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Comparison of explicit calculations for $n=3-8$ dielectronic satellites of the Fe XXV $K\alpha$ resonance line with experimental data from the tokamak fusion test reactor

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Dielectronic satellite spectra of the Fe XXV $K\alpha$ resonance line observed from tokamak fusion test reactor plasmas have been compared with recent explicit calculations for the $n=3-8$ dielectronic satellites as well as the earlier theoretical predictions, which were based on the $1/n^3$ scaling law for $n>4$ satellites. The analysis has been performed by least-squares fits of synthetic spectra to the experimental data. The synthetic spectra constructed from both theories are in good agreement with the observed data. However, the electron-temperature values obtained from the fit of the present explicit calculations are in better agreement with independent measurements.

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It is well known [1–5] that the $K\alpha$ resonance line of heliumlike ions is blended with lithiumlike dielectronic satellites due to transitions $1s^2nl$-$1s2pnl$ with $n \geq 3$. These unresolved satellites lead to a significant increase in both the apparent width and intensity of the resonance line, which must be taken into account for Doppler-broadening and Doppler-shift measurements as well as the evaluation of satellite-to-resonance-line ratios, which are used for diagnostics of solar flares and tokamak plasmas [5–10]. In view of these important diagnostic applications, it is necessary to determine the contribution of these satellites as well as possible. However, explicit calculations of the high-n-satellite line strengths are difficult, due to the fact that the number of intermediate resonance states increases rapidly with the principal quantum number n of the outermost occupied shell of the resonance state. As a result, explicit calculations [1,11–15] have been limited so far to low-lying resonance states with $n \leq 4$, while an approximate $1/n^3$ scaling law has generally been used to extrapolate the satellite intensity factors for $n>4$.

In order to test the validity of this approximation, Karim and Bhalla have recently performed explicit calculations of $n=3-8$ dielectronic satellite line strengths using the Hartree-Fock atomic model for Ne VII, Si XIII, Ar XVII, Ti XXI, Cr XXIII, and Ni XXVII [16]. They found that the n threshold above which the $1/n^3$ scaling law provides a good approximation varies with Z. For high-Z ions, the $1/n^3$ scaling law can be applied if $n \geq 5$, whereas for low-Z ions ($Z \leq 14$) it can only be applied if $n \geq 8$. The purpose of this paper is to compare recent explicit Hartree-Fock model calculations for the $n=3-8$ dielectronic satellites of Fe XXV and the earlier theoretical results from Bely-Dubau, Gabriel, and Volonté [1] who used the $1/n^3$ scaling law for dielectronic satellites with $n>4$, with experimental spectra.

The experimental data were recorded from ohmically heated tokamak-fusion-test-reactor (TFTR) plasmas with a central major radius $R=2.70$ m and minor radius $a=0.95$ m, which were fueled by the injection of solid deuterium pellets. There was also a small amount of radio-frequency heating (0.5, 0.6, and 1.0 MW, respectively, for each of the three discharges we analyzed) from 3.3 to 3.8 s. Pellet injections result in large electron-density increases, as shown in Fig. 1, which are correlated with a sudden drop of the electron temperature. As a result, pellet injections in ohmically heated discharges provide ideal experimental conditions for the study of high-n dielectronic satellites, which are then very pronounced due to the facts that (1) the intensities of the dielectronic satellites relative to the resonance line increase with decreasing electron temperatures, and (2) the Doppler broadening of the lines is substantially reduced since the ion temperatures T_i are low ($T_i \approx T_e$), so that a large

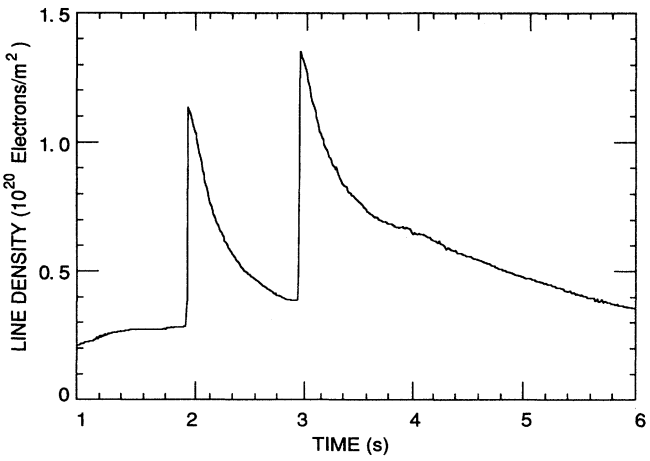

FIG. 1. Line-averaged electron density as a function of time from a TFTR discharge with injection of solid deuterium pellets at 2 and 3 s. The data were measured with the TFTR infrared interferometer at a plasma major radius $R=2.47$ m. The plasma center was at $R=2.70$ m, as determined by the magnetic axis.

fraction of the $n=3$ satellites is resolved from the resonance line.

Figure 2 presents spectra obtained after the injection of the second pellet during the period from 4.5 to 5.0 s from the TFTR high-resolution vertical x-ray crystal spectrometer [17] at a plasma major radius $R=2.41$ m. The data have been accumulated from three very similar discharges in order to reduce the statistical errors. Since most of the $n \geq 3$ dielectronic satellites are blended with the $K\alpha$ resonance line, we performed a least-squares fit of synthetic spectra constructed from the present calculations [Fig. 2(a)] and from the theory of Bely-Dubau, Gabriel, and Volonté [1] [Fig. 2(b)] to the experimental data. The results from both fits, which include the individual contributions from the different n shells, are shown in Fig. 2 by solid lines. The present calculations were performed using the Hartree-Fock atomic model for the following cases: $1s2pnp$ ($n=2$–8), $1s2pns$ ($n=2$–8), $1s2pnd$ ($n=3$–8), $1s2pnf$ ($n=4$–8), and $1s2snp$ ($n=2$–8); the details of the calculations are given in Ref. [16]. On the other hand, the calculations of Bely-Dubau, Gabriel, and Volonté [1] are based on the scaled Thomas-Fermi atomic model and used the $1/n^3$ scaling law for dielectronic satellites with $n=5$–16. The synthetic spectrum from the present explicit calculations shown in Fig. 2(a) is composed of approximately 100 spectral lines. Since these calculations have been carried out only up to $n=8$, we have taken the extrapolated data of Bely-Dubau, Gabriel, and Volonté [1] only up to $n=8$ in order to make a sensible comparison of the two theories. Since the spectrometer has no absolute wavelength calibration, the experimental wavelengths have been normalized to the value of 1.85026 Å for the $K\alpha$ resonance line obtained by Briand *et al.* from an absolute wavelength measurement in beam-foil experiments [18]. Similarly, the theoretical wavelengths from the present calculations have been shifted by a constant

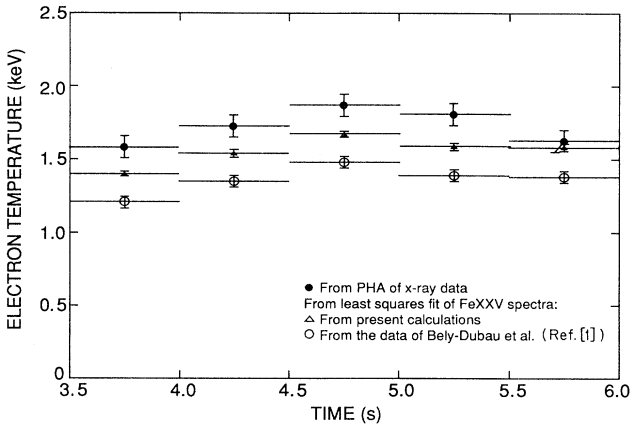

FIG. 3. Comparison of the electron-temperature values derived from least-squares fits of the synthetic spectra constructed from the present calculations and the theory of Bely-Dubau, Gabriel, and Volonté (Ref. [1]) with the results from the PHA system.

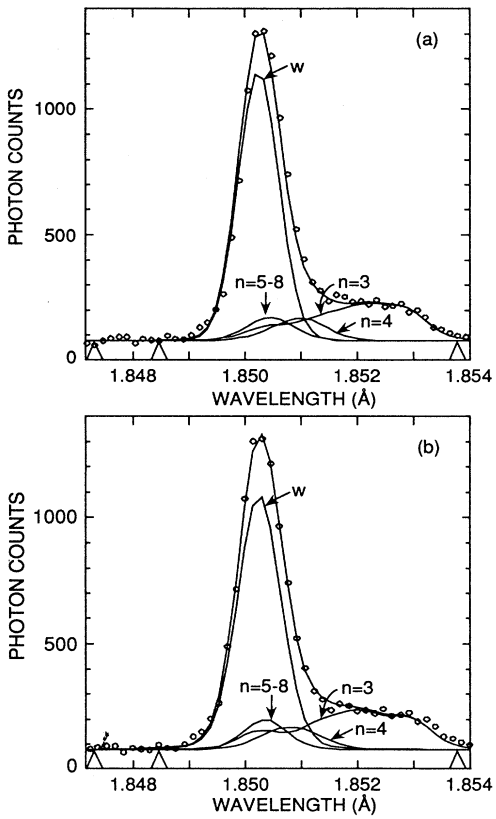

FIG. 2. Spectra of the Fe XXV $K\alpha$ resonance line accumulated from three very similar TFTR discharges during the period from 4.5 to 5.0 s after the injection of the second pellet (circles). The solid lines represent least-squares fits of synthetic spectra constructed from (a) present calculations and (b) the theory of Bely-Dubau, Gabriel, and Volonté (Ref. [1]) to the experimental data. Shown are the individual contributions from the resonance line and the $n=3$, $n=4$, and $n=5$–8 satellites, as well as the sum of these components.

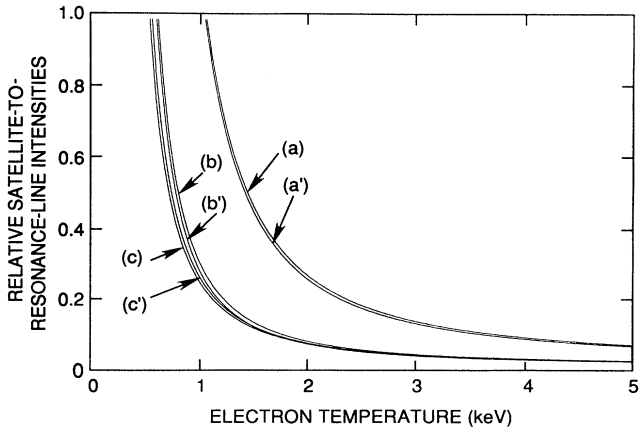

FIG. 4. Theoretically predicted intensity ratios of the dielectronic satellites to the resonance line as a function of the electron temperature. Contributions from the $n=3$, $n=4$, and $n=5$–8 shells are labeled (a), (b), and (c), respectively, for present calculations and (a'), (b'), and (c') for the theory of Bely-Dubau, Gabriel, and Volonté (Ref. [1]).

amount of 1.86 mÅ, and the wavelengths from Bely-Dubau, Gabriel, and Volonté [1] were shifted by 0.36 mÅ.

The least-squares fits allowed us to determine best values for the electron temperatures, upon which the ratios of the dielectronic satellites to resonance line intensity solely depend [1,19]. The T_e results from these fits have been compared with the values provided by independent measurements from the TFTR pulse-height analysis (PHA) system [20], and are shown in Fig. 3 for five time intervals of 500 ms ranging from 3.5 to 6.0 s. The PHA values shown in Fig. 3 were obtained from an interpolation of results measured at $R=2.08$ and 2.70 m, using radial profiles of the electron-cyclotron emission which was measured by the TFTR radiometer. The estimated errors for these PHA results are typically of the order of 10%. The error bars for the T_e values obtained from the least-squares fits were typically of the order of 50 eV. These error bars reflect the good agreement between the synthetic and observed spectra, since the statistical errors of the experimental data were small.

The T_e values obtained from the fit of the present explicit calculations are in better agreement with the PHA results than the one obtained from the fit of the data of Bely-Dubau, Gabriel, and Volonté [1] using the $1/n^3$ scaling law. The difference of typically 200 eV in the electron-temperature results obtained from the two theories cannot be ascribed to differences in the theoretical predictions for the satellite-to-resonance-line intensity ratios, which are in fact very similar for both theories, as shown in Fig. 4: This confirms previous findings from Karim and Bhalla [16] that the $1/n^3$ scaling law should be applicable for iron. We assume that the difference in the T_e values obtained from both theories can be explained by small differences in the predicted wavelengths. We note that in the calculation of Bely-Dubau, Gabriel, and Volonté [1], the wavelengths for the dielectronic satellites from each n shell with $n \geq 5$ were grouped under a unique value, which was also determined by a scaling law, while the wavelengths were explicitly calculated for each line in the present paper.

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