THE X-RAY SPECTRUM OF Fe$^{16+}$ REVISITED WITH A MULTI-ION MODEL

Rami Doron$^{1,2}$ and Ehud Behar$^3$

Received 2002 February 7; accepted 2002 March 31

ABSTRACT

The theoretical intensities of the soft X-ray Fe$^{16+}$ lines arising from 2l–3l′ transitions are reexamined using a three-ion collisional-radiative model that includes the contributions to line formation of radiative recombination (RR), dielectronic recombination (DR), resonant excitation (RE), and inner-shell collisional ionization (CI), in addition to the usual contribution of collisional excitation (CE). These additional processes enhance mostly the 2p–3s lines and not the 2p–3d lines. Under coronal equilibrium conditions, in the electron temperature range of 400–600 eV where the Fe$^{16+}$ line emissivities peak, the combined effect of the additional processes is to enhance the 2p–3s lines at 16.78, 17.05, and 17.10 Å, by ~25%, 30%, and 55%, respectively, compared with their traditional, single-ion CE values. The weak 2p–3d line at 15.45 Å is also enhanced by up to 20%, while the other 2p–3d lines are almost unaffected. The effects of DR and RE are found to be dominant in this temperature range (400–600 eV), while that of CI is 3% at the most, and the contribution of RR is less than 1%. At lower temperatures, where the Fe$^{16+}$/Fe$^{17+}$ abundance ratio is high, the RE effect dominates. However, as the temperature rises and the Fe$^{17+}$ abundance increases, the DR effect takes over. The newly calculated line powers can reproduce most of the often observed high values of the (I$_{17.05}$/I$_{15.01}$) intensity ratio. The importance of ionization and recombination processes to the line strengths also helps to explain why laboratory measurements in which CE is essentially the sole mechanism agree well with single-ion calculations but do not reproduce the astrophysically observed ratios.

Subject headings: atomic processes — line: formation — techniques: spectroscopic — X-rays: general

1. INTRODUCTION

The soft X-ray emission-line spectrum of Ne-like iron (Fe$^{16+}$, Fe xvi) is one of the most extensively investigated spectroscopic systems in astrophysics. Owing to the high abundance of Fe and to the closed electronic shell structure of the Ne-like ground configuration 2s$^2$2p$^6$, Fe$^{16+}$ forms over a wide range of temperatures ($kT = 100$–1000 eV). Hence, many spectra of hot astrophysical objects exhibit prominent Fe$^{16+}$ lines. A better understanding of the spectrum of Fe$^{16+}$ is even more important in light of the multitude of high-resolution X-ray spectra obtained with the grating spectrometers on board the Chandra and XMM-Newton observatories. The brightest lines of Fe$^{16+}$ in the X-rays arise from the 2p–3d and 2p–3s transitions, which appear roughly at 15 and 17 Å, respectively. The analysis of X-ray spectra emitted during solar flares has shown the potential of these lines to serve as diagnostic tools, mainly for the diagnostics of electron temperature (Raymond & Smith 1986; Smith et al. 1985), electron density (Schmelz, Saba, & Strong 1992; Waljeski et al. 1994; Phillips et al. 1996), and elemental abundances (Waljeski et al. 1994).

However, the usefulness of the Fe$^{16+}$ lines has been hampered by two persistent problems, which emerge from extensive comparisons between observations, laboratory measurements, and theoretical models. The first is that the strongest line at 15.01 Å arising from the 2p$^6$ 3S$_0$–2p$^5$3d$^1$P$_1$ transition appears to be significantly weaker than its predicted relative intensity. In particular, the intensity ratio of that line to the 2p$^6$ 3S$_0$–2p$^5$3d$^1$D$_1$ line at 15.26 Å, commonly labeled I$_{3D}$/I$_{3P}$ (Parkinson 1973), is consistently lower than the ratio calculated for a wide range of plasma parameters. This has led to the suggestion that the high oscillator-strength line at 15.01 Å is quenched by resonant scattering (Rugge & McKenzie 1985; Schmelz et al. 1992; Waljeski et al. 1994; Schmelz et al. 1997; Phillips et al. 1996; Phillips et al. 1997; Bhatia & Kastner 1999; Saba et al. 1999). The continuing discrepancies between observations and theory have prompted several laboratory studies in which the plasma elemental composition, and to a large extent also the plasma conditions, can be controlled. In particular, the EBIT (electron beam ion trap) device offers the opportunity to isolate nearly entirely the Fe$^{16+}$ ions from neighboring charge states and to measure their atomic properties with high accuracy. The EBIT measurements of Brown et al. (1998) first supported the claim that the line at 15.01 Å is affected by resonance scattering, although to a lesser extent than originally believed. However, as suggested by Behar, Cottram, & Kuhn (2001a) and later demonstrated in an EBIT measurement (Brown et al. 2001), a satellite line of Fe$^{15+}$ that coincides in wavelength and blends with the 15.26 Å line can explain most of the observed I$_{3C}$/I$_{3P}$ ratios without needing to invoke resonant scattering. This conclusion is also supported by measurements in the Princeton Large Torus tokamak (Beiersdorfer et al. 2001).

The second problem with the Fe$^{16+}$ lines is the overall intensities of the 2p–3s lines, which often appear enhanced relative to theoretical predictions when compared with the intensities of the 2p–3d lines. This has led to suggestions that 2p inner-shell ionization of Na-like Fe$^{15+}$ (ground configuration 2p$^6$3s) might contribute to the population of the 2p$^5$3s levels (Feldman 1995). Other explanations suggested

---

1 Institute for Computational Sciences and Informatics, George Mason University, Fairfax, VA 22030.
2 E. O. Hulburt Center for Space Research, Naval Research Laboratory, Code 7670D, Washington, DC 20375; rdoron@ssd5.nrl.navy.mil.
3 Columbia Astrophysics Laboratory and Department of Physics, Columbia University, 550 West 120th Street, New York, NY 10027; behar@astro.columbia.edu.
possible contributions to these level populations from dielectronic recombination (DR) of F-like Fe$^{17+}$ ($2p^5$) followed by radiative cascades (Saba et al. 1999; Liedahl 2000; Laming et al. 2000). An EBIT measurement that focused on the overall intensity ratio of the 2$p$-3$s$ lines relative to the 2$p$-3$d$ lines (Laming et al. 2000) yielded a ratio that generally agrees with theoretical predictions but is significantly lower than most astrophysical measurements. This further suggested that ionization and recombination processes, which are by and large absent from EBIT experiments and are also neglected in the theoretical models, play an important role in producing the Fe$^{16+}$ lines in cosmic sources.

The recent high-resolution observations of stellar coronae with Chandra (Brinkman et al. 2000; Canizares et al. 2000; Behar et al. 2001a; Ayres et al. 2001; Drake et al. 2001; Huenemoerder, Canizares, & Schulz 2001; Ness et al. 2001; Mewe et al. 2001) and XMM-Newton (Brinkman et al. 2001; Güdel et al. 2001a, 2001b; Audard, Güdel, & Mewe 2001a; Audard et al. 2001b) produced a variety of 2$p$-3$s$/2$p$-3$d$ intensity ratios. However, none of the observed ratios are fully consistent with existing theoretical models, further demonstrating that the above problems occur for a wide range of coronal sources. In addition, thanks to the high dispersion and efficiency of the Reflection Grating Spectrometer (RGS) on board XMM-Newton, Fe$^{16+}$ line spectra can now be obtained not only for stellar coronae (point sources) but also for extended sources. In observations of supernova remnants (Behar et al. 2001b) and elliptical galaxies (Xu et al. 2002), the relative Fe$^{16+}$ line intensities show the same discrepancies with available models. In fact, for the analysis of the X-ray spectrum of NGC 4636, Xu et al. (2002) were required to invoke the empirical Capella spectrum into their model, because even the most updated theoretical models could not reproduce the observed emission. The pervasive discrepancies between the calculated spectra and those measured for a wide variety of hot astrophysical sources strongly suggest that the problems lie in the shortcomings of the atomic models for line formation rather than in the uncertainties associated with the astrophysical environments.

In an effort to improve the existing atomic models, which neglect atomic processes that involve neighboring ions, we construct a three-ion collisional-radiative model that includes levels of F-like, Ne-like, and Na-like Fe. Such a model allows one to consider collisional excitation (CEs) as well as the effect of recombination and ionization simultaneously. The main drawback of a naive, all-inclusive three-ion model, in which rate equations for the three ionization states are solved simultaneously, is that the fractional ion abundances, which self-consistently result from the model, would be clearly erroneous. In order to obtain correct results for the ionization balance in a collisional-radiative model for a wide range of temperatures, one would have to include more than three ionization states, as well as numerous levels for each charge state (to adequately account for DR), which makes this approach impractical. Since we are interested in the line spectrum and not the ionization balance, we can circumvent this difficulty by adopting the approach formerly used in Doron et al. (1998, 2000), by which an independent ionization balance is imposed on the level-by-level, multi-ion model. The details of the current three-ion method are given in § 2. In § 3, we give the results of the three-ion model for the line-emission of Fe$^{16+}$ and compare them with results obtained with a basic, single-ion model typical of those that have been used until now.

### 2. Theoretical Method

Collisonally ionized, astrophysical plasmas are characterized by relatively high temperatures and low densities. The most common atomic model used to describe the line emission from a particular ionic species (say Fe$^{16+}$) under these conditions includes only electron impact excitations from the ground state and subsequent radiative decays, either directly to the ground state or via cascades. In the present work, we wish to extend this standard model and take into account also atomic processes involving neighboring ionization states. Specifically, we include dielectronic and radiative recombination from F-like Fe$^{17+}$, inner-shell ionization from Na-like Fe$^{15+}$, and resonant excitation (RE) through doubly excited levels of Fe$^{15+}$ (i.e., dielectronic capture followed by autoionization to excited levels). We assume the plasma is optically thin and collisionally ionized; i.e., photoexcitation and photoionization are unimportant. Assuming that the free electron energy distribution is Maxwellian, corresponding to an electron temperature $T_e$, the general set of rate equations for the density (population) $n_{j q}^{\pm}$ of an ion with charge $q$ in a level $j$ in a steady state can be written as

$$
\frac{d}{dt} n_{j q}^{\pm} = n_e \sum_{k \neq j} n_k^{\pm q} \left[ Q_{kj} (T_e) + Q_{jk}^{\pm} (T_e) \right] + \sum_{k > j} n_k^{\pm q} A_{kj} - n_j^{\pm q} \left[ \sum_{k < j} A_{kj} + \sum_{j' > j} A_{jj'}^{\pm q} \right] + n_e \left[ \sum_{j''} n_{j''}^{(q-1)^+} S_{jj''} (T_e) \right.
\left. + \sum_{j'} n_{j'}^{(q+1)^+} \left[ \alpha_{jj'}^{DC} (T_e) + \alpha_{jj'}^{RR} (T_e) \right] \right]
\left. - n_j^{\pm q} n_e \left[ \sum_{j''} S_{jj''} (T_e) + \sum_{j'} \left[ \alpha_{jj'}^{DC} (T_e) + \alpha_{jj'}^{RR} (T_e) \right] \right] \right) = 0 ,
$$

(1)

where $j'$ and $j''$ are levels pertaining to ions with charges $(q - 1)^+$ and $(q + 1)^+$, respectively. The terms $Q(T_e)$ and $Q^{\pm}(T_e)$, respectively, represent the rate coefficients for direct and resonant (RE) electron-impact excitation or deexcitation. The terms $A$ and $A^{\pm}$ denote the rate coefficients for spontaneous radiative decay and for autoionization, respectively. The terms $S(T_e)$ stand for the rate coefficients for collisional ionization (CI), and $\alpha^{DC}(T_e)$ and $\alpha^{RR}(T_e)$ are the rate coefficients for dielectronic capture and for radiative recombination, respectively. The electron density is denoted by $n_e$. The entire set of equations that needs to be solved consists also of the appropriate rate equations for $n_{j q}^{(q-1)^+}$ and $n_{j q}^{(q+1)^+}$, consistent with the atomic processes that appear in equation (1). Throughout this work, we use $q = 16$. Densities for ions other than the three considered are taken as zero. In order to obtain a unique solution, one of the rate equations in equation (1) is replaced by a
normalization condition, such as

$$\sum_j n_j^{(q-1)+} + \sum_j n_j^q + \sum_j n_j^{(q+1)+} = 1,$$

which leaves us with $N - 1$ independent equations for the $N$ levels included in the model.

A straightforward solution for equation (1) necessarily yields the ionization balance through the results for the level populations $n_j^{(q-1)+}$, $n_j^q$, and $n_j^{(q+1)+}$. As argued above, this resulting ionization balance will be wrong for most temperatures, as the set of equations consists of only three ionization states and, practically, an insufficient number of levels to determine the correct ionization balance. In order to avoid this error, the set of rate equations is solved by imposing the following constraints:

$$\sum_j n_j^{(q-1)+} / \sum_j n_j^q = f_{q-1}/f_q, \quad (2)$$

$$\sum_j n_j^{q+} / \sum_j n_j^{(q+1)+} = f_q/f_{q+1}, \quad (3)$$

where $f_{q-1}$, $f_q$, and $f_{q+1}$ represent the relevant ion fractions and are calculated independently. In other words, we impose the ionization balance and only seek for the consequential population distribution among the individual levels. We are primarily interested in levels $j$ of the ion with charge $q+1$. In the coronal approximation, where the ions are essentially in their ground state, and in the absence of metastable levels, it is sufficient to apply the constraints only through the ground levels of the three charge states. Moreover, collisional transitions among excited levels can be neglected. For Fe$^{16+}$, this approximation holds for $n_e \leq 10^{12}$ cm$^{-3}$. For the present study, we have adopted the fractional abundances calculated by Mazzotta et al. (1998). Table 1 presents the ion fractions of Fe$^{15+}$ through Fe$^{17+}$ for several chosen electron temperatures in the relevant range of 200–1000 eV. The last column in the table gives the combined fraction of these three ions as a function of temperature. These total values are provided in order to give an idea of the collective importance of these ions in astrophysical plasmas at each temperature.

For Fe$^{16+}$ we include in the model the configurations $2s^22p^6$, $2s^22p^5nl$ ($n = 3-7$), $2s^22p^6nl$ ($n = 3-7$), $2s^22p^43p^3l^p$, $2s^22p^53p^3l$, $2s^22p^3d^3l$, and $2s^22p^4d^3l$. For Fe$^{17+}$, the configurations $2s^22p^7$ and $2s^22p^43l$ are taken into account. Finally, the ground configuration $2s^22p^63s$ of Fe$^{15+}$ is also included. All of these configurations add up to 2111 levels. In fact, the inclusion of the RE processes ($Q^{RE}$ in rate equation (1)) is equivalent to including the doubly excited configurations of Fe$^{15+}$. Since we are not interested specifically in the population of the Fe$^{15+}$ levels, we have incorporated the RE rate coefficients from the literature (instead of including all of the appropriate doubly excited levels of Fe$^{15+}$), and by doing so, we significantly reduce the number of rate equations to be solved. The singly excited configurations of Fe$^{16+}$ up to $n = 7$ have been shown to account for most of the radiative-cascades effects (Liedahl 2000) and are taken into account in all of our models. The Fe$^{16+}$ doubly excited configurations that are included here explicitly produce about $50\%$ of the total DR effect in the entire 200–800 eV temperature range. The contribution of higher DR resonances is obtained by means of extrapolation based on the total DR rates published by Chen (1988). In order to account for the RR contribution onto high electronic shells with $n > 7$, we have employed a hydrogenic extrapolation method.

The solutions for rate equation (1), which are the normalized level populations $n_j^{(q+1)+} / \sum_k n_k^{(q+1)+}$, are used to obtain the line power $I_j^p$, which is defined here by:

$$I_j^p = \frac{n_j^{(q+1)+}}{\sum_k A_{jk} n_k} f_j n_e , \quad (4)$$

where $A_{jk}$ is the iron elemental abundance and $n_e$ is the hydrogen density.

The basic atomic quantities used in this work were generated by means of the multiconfiguration, relativistic HULLAC (Hebrew University Lawrence Livermore Atomic Code) computer package developed by Bar-Shalom, Klapisch, & Oreg (2001). Resonance excitation rates are not calculated explicitly but incorporated from Chen & Reed (1989) for the $2p^6$ to $2p^53l$ ($l = s, p$) excitations of Fe$^{16+}$. Following those authors, resonant excitation to $2p^53d$ levels is assumed to be unimportant because of their high energies and has been neglected.

### 3. RESULTS AND DISCUSSION

We have employed the model described above to calculate the Fe$^{16+}$ level populations and line intensities for various temperatures in the range 200–1000 eV. In the following, we focus our presentation on the results for the seven most intense Fe$^{16+}$ lines, which fall in the range 13.5–17.5 Å. The corresponding transitions, their labels, and measured wavelengths ($\lambda$) from Brown et al. (1998) are given in Table 2. Since in optically thin plasma, the relative intensities of these lines show negligible sensitivity to the electron density, the present results are valid for electron densities below $10^{12}$ cm$^{-3}$.

#### 3.1. Line Powers

The calculated line powers (defined in § 2, eq. [4]) as a function of the electron temperature for the seven transitions listed in Table 2 are given in Figures 1 and 2 by the solid curves. For comparison, we also give the line powers calculated with a single-ion model, i.e., a model that takes into account only direct electron impact excitations and
subsequent radiative decays. The data points in the plots throughout this paper mark the explicitly calculated values, while the curves represent a spline interpolation between these points. It can be seen from this comparison that the 2p–3s lines (Fig. 1), as well as the weak 2p–3d line at 15.45 Å (Fig. 2), are significantly affected by processes involving neighboring ions over a wide range of temperatures, while the two strong 2p–3d lines at 15.01 and 15.26 Å, as well as the 2s–3p line at 18.33 Å, are much less affected by these processes. In particular, the intensity of the strongest 2p–3d line at 18.33 Å is almost identical in the two types of models, while the intensity of the 2p–3s line at 17.10 Å roughly doubles when contributions from neighboring ionization states are considered.

3.2. Contribution of the Various Mechanisms to Upper Level Population

In order to obtain an insight into the dramatic differences between the results of the three-ion model and the single-ion model, we investigate the relative importance of each atomic process separately. This is done by running a sequence of three-ion models, where in each run we turn off one of the atomic processes: resonant excitation, dielectronic recombination, or collisional ionization. The resulting line powers in each of these models are presented in Table 3 for several electron temperatures in the range 200–800 eV. The results obtained with a traditional single-ion model, which includes direct collisional excitation alone, are also given for comparison. The first column in the table indicates the electron temperature, and the second column describes the model. The following columns give the line power for each of the seven lines. In general, it can be seen from Table 3 that among the additional atomic processes, which are included in the three-ion model, RE and DR are the most important.

At an electron temperature of 400 eV, the power of the 17.10 Å line, which is the most affected, receives contributions of 17%, 11%, 0.5%, and 3% from RE, DR, RR, and CI, respectively, which together enhance the line by 47% compared with the value obtained when calculating direct CE alone. At 600 eV, where the absolute Fe16+ line powers are still very high, the additional processes enhance the CE value for the 17.10 Å line by 57%, where RE, DR, RR, and CI produce, respectively, 10%, 21.5%, 0.5%, and 2.5% of the total line power. The other 2p–3s lines at 16.78 and 17.05 Å are also enhanced by the non-CE processes, albeit to a somewhat lesser degree (20%–30%). The main reason for this is DR, which preferentially populates the upper level of the 17.10 Å line. In addition, CI processes to that level are about twice as effective as CI to any other upper level of the 2l–3p transitions. The weak 2p–3d line at 15.45 Å is also enhanced, mostly by DR (RE processes toward the 2p83d levels are neglected). At 600 eV, 13.5% of the 15.45 Å line power is due to DR.

The trends of the various contributions with temperature are also interesting to note. The RE effect is predominant at low temperatures. It represents about twice as effective as CI to any other upper level of the 2l–3p transitions. The weak 2p–3d line at 15.45 Å is also enhanced, mostly by DR (RE processes toward the 2p83d levels are neglected). At 600 eV, 13.5% of the 15.45 Å line power is due to DR.
DR reaches almost 30% at 800 eV. These two opposing effects are a direct consequence of the strong variations in the fractional ionic abundances with temperature and the fact that the RE effect is correlated with the Fe$^{16+}$ abundance, while that of DR depends strictly on the Fe$^{17+}$ abundance. As can be inferred from Table 1 and from Mazzotta et al. (1998), the abundance of Fe$^{16+}$ dominates at temperatures up to $\sim$400 eV, while that of Fe$^{17+}$ peaks at $\sim$600 eV. Interestingly, through most of the temperature range in which the Fe$^{16+}$ line powers are relatively high, say 300–700 eV (see Figs. 1 and 2), both RE and DR are important, which means neither can be neglected when accurate line powers are needed. Recent unpublished calculations by Chen & Pradhan (2002) claim that Chen & Reed (1989) have underestimated the RE rate coefficients. Indeed, higher RE rates would imply an even more pronounced enhancement to the line powers than demonstrated here, especially in the low-temperature regime, where RE is important. Unfortunately, the absence of full level-by-level RE rate coefficients in that paper precludes us from estimating this effect quantitatively. Notwithstanding, the DR and CI enhancements calculated in this work are by and large independent of the RE effect.

It is important to distinguish between the DR enhancement of Fe$^{16+}$ lines calculated in this work and the effect of Fe$^{15+}$ DR satellite lines, which was traditionally incorporated in plasma models (see, e.g., Raymond & Smith 1986). The DR effect, which is discussed here, produces the exact same parent lines of Fe$^{16+}$ (i.e., $2p^53l^2p^6$), by means of DR processes that populate the upper levels of these transitions (e.g., $2p^53l^3l^02p^6$). This should not be confused with DR satellites emitted by lower charge states at slightly longer wavelengths (e.g., $2p^53l^3l^02p^6$ in Fe$^{15+}$). The latter, in many cases, can be resolved from the parent lines by high-resolution spectrometers. Note, however, that the radiative decays ($2p^53l^3l^02p^6$) that populate the upper levels of the Fe$^{16+}$ lines, are, in fact, associated with DR satellites of Fe$^{17+}$. This line emission is explicitly included in our calculations and is illustrated in the spectra shown below in § 3.4.

### 3.3. Line Intensity Ratios

The large impact of the additional atomic processes considered in the three-ion model on some of the line intensities directly affects the line ratios, and thus the diagnostic applications of the Fe$^{16+}$ system. In Figures 3–5, we present the

### Table 3

| Line Power (x10^{-12} cm^3 s^{-1}) | 2s–3p (13.83 Å) | 2p–3d (15.01 Å) | 2p–3d (15.26 Å) | 2p–3d (15.45 Å) | 2p–3s (16.78 Å) | 2p–3s (17.05 Å) | 2p–3s (17.10 Å) |
|-----------------------------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|
| **200 eV**                        |                |                |                |                |                |                |                |
| Complete ...                      | 0.128          | 2.96           | 0.897          | 0.152          | 2.39           | 3.02           | 2.52           |
| No RE ...                         | 0.128          | 2.96           | 0.897          | 0.152          | 1.69           | 2.07           | 1.66           |
| No DR ...                         | 0.128          | 2.96           | 0.895          | 0.151          | 2.38           | 3.00           | 2.49           |
| No RR ...                         | 0.128          | 2.96           | 0.897          | 0.152          | 2.39           | 3.02           | 2.52           |
| No CI ...                         | 0.128          | 2.96           | 0.897          | 0.152          | 2.36           | 2.98           | 2.46           |
| CE only ...                       | 0.128          | 2.96           | 0.894          | 0.150          | 1.64           | 2.00           | 1.56           |
| **400 eV**                        |                |                |                |                |                |                |                |
| Complete ...                      | 2.78           | 39.7           | 11.8           | 1.60           | 25.0           | 31.4           | 25.8           |
| No RE ...                         | 2.78           | 39.7           | 11.8           | 1.60           | 21.3           | 26.4           | 21.4           |
| No DR ...                         | 2.76           | 39.6           | 11.7           | 1.49           | 24.2           | 29.8           | 22.9           |
| No RR ...                         | 2.78           | 39.7           | 11.8           | 1.60           | 25.0           | 31.2           | 25.7           |
| No CI ...                         | 2.77           | 39.7           | 11.8           | 1.57           | 24.6           | 30.8           | 25.0           |
| CE only ...                       | 2.75           | 39.6           | 11.7           | 1.45           | 20.1           | 24.2           | 17.6           |
| **600 eV**                        |                |                |                |                |                |                |                |
| Complete ...                      | 3.16           | 37.5           | 11.1           | 1.33           | 21.5           | 26.3           | 22.6           |
| No RE ...                         | 3.16           | 37.5           | 11.1           | 1.33           | 19.5           | 23.6           | 20.3           |
| No DR ...                         | 3.13           | 37.4           | 10.9           | 1.15           | 20.1           | 24.5           | 17.6           |
| No RR ...                         | 3.16           | 37.5           | 11.1           | 1.32           | 21.5           | 26.2           | 22.4           |
| No CI ...                         | 3.15           | 37.5           | 11.1           | 1.33           | 21.1           | 25.8           | 22.0           |
| CE only ...                       | 3.12           | 37.4           | 10.9           | 1.13           | 17.7           | 21.2           | 14.4           |
| **800 eV**                        |                |                |                |                |                |                |                |
| Complete ...                      | 1.01           | 10.9           | 3.22           | 0.366          | 5.87           | 7.48           | 6.33           |
| No RE ...                         | 1.01           | 10.9           | 3.22           | 0.366          | 5.48           | 6.95           | 5.87           |
| No DR ...                         | 0.99           | 10.8           | 3.14           | 0.292          | 5.33           | 6.48           | 4.35           |
| No RR ...                         | 1.01           | 10.9           | 3.22           | 0.361          | 5.87           | 7.44           | 6.30           |
| No CI ...                         | 1.00           | 10.9           | 3.20           | 0.365          | 5.80           | 7.35           | 6.19           |
| CE only ...                       | 0.98           | 10.8           | 3.12           | 0.287          | 4.84           | 5.78           | 3.72           |
most interesting line intensities normalized in most cases to the 2p–3d line at 15.01 Å, which is the strongest Fe $^{16+}$ line at most temperatures and also the least affected by the additional processes (see Table 3). As in Figures 1 and 2, the solid curves represent the results of the (complete) three-ion model, and the dotted curves represent the single-ion model. The most pronounced effect is found for the ratios involving the 2p–3s lines in Figure 3. Since the spectral resolution of contemporary spectrometers, such as the RGS aboard XMM-Newton and the LETGS aboard Chandra, is hardly sufficient to resolve the two 2p–3s lines at 17.10 and 17.05 Å, we also show the corresponding curve for the summed intensities of these two lines. The ratio involving the third 2p–3s line at 16.78 Å is given separately in Figure 4 to avoid overcrowding the plot. The calculated ratios shown in Figure 3 shed new light on the discrepancy as yet between the observed and calculated values for the ratio of the 17.10 and 17.05 Å lines to the line at 15.01 Å. Using the single-ion model, one obtains (in the relevant temperature range) a maximum value of 1.2 for the ratio $I_{17.10} + I_{17.05}$/$I_{15.01}$, while the observed ratios from various coronal sources, including many observations of the Sun, are in the range of $\sim$1.5–2.6. A list of various measured ratios for these lines is presented in Table 4. The inclusion of RE, DR, and CI processes in the calculations by means of the three-ion model yields values of $\sim$1.4–1.9 for this ratio at temperatures of 200 eV and higher, where Fe $^{16+}$ forms predominantly. Even higher values, which are observed mostly in active regions on the Sun (e.g., Phillips et al. 1997; Saba et al. 1999) can be attained for this ratio at lower temperatures, which are realistic for these environments. In the special case of spatially resolved observations of the Sun, resonant scattering of the 15.01 Å line is also plausible. Alternatively, nonequilibrium ionization (NEI) conditions can also play a role in enhancing the 2p–3s/2p–3d ratios. In particular, NEI conditions make the effects of ionization and recombination on line formation more pronounced than in equilibrium and would tend to enhance the 2p–3s lines even further. In conclusion, the major part of the observed ratios can be explained in terms of the three-ion coronal-equilibrium model. For the abnormally high ratios observed mostly in the Sun, resonant scattering and NEI are also plausible.

The present results can shed more light on the interpretation of laboratory measurements. Laming et al. (2000) found for the 2p–3s/2p–3d ratios good agreement between their EBIT measurements and simple, single-ion models. In the EBIT experiment, the selectivity of the ionic charge Fe $^{16+}$ is supposed to be very high, and the presence of Fe $^{15+}$ and Fe $^{17+}$ can therefore be minimized. In addition, Laming et al. (2000) used a relatively high energy ($\sim$1 keV) electron beam. Under such conditions, the contributions of RE, DR, and CI are expected to be very small, and a single-ion CE model could therefore be adequate for reproducing the experimental results. However, in a very recent EBIT experiment, also with a high-energy beam (>0.8 keV), P. Beiersdorfer et al. (2002, unpublished) measure...
$2p-3s/2p-3d$ ratios that are almost a factor of 2 higher than those measured by Laming et al. (2000). These recent results could imply that even the basic CE models may be inadequate, or that high-lying resonances do contribute to RE even at these high energies, or a combination thereof. In any event, the effects of the additional processes, which are put forward in this work, are relevant to all plasmas in collisional equilibrium, and as such they ubiquitously enhance the CE (+ additional RE) rates measured with EBIT. Another indication for additional processes in plasma sources that are not present in EBIT experiments comes from the relative intensities of the 17.05 and 17.10 Å lines. In the EBIT measurements of Brown et al. (1998) the line at 17.05 Å is significantly stronger than the line at 17.10 Å, while in many astrophysical observations the two lines have comparable intensities (e.g., Rugge & McKenzie 1985; Huene-emoerder et al. 2001; Behar et al. 2001a). This difference is consistent with our results as presented in Table 3, where DR enhances the 17.10 Å line much more than it does the 17.05 Å line.

As can be seen in Figure 3, for $kT_e \leq 600$ eV, the newly calculated $2p-3s/2p-3d$ ratios are more sensitive to the electron temperature than those calculated with the single-ion model, while at higher temperatures, the little sensitivity that existed in the single-ion model is, in fact, lost in the new model. In particular, the major role played by the RE processes at low temperatures significantly increases the temperature sensitivity in this regime. The $\left(I_{17.05} + I_{17.10}\right)/I_{15.01}$ ratio decreases from 1.9 to 1.4 from 200 to 600 eV. The temperature sensitivity of these ratios diminishes rapidly thereafter, but in any case the absolute power of these lines drops sharply beyond 600 eV (see Figs. 1 and 2). Therefore, in multitemperature sources often unresolved in astrophysical observations, the high-temperature contribution to the integrated spectrum of Fe$^{16+}$ would be very small. In Figure 4, one can see that the values obtained for the ratio $I_{15.01}/I_{15.26}$ in the three-ion model are not very different ($<3\%$) than the single-ion model values in the entire temperature range. We note that our single-ion calculations for the ratio $I_{15.01}/I_{15.26}$ yield a value of 3.4. The present model includes configurations up to $n = 7$. The inclusion of even higher configurations would have only a negligible effect on the ratio. A value of 3.4 is about 12% higher than the value measured by Brown et al. (1998) in EBIT with a monenergetic beam at 1.15 keV and about 15% higher than the EBIT ratio measured by Laming et al. (2001) with a beam energy of 0.9 keV. The EBIT values are associated with errors of about 5%. Both measurements are just within the 15% accuracy range expected from the CE rate coefficients produced by the HULLAC code for this kind of atomic system.

The ratio of the weak $2p-3d$ line at 15.45 Å to the $2p-3s$ resonance line at 15.01 Å is also enhanced, albeit to a lesser extent than the $2p-3s$ lines, as can be seen in Figure 5. The $2s-3p$ line at 13.83 Å is only very slightly affected by the additional processes (Fig. 5). The 15.45 Å line is enhanced for the most part by DR, while the effects of CI and RR are very small. The DR effect increases with temperature because of the increase in the abundance of Fe$^{15+}$. The CI effect, on the other hand, depends on both the CI rate coefficients that increase with temperature but also on the decreasing Fe$^{15+}$ abundance. Since at low temperatures, the rate coefficients for inner-shell ionization (CI) are very small while the Fe$^{15+}$ abundance is high and vice versa at high temperatures, the CI effect is suppressed in ionization equilibrium conditions throughout the relevant temperature range. In NEI, however, the CI effect could be more pronounced. Note that following Chen & Reed (1989), RE processes to $2p^53d$ levels are neglected in our model. However, according to Chen & Pradhan (2002), RE processes do, in fact, populate the upper level of the 15.45 Å line and enhance this ratio to values of 0.08 and higher. On the other hand, the measurements of P. Beiersdorfer et al. (2002, unpublished) show a value of 0.04 for this ratio, which is totally consistent with the present results. Either way, the DR effect on this ratio demonstrated in Figure 5 remains. Admittedly, the ratios in Figure 5 could be rather hard to use for diagnostics because of their weakness in most sources. However, in bright sources, such as Capella for instance, the 13.83 Å line could be intense enough to provide useful temperature diagnostics (Behar et al. 2001a).

We point out that the present line ratios have been compared with those calculated by M. Gu (2002, private communication) using a similar model based on the FAC atomic code (Gu 2002). The overall $2p-3s/2p-3d$ intensity ratios obtained with the two codes agree to within 1%. The agreement between ratios for individual lines is $\sim 5\%$.

---

**TABLE 4**

| Source                  | Spectrometer       | $(I_{17.05} + I_{17.10})/I_{15.01}$ | Reference |
|-------------------------|--------------------|-----------------------------------|-----------|
| Sun                     | Solex B RAP       | 1.95$^a$                          | 1         |
| Solar flares            | Flat crystal      | 1.93$^a$                          | 2         |
| Solar active region     | Flat crystal      | 2.2$^a$                           | 2         |
| Solar active region     | Flat crystal      | 2.6$^a$                           | 3         |
| Capella                 | Chandra HETGS     | 1.67$^a$                          | 4, 5      |
| Capella                 | Chandra LETGS     | 1.62$^a$                          | 6         |
| Capella                 | Chandra LETGS     | 1.52$^a$                          | 7         |
| HR 1099                 | Chandra HETGS     | 1.67$^a$                          | 8         |
| II Pegasi               | Chandra HETGS     | 2.10$^a$                          | 9         |
| NGC 4636....            | XMM-Newton RGS    | 1.59$^a$                          | 10        |

$^a$ Averaged over many observations.
3.4. Synthetic Spectra

As seen in §§ 3.2 and 3.3, additional processes to direct CE have a major role in producing the soft X-ray lines of Fe\textsuperscript{16+}. In order to provide a more visual illustration of the overall effect on the spectrum, total and partial synthetic spectra calculated for 400 eV are presented in Figure 6. The upper trace in the figure gives the total spectrum, while the lower trace shows the explicit contribution of the CE processes alone. The middle trace represents the complementary contribution of non-CE processes. The different plots in Figure 6 are all on the same scale. The spectra clearly show the importance of the non-CE processes to the 2\textit{p}–3\textit{s} lines at \(\sim 17 \, \text{Å}\). The 2\textit{p}–3\textit{d} lines (\(\sim 15 \, \text{Å}\)) are almost unaffected by these mechanisms. The spectra also include lines of Fe\textsuperscript{17+}, around 14.2 Å (2\textit{p}–3\textit{d}) and 16 Å (2\textit{p}–3\textit{s}), which are produced self-consistently by the model and are rather weak at 400 eV. The line intensities for Fe\textsuperscript{17+}, however, should be viewed with caution, since the model for Fe\textsuperscript{17+} is limited. Particularly, DR processes from Fe\textsuperscript{18+} are not taken into account. In addition, the model does not include the DR satellite lines of Fe\textsuperscript{15+}, and therefore these are absent from the plots in Figure 6. At 400 eV, these DR satellites are expected to produce weak line emission mostly around 15.26 Å, as mentioned above in § 1.

4. CONCLUSIONS

We have constructed a three-ion model to account for ionization and recombination processes that produce the Fe\textsuperscript{16+} emission lines, in addition to the collisional and radiative processes among Fe\textsuperscript{16+} levels. It is shown that recombination (radiative and dielectronic), inner-shell collisional ionization, and resonant excitation processes contribute significantly to the line powers and can resolve the existing discrepancies between observations and previous calculations within the framework of a coronal equilibrium model. Among the additional processes considered, RE and DR (of Fe\textsuperscript{17+}) are found to play a major role in producing the Fe\textsuperscript{16+} lines. The present calculations reproduce the systematically high values observed for the 2\textit{p}–3\textit{s}/2\textit{p}–3\textit{d} intensity ratios in many astrophysical sources. Only abnormally high ratios observed mostly on the Sun may still require one to invoke resonant scattering of the 15.01 Å line, or less likely transient conditions that depart from ionization equilibrium. Since nonequilibrium conditions are not required to explain most of the observed ratios, we defer the study of those cases to future work. The fact that recombination and ionization are important makes the present predictions dependent upon the ionization balance of Fe\textsuperscript{15+}–Fe\textsuperscript{17+}. We expect similar effects of inner-shell ionization and of recombination on the 2\textit{l}–3\textit{l'} lines to be present in more highly ionized systems (Fe\textsuperscript{19+}–Fe\textsuperscript{21+}) as well. However, a reliable assessment of this effect will require detailed models similar to the one employed here. The results of the present, elaborate, three-ion model should also be important for analyzing the intensities of other lines that arise from the decay of the 2\textit{p}3\textit{s} levels, i.e., 3\textit{l}–3\textit{l'} transitions. In the case of Fe\textsuperscript{16+}, these transitions fall in the EUV range. In lighter Ne-like ions, these 3\textit{l}–3\textit{l'} transitions are clearly observed in the UV solar spectra obtained by the Solar and Heliospheric Observatory (SOHO) and the Solar Ultraviolet Measurements of Emitted Radiation spectrometer on board the Solar and Heliospheric Observatory satellite.

E. B. acknowledges ongoing work and many useful discussions with Steven Kahn on the complexity of the line intensity patterns of Fe\textsuperscript{16+} and their manifestation in X-ray observations. We are grateful to Ming Feng Gu for useful comparisons of the present results with some of his own calculations. We thank Daniel Savin for reading the manuscript carefully prior to its submission. R. D. was supported by a NASA Solar Physics Guest Investigator Grant S137816.

REFERENCES

Audard, M., Behar, E., Güdel, M., Raassen, A. J. J., Porquet, D., Mewe, R., Foley, C. R., & Bromage, G. E. 2001b, A&A, 365, L329
Audard, M., Güdel, M., & Mewe, R. 2001a, A&A, 365, L318
Ayres, T. R., Brown, A., Osten, R. A., Huenemoerder, D. P., Drake, J. J., Brickhouse, N. S., & Linsky, J. L. 2001, ApJ, 549, 554
Bar-Shalom, A., Klapisch, M., & Oreg, J. 2001, J. Quant. Spectrosc. Radiat. Transfer, 71, 169
Behar, E., Cottam, J., & Kahn, S. M. 2001a, ApJ, 548, 966
Behar, E., Rasmussen, A. P., Griffiths, R. G., Dennerl, K., Audard, M., Aschenbach, B., & Brinkman, A. C. 2001b, A&A, 365, L242
Beiersdorfer, P., Von Goeler, S., Bitter, M., & Thorn, D. B. 2001, Phys. Rev. A, 64, 2705
Bhatia, A. K., & Kastner, S. O. 1999, ApJ, 516, 482
Brinkman, A. C., et al. 2000, ApJ, 530, L111
Brown, G. V., Beiersdorfer, P., Chen, H., Chen, M. H., & Reed, K. J. 2001, ApJ, 557, L75
Brown, G. V., Beiersdorfer, P., Liedahl, D. A., Widman, K., & Kahn, S. M. 1998, ApJ, 502, 1015 (erratum 532, 1245 [2000])
Canizares, C. R., et al. 2000, ApJ, 539, L41
Chen, G. X., & Pradhan, A. K. 2002, preprint (astro-ph/0201513)
Chen, M. H. 1988, Phys. Rev. A, 38, 2332
Chen, M. H., & Reed, K. J. 1989, Phys. Rev. A, 40, 2292
Doron, R., Behar, E., Frankev, M., Mandelbaum, P., Schwoh, J. L., Zigler, A., Faenov, A.Y., & Pikuz, T. A. 1998, Phys. Rev. A, 58, 1859
Doron, R., Behar, E., Mandelbaum, P., & Schwob, J. L. 2000, J. Quant. Spectrosc. Radiat. Transfer, 65, 161
Drake, J. J., Brickhouse, N. S., Kashyap, V., Laming, J. M., Huememoerder, D. P., Smith, R., & Wargelin, B. J. 2001, ApJ, 548, L81
Feldman, U. 1995, Comments At. Mol. Phys., 31, 11
Gu, M. F. 2002, Comput. Phys. Commun., in press
Güdel, M., Audard, M., Magee, H., Franciosini, E., Grosso, N., Cordova, F. A., Pallavicini, R., & Mewe, R. 2001a, A&A, 365, L344
Güdel, M., et al. 2001b, A&A, 365, L336
Huenemoerder, D. P., Canizares, C. R., & Schulz, N. S. 2001, ApJ, 559, 1135
Laming, J. M., et al. 2000, ApJ, 545, L161
Liedahl, D. A. 2000, in Atomic Data Needs for X-Ray Astronomy, ed. M. A. Bautista, T. R. Kallman, & A. K. Pradhan (NASA CP-2000-209968; Washington: NASA), 151
Mazzotta, P., Mazzitelli, G., Colafrancesco, S., & Vittorio, N. 1998, A&AS, 133, 403
Mewe, R., Raassen, A. J. J., Drake, J. J., Kaastra, J. S., Van Der Meer, R. L. J., & Porquet, D. 2001, A&A, 368, 888
Ness, J.-U., et al. 2001, A&A, 367, 282
Parkinson, J. H. 1973, A&A, 24, 215
Phillips, K. J. H., Greer, C. J., Bhatia, A. K., Coffey, I. H., & Keenan, F. P. 1997, A&A, 324, 381
Phillips, K. J. H., Greer, C. J., Bhatia, A. K., & Keenan, F. P. 1996, ApJ, 469, L57
Raymond, J. C., & Smith, B. W. 1986, ApJ, 306, 762
Rugge, H. R., & McKenzie, D. L. 1985, ApJ, 297, 338
Saba, J. L. R., Schmelz, J. T., Bhatia, A. K., & Strong, K. T. 1999, ApJ, 510, 1064
Schmelz, J. T., Saba, J. L. R., Chauvin, J. C., & Strong, K. T. 1997, ApJ, 477, 509
Schmelz, J. T., Saba, J. L. R., & Strong, K. T. 1992, ApJ, 398, L115
Smith, B. W., Raymond, J. C., Mann, J. B., & Cowan, R. D. 1985, ApJ, 298, 898
Waljeski, K., Moses, D., Dere, K. P., Saba, J. L. R., Web, D. F., & Zarro, D. M. 1994, ApJ, 429, 909
Xu, H., Kahn, S. M., Peterson, J. R., Behar, E., Paerels, F. B. S., Moshutzy, R. F., Jernigan, J. G., & Makishima, K. 2002, preprint (astro-ph/0110013)