differential cross sections in the $0.3–1.1$ keV energy range of the Fe XVII $3s$ $(3F+3G+M_2)$ and $3d$ $(3C+3D+3E)$ emissions that are driven by DR, DE, and RE processes. Using an electron beam ion trap (EBIT), we produced an ion population mainly consisting of Fe XVII ions and scanned the electron beam energy with an energy spread of only $5$ eV full-width-at-half-maximum (FWHM). This, together with three orders of magnitude higher counts compared to previous experiments, allows us clearly to distinguish narrow RE and DR features from DE ones as a function of electron beam energy. Furthermore, we perform calculations of $3s$ and $3d$ line emission cross sections using both state-of-the-art distorted-wave (DW) and many-body perturbation theory (MBPT) methods. We found overall agreement of the experimental $3s$ cross sections with both DW and MBPT predictions, thus benchmarking the DE cross sections with respective cascades and the strong RE features. On the other hand, we observe discrepancies between both theories and the experimental $3d$ cross section, consistent with previous laboratory measurements, solar, and astrophysical observations of $(3G+M_2)/3C$ ratio and $3s/3d$ or $(3F+3G+M_2)/(3C+3D+3E)$ ratios. Our results indicate that a fundamental discrepancy in $3d$ formation likely causes the reported inconsistencies of models with laboratory and astrophysical observations.

2. Experimental Technique

We used FLASH-EBIT (Epp et al. 2007, 2010) at the Max-Planck-Institut für Kernphysik in Heidelberg to produce Fe XVII ions from a molecular beam of iron pentacarbonyl. The monoenergetic electron beam induces a negative space-charge potential that radially traps the ions; in the axial direction, a set of cylindrical drift tubes electrostatically confines them. In the trap, the electrons have a well defined kinetic energy due to the acceleration potentials corrected by the space-charge contributions of the electron beam and trapped ions. Collisions between beam electrons and trapped ions efficiently drive ionization, excitation, and recombination processes. The generated X-rays are registered at $90^\circ$ to the beam axis with a silicon-drift detector (SDD) with a photon-energy resolution of $\approx120$ eV FWHM at $6$ keV, which separate transitions from the $3s$ and $3d$ manifolds; see the bottom left inset of Figure 1.

To maximize Fe XVII purity, a sawtooth scan consists of a breeding time of $0.5$ s at $1.15$ keV beam energy (below the Fe XVII ionization threshold at $1.26$ keV), followed by a $40$ ms long energy scan from $0.3$ to $1.1$ keV during which only a small fraction of the ions recombine. This method efficiently suppressed lower charge states, as only very faint LMM DR resonances from Fe XV–XVI are obtained. Measurements at a breeding energy of $0.5$ keV, just above the Fe XVI ionization threshold, allowed us to separately identify those weak contributions. The DR paths are named in analogy to Auger nomenclature, e.g., LMM implies the $L \rightarrow M$ resonant excitation due to a free electron recombining into the $M$-shell. Moreover, the spectra taken on the upward and downward energy scans show differences of less than $2\%$ and confirm a nearly constant population of Fe XVII ions.

During the fast energy scans, the beam current $I_e$ was also adjusted synchronously with $E$ to keep the electron density $n_e \propto I_e/\sqrt{E}$ constant (Savin et al. 2000), minimizing a modulation of the space-charge potential, and concomitant heating that causes ion losses. The trap was emptied every $5$ s to prevent accumulation of unwanted (Ba, W) ions emanating from the electron-gun cathode.

In this work, we reached an electron beam energy spread of $\sim$5 eV FWHM at $800$ eV, a six-to-ten-fold improvement over previous works (Brown et al. 2006; Gillaspay et al. 2011; Beiersdorfer et al. 2017) in this energy range by an application of forced evaporative cooling technique (Penetrante et al. 1991). Here, the cooling of ions optimized by lowering as much as possible the axial trapping potential. Within the radial trapping potential generated by the space-charge potential of the electron beam, the cooled ions are more concentrated at the bottom, thus reducing the energy dispersion due to the space charge. The details of this technique are discussed in Beilmann et al. (2009, 2010, 2011), Shah et al. (2016a, 2018), and Micke et al. (2018). Because the ion trapping parameters were kept constant during the electron beam energy scan, this technique does not introduce any systematic effects on the present measurements.

3. Theory

Within an independent resonance approximation model, the DR and RE processes can be described as a two-step process. First, a doubly excited state is formed by dielectronic capture (DC), i.e., a capture of a free electron by an ion with excitation of a bound electron. Here, we focus on the $L$-shell. While in DR this excited state decays radiatively, RE includes an autoionization process that leaves an $L$-shell hole that relaxes by photon emission.

We used the parallel version of the Flexible Atomic Code\textsuperscript{5} (FAC v1.1.5) (Gu 2008) to compute the electronic structures of Fe XVII–XVI ions. We evaluated DR, DE, and RE with extended sets of configurations, full-order configuration mixing, and Breit interaction (Amaro et al. 2017; Shah et al. 2018). For DC channels of both DR and RE, we included $2s^22p^5nl'nl''$ and $2s2p^6nl'nl''$ configurations. All the DR

\textsuperscript{5} https://github.com/flexible-atomic-code/fac
radiative paths of these states were included \((2s^22p^6n'l')\), which corresponds to the main radiative recombination (RR) paths. Additionally, all Auger paths addressing RE are taken into account \((2s^22p^6n'n'l'\) and \(2s^22p^6n'l'\)). They are also the main paths of DE. In all sets of configurations, we included principal quantum numbers and orbital angular momentum quantum numbers of \(n \leq 7\), \(n' \leq 60\) and \(\ell, \ell' < 8\) that resulted into roughly half-a-million eigenstates in our calculations. The output was fed into the collisional-radiative model of FAC (Gu 2008) for obtaining steady-state populations of Fe XVII–XVI states connected by the aforementioned processes and radiative cascades. It solves a system of coupled rate equations on a fine grid of electron beam energies and electron density matching the experimental conditions. The resulting level populations are used to calculate the line emission for comparison with the measurement.

For the DE cross sections, we used the MBPT implementation of FAC. The treatment of DE with the MBPT method is described by Gu (2009). In essence, a combined configuration interaction and second-order MBPT method (Gu et al. 2006) is used to refine the energy levels and multipole transition matrix elements. Collision strengths of DE under the DW approximation can be split into direct and exchange interaction contributions. Allowed transitions such as \(3C\) and \(3D\) lines of Ne-like ions have a dominant contribution of the direct interaction that is proportional to the corresponding matrix elements. We therefore use the MBPT-corrected matrix elements to scale the direct contribution to the DW collision strength and obtain correlation corrections to the DE cross sections.

Due to the unidirectional electron beam and the side-on X-ray observation, both polarization and emission anisotropy must be accounted for (Beiersdorfer et al. 1996; Shah et al. 2015). We also used FAC to calculate the X-ray polarization following DR, DE, and RE. Depolarization due to radiative cascades and cyclotron motion of the electrons was taken into account (Beiersdorfer et al. 1996; Gu et al. 1999). The transversal electron-energy component due to the cyclotron motion of electrons inside the electron beam was estimated in our previous work (Shah et al. 2018). For the present experimental conditions, the depolarization due to this essentially resulted in no change in the total X-ray polarization.

All theoretical data on cross sections and polarization presented in Figures 2–4 are listed in the accompanying machine-readable table.
Figure 2. Black curves: experimental cross sections observed at 90° vs. electron beam energy for the 3d (3C+3D+3E) manifold. Gray band: total (1σ statistical + systematics) uncertainty. (a) Measured DR cross sections below the DE threshold. Dotted magenta curve: independently calibrated high-resolution results from the Test Storage Ring (TSR) in Heidelberg (Schmidt et al. 2009) that were folded with a 5 eV Gaussian for comparison. Blue solid curve: our FAC-DW predictions. Inset: DR resonance used for normalization of the 2D map to our FAC results (Figure 1). (b) DE cross sections including above-threshold RE peaks. FAC-DW predictions: blue solid (DE + RE) and dashed (DE only) curves. FAC-MBPT predictions: orange solid (DE + RE) and dashed (DE only) curves. Green dotted curve: Breit–Pauli R-matrix predictions of Chen (2011). Solid circles: measured LLNL-EBIT cross sections (Brown et al. 2006). For comparison with Brown et al. (2006) and Chen (2011) data, 3E cross sections are added from our FAC-DW theory. Hollow circles: Brown et al. (2006) data without the addition of the 3E line (~7%).

(The data used to create this figure are available.)

4. Data Analysis

Figure 1 shows the X-ray intensity as a function of the electron beam (abscissa) and the X-ray energies (ordinate). Features due to electron recombination can be recognized above and below the DE threshold. Above it, we resolve DR channels populating the 3d manifold from LMM to LMT, while unresolved L Mn DR channels up to \( n > 60 \) pile up near the 3d threshold. Below the threshold, photon emissions produced after DE of L-shell electrons appear as horizontal bright band comprising both the 3d and 3s manifolds. Bright spots on top of the continuous DE emission band are RE features; see the bottom right inset of Figure 1.

Two horizontal regions of interest (ROIs) with an X-ray energy width of ±30 eV and centered on the respective line centroids were carefully selected on the 2D map for distinguishing the contributions of the 3s and 3d manifolds. X-ray photon counts within these ROIs were then projected onto the electron-energy axis; see Figures 2 and 3. In front of the windowless SDD detector, a 1 \( \mu \)m carbon foil blocks UV light from the trapped ions. At the X-ray energies of interest varying from 650 to 900 eV, the foil has a transmission of 26%–52%. We normalized counts with known transmission coefficients (Henke et al. 1993). To verify them, we carried out measurements of Lyα and RR emissions from O VIII and Ne X, and found them to be in agreement within 3%. Furthermore, X-ray yields were also normalized to the cyclically time-varying electron beam current density. After that, we determine the relative differential cross sections.

Previously, Brown et al. (2006) determined the 3C and 3D cross sections using an X-ray microcalorimeter by normalizing their experiment with theoretical RR cross sections. This was not possible in the present experiment due to pileup and contamination of the RR band, as the detector does not resolve RR transitions into the 3s, 3p, and 3d sub-shells. We thus selected a single DR resonance, \( [1s^{2}2s^{2}2p_{1/2}^{2}2p_{3/2}^{2}3d_{3/2}3d_{5/2}]^{2}S_{1/2} \) at \( \sim 412 \) eV electron beam energy for normalizing the 3s and 3d projections; see the inset of Figure 2. An ab initio calculation for this resonance using FAC under DW approximation was employed. Its strength can be traced to a single and strong resonance in the LMM channel. This channel has the simplest structure of all DR channels and this presumably makes its prediction theoretically more reliable. Moreover, theoretical
treatments of DR and RE are more reliable than the DE due to the involvement of only one continuum state in DR and RE, in contrast to two continuum states in the DE treatment. By fitting the experimental and the theoretical projections (convoluted with a Gaussian function), a normalization factor of $1.42 \times 10^{11}$ counts per cm$^2$ with a 2% fitting error was found. The complete projection was accordingly rescaled, yielding the differential cross sections for both the 3$d$ and 3$s$ manifolds at 90°; see Figure 2.

To verify our normalization factor, we also used a theoretical cross-section value of single RE-LMP resonance at $\sim 734$ eV electron beam energy and found a normalization factor of $1.46 \times 10^{11}$ counts per cm$^2$ with a 3% fitting error. We select this RE resonance because it is relatively free from the DE background. Moreover, we further normalized our experiment with measured cross sections of 3$C$ and 3$D$ by Brown et al. (2006), which are normalized to RR cross sections, at $\sim 964$ eV electron beam energy. All three normalization procedures show consistency in inferred cross sections within their uncertainties.

We also utilized the DR rate coefficients independently measured at the Test Storage Ring (TSR) at the Max-Planck-Institut für Kernphysik in Heidelberg by the merged-beam method. There, a cooled Fe XVII ion beam is brought to overlap with an electron beam as the electron target (Schmidt et al. 2009). The yield of Fe XVI ions, not X-ray photons, is detected, resulting in high-resolution absolute total recombination-rate coefficients with an estimated total uncertainty of 20%, which we corrected for observations at 90° and convoluted to a 5 eV Gaussian for the comparison. In the Figure 2, the independently calibrated TSR data (without any normalization) are shown for the comparison along with the present EBIT data. We not only found a very good agreement for the DR resonance we used for the normalization, but also an overall consensus between TSR and EBIT data for all measured DR resonances. Moreover, we also compared our inferred cross sections with those measured at the LLNL-EBIT by Brown et al. (2006) at 910 and 964 eV energies. Both EBIT data are in agreement within their reported uncertainties and consistent with or without the addition of 3$E$ cross sections. This overall agreement of three independent experiments for the 3$d$ line manifold is shown in Figures 2(a) and (b).

We further check the effect of the 3$s$–3$d$ ROI selection, as even though our detector resolves them, the wings of both transitions partially overlap. This is evident in Figure 1: the low-energy tail of the 3$d$ peak contaminates the 3$s$ manifold. To check those blends, we shifted the 3$s$ and 3$d$ ROIs up to $\pm 15$ eV from their respective centroids, leading to effects on the normalization factor of 9%. We conservatively add this $\sim 9%$ uncertainty to our normalization factor, in addition to the $\sim 2%$ uncertainty from the LMM fits. Total uncertainty sources are thus: $\sim 2%$ from statistics, $\sim 3%$ from the carbon-foil transmission, and $\sim 9%$ from the normalization factor. The resulting cross sections with their overall uncertainties of DR, RE, and DE driven 3$d$s line emissions are shown in Figures 2 and 3, respectively, and compared with FAC-MBPT and FAC-DW calculations performed in this work as well as previous works of Chen (2011), Pindzola et al. (2006).

The ratios of normalized cross sections of 3$s$ and 3$d$ line manifold are also shown in Figure 4 (dubbed Analysis 1) as a function of electron beam energies. These 3$s$/3$d$ ratios are then compared with LLNL-EBIT ratios measured with three different high-resolution X-ray spectrometers (Beiersdorfer et al. 2002). We found a good agreement with LLNL-EBIT data; however, disagreement with a microcalorimeter measurement of Laming et al. (2000).

In the second analysis, we did not rely on our normalization procedure in order to obtain 3$s$/3$d$ line ratios. As can be seen in the bottom left inset of Figure 1, we can clearly separate X-ray peaks of 3$s$ and 3$d$ by selecting a particular ROI (vertical slices) along the electron beam energy axis where both do not overlap, e.g., at 690 eV and at 745 eV for 3$d$ and 3$s$, respectively. By fitting a Gaussian with a low-energy Compton wing, we extracted the line centroids and widths of 3$s$ and 3$d$ peaks. We then selected several other ROIs along the electron beam energy axis with $\pm 25$ eV widths, and projected X-ray counts within these ROIs onto X-ray energy axis. Here 3$s$ and 3$d$ peaks are not separated; however, line intensities of both 3$s$ and 3$d$ manifolds can still be extracted by fitting Gaussians while fixing line centroids and widths to previously obtained values in the fitting procedure. The inferred 3$s$/3$d$ ratios by this method (dubbed Analysis 2) are shown in Figure 4. Both analysis methods are in very good agreement with each other.

Figure 3. Same as in Figure 2(b), except for the 3$s$ (3$F$+3$G$+M2) manifold. Green dotted line: 30 eV broadened 2$p^5$3$s$ cross sections presented by Pindzola et al. (2006). Note that the data behind the figure for Figure 2 also contains data for Figure 3.
as well as with the LLNL-EBIT data of Beiersdorfer et al. (2002). This, in turn, reassures our normalization procedure to obtain the 3s and 3d cross sections. We again emphasize that our normalization is based on a single theoretical value of the DR resonance at ~412 eV electron beam energy.

5. Results and Discussions

Overall, we observe an agreement over a wide range of electron energies. However, a few discrepancies are noticeable. The comparison of TSR DR data with the present experiment in Figure 2(a) shows minor differences in the baseline, as for clarity the contributions to the total cross section from $n = 4$ -- 2 photon emission that are visible in the 2D plot at ~1 keV photon energies (see Figure 1) were left out, while they are present in the TSR data. The TSR data do not include DE and RE processes, thus its signal disappears above the threshold at 0.8 keV.

Another discrepancy in Figure 3 at electron energies of 0.72 keV could not be attributed to the 3s ROI selection or contamination by a DR feature at 0.83 keV photon energy. Moreover, Fe XVII (2p$^3$3nl) DR channels at similar electron energy also predict negligible contributions at ~0.7 keV photon energy. Calculations assuming ~10% of Fe XVI, which is five times the predicted concentration based on comparison of upward and downward scans, still predict a negligible contribution of Fe XVI at this energy.

We also checked possible contaminations due to oxygen ions producing O VIII Ly$\beta$ and Ly$\gamma$ lines (Beiersdorfer et al. 2002; Gillaspy et al. 2011). These contributions can be estimated by checking the presence of KLL DR resonances of O VII-V in the electron-energy range of 0.42–0.55 keV, which is free from low-energy contamination from Fe XVII DR resonances; see Figure 1. We found out less than 1% K$\alpha$ X-ray counts after correcting for detector efficiency, which could be due to O VIII-III KLL DR, compared to the strong Fe LMM features. Moreover, simultaneous measurements with a vacuum-ultra-violet (VUV) spectrometer in the 40–140 nm wavelength range, which we also used to monitor impurity ions, did not show any fluorescent lines of O IV–V, as well as strong fine-structure 2s–2p transitions of O VI. This clear absence of any fluorescent X-ray or VUV lines essentially shows that there are no oxygen ions co-trapped with Fe ions in our EBIT, and rules out O VIII Ly$\beta$ and Ly$\gamma$ lines as source systematics in our measurements. Thus, oxygen impurity lines can be disregarded as a cause of observed discrepancies between the present experiment and theory.

We further investigated the contribution of charge-exchange recombination X-rays in our experiment. Charge exchange (CX) can also produce Fe XVI ions by recombining an electron from residual gases with Fe XVII ions. However, X-rays due to CX do not directly affect Fe XVII $n = 3–2$ transitions. It only indirectly affects the emission due to the large fraction of Fe XVI ions that may produce satellites due to the inner-shell excitation. A comparison between LMM DR scans above and below the production threshold of Fe XVII shows only a negligible contribution of Fe XVI ions in our trap. CX into Fe XVIII producing Fe XVII can also be neglected because the upper electron beam energy scan limit (~1.12 keV) is below the production threshold of Fe XVIII ions (~1.27 keV). Moreover, we used a four-stage differential pumping system to inject the iron pentacarbonyl compound. In the present experiment, the injection pressure at the second stage was set too low (~10$^{-9}$ mbar) which follows two additional stages of cryogenic differential pumping at 45 and 4 K temperature shield apertures at the Heidelberg FLASH-EBIT (Epp et al. 2010). Due to this, at the vacuum level well below $\lesssim 1 \times 10^{-11}$ mbar in the trap region, CX rates reduce by three orders of magnitudes. Our previous CX measurements with highly charged S, Ar, and Fe ions show that the additional two-to-three orders of magnitude raised in the injection pressure are required to observed CX X-ray features (Shah et al. 2016b). Therefore, CX can be neglected as a cause of these discrepancies.

The 3s emission in Figure 3 shows a dominant contribution of RE in the proximity of the excitation threshold.

![Figure 4. Measured 3s (3F+3G+M2) to 3d (3C+3D+3E) line intensity ratios as a function of the electron beam energy. Black curve: present experiment (based on DR-normalization procedure–Analysis 1). Gray shaded area: 1σ statistical + systematic error. Solid circles: present experiment (independent of normalization–Analysis 2). Open circles: LLNL-EBIT microcalorimeter (Beiersdorfer et al. 2002). The blue solid and dashed curves show distorted-wave (DW) predictions that include (DE + RE) and exclude RE (DE only), respectively. Similarly, the orange solid and dashed curves show the many-body perturbation theory (MBPT) predictions.](image-url)
(0.73–0.8 keV) of the total photon emission, This can be traced back to the LMP (2p⁵ 3l 6l') and LNN (2p⁵ 4l 4l') resonances. Previously, Pindzola et al. (2006) predicted the LMP RE contribution to the 2p⁵3s DE cross section at ≈750 eV. In addition to this, we observe RE channels up to LPP (2l 6l'6l''), which are necessary to fully understand our data up to E ≈ 0.11 keV. Furthermore, DE processes populate states having non-dipole (e.g., 2p³3p) decays to the ground state, feeding the 3s manifold through radiative cascades. The excitation thresholds of such states are apparent in the stepwise shape of the non-RE theoretical prediction in Figure 3. Excellent agreement is observed when all these atomic processes are taken into account and compared with both DW and MBPT theoretical methods. Table 1 lists theoretical and experimental total cross sections, as well as the contribution of RE and DE, showing detailed agreement between both theories and experiment for the 3s manifold.

On the other hand, the 3d emission shown in Figure 2(b) and its total cross section in Table 1 demonstrate an overestimation of DW theory by 20%, while MBPT overpredicts by only 9%. Such differences also appear in earlier predictions (Chen & Pradhan 2002; Loch et al. 2006; Chen 2007, 2008a, 2011). For example, previous predictions for the 3d cross sections reported by Loch et al. (2006) and Chen & Pradhan (2002) differ by 14% and 17% from our measurements, respectively. The difference between our present MBPT and experiment is likely due to the 3C component of the 3d manifold (see Figure 7 of Gu 2009). As discussed by Chen (2007, 2008b), Gu (2009), Chen (2011), and Santana et al. (2015), the main difference between theoretical methods evaluating the 3C component can be traced back to the completeness of electron correlation, and not to the theoretical scattering implementation, i.e., regardless of using DW, close-coupling, or R-matrix methods. The MBPT-corrected cross sections presented here give a better agreement with the measurements because of their more complete treatment of correlation effects in comparison with our DW cross sections. We note that the remaining discrepancy on the 3C component indicates that higher-order correlation effects second order need to be considered (Safronova et al. 2001; Santana et al. 2015), as also confirmed in the earlier findings (Bernitt et al. 2012). Laboratory measurements (Brown et al. 2006) performed at the LLNL-EBIT are within our uncertainties (see Figure 2), and share the same conclusion that the actual 3C cross sections are lower than theoretical predictions. Here, we note that the present measurement resolved RE components for the 3d manifold and found their overall contributions to be ≈8%, which is also consistent with values reported by Brown et al. (2006).

The ratios of 3s/3d, which are independent of cross-section normalization and are of astrophysical preeminence, plotted in Figure 4 as a function of electron beam energies, are also in good agreement with the LLNL-EBIT results of Beiersdorfer et al. (2002). We found an ~18% discrepancy in 3s/3d ratios between our results and DW predictions. Similar to the previous reasoning, including a more complete treatment of electron correlation for the 3C through the MBPT method reduces these discrepancies to ~11%. Figure 4 also demonstrates the substantial contribution of RE (~25%); thus, it is important to take into account RE in evaluating 3s/3d ratios.

6. Summary and Conclusions

In this work, we reported a first systematic measurement of the soft X-ray emission in Fe XVII after electron recombination with a sixfold improved electron-energy resolution and threefold improved counting statistics for both the 3s and 3d line manifolds. In contrast to previous work where excitation cross sections were measured only for a few electron energies, we measured Fe XVII line emission cross sections for continuous electron beam energies from 0.3 to 1.1 keV. We demonstrated that predictions have to include substantially larger sets of configurations and the corresponding contributions of DR and RE to the main DE process, as well as the effect of forbidden transitions driving the line emission through radiative cascades. Our DW and MBPT predictions show good agreement with the measured 3s cross sections. On the other hand, the discrepancy for the 3d excitation and for 3s/3d ratios found in earlier studies were broadly confirmed in this work. The agreement between our measurements and previous laboratory data based on storage ring, ion trap, and tokamak measurements, and the reproducibility of the observed discrepancy in the 3d manifold, let us conclude in accord with earlier works that the main disparities between models and astrophysical observations in the 3s/3d, 3C/3D, and 3C/ (3G+M₂) are due to an overestimation of the 3C component.

Our experimental data and dedicated calculations may contribute to a better understanding of these line ratios, which are used for estimating opacity and turbulence velocities in galaxies (Beiersdorfer et al. 2004; de Plaa et al. 2012). Moreover, measured DR satellites associated with Fe XVII can provide an excellent diagnostics of coronal temperatures of stars (Beiersdorfer et al. 2018). Our results can be employed to benchmark widely used spectral codes, such as SPEX (Kaastra et al. 1996; Gu et al. 2019), ATOMDB (Foster et al. 2012), and CHIANTI (Dere et al. 2019). Validation of such codes is, indeed, an urgent task in view of the upcoming launch of the X-ray microcalorimeter-

| Line | E, Range (eV) | Integral Cross Sections (10⁻¹⁸ cm² eV) | % Contribution of Processes | % MBPT Correction to DW theory | % Correction Required to theory |
|------|--------------|---------------------------------------|-----------------------------|-------------------------------|--------------------------------|
|      |              | DW Theory | MBPT Theory | DW Theory | MBPT | DE only | DE + RE | DE only | DE only | DE only | DE only |
| 3s   | 710–1120     | 110.6 ± 5.7 | 108.29 | 60.82 | 60.35 | 43.8 | 56.2 | −0.8 | 2.2 | 2.6 |
| 3d   | 830–1120     | 47.6 ± 4.2 | 57.19 | 52.69 | 47.56 | 7.9 | 92.1 | −10.8 | −20.1 | −9.4 |
| 3s/3d| 830–1120     | 1.64 ± 0.17 | 1.35 | 1.02 | 1.11 | 24.6 | 75.4 | 8.0 | 17.5 | 10.6 |

Note. The predicted contributions of various processes from DW and MBPT calculations are compared with experimental values.
based XRISM satellite (Hitomi Collaboration et al. 2018; Tashiro et al. 2018; Betancourt-Martínez et al. 2019). The expected scientific harvest of this mission, and future missions Arcus (Smith et al. 2016) and Athena (Barret et al. 2016), should revolutionize X-ray astrophysics, as the few but nonetheless, excellent measurements of the ill-fated Hitomi mission have shown (Hitomi Collaboration et al. 2016, 2017).

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