New Benchmarks from Tokamak Experiments for Theoretical Calculations of the Dielectronic Satellite Spectra of Heliumlike Ions

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Dielectronic satellite spectra of heliumlike argon, recorded with a high-resolution x-ray crystal spectrometer at the National Spherical Torus Experiment, were found to be inconsistent with existing predictions resulting in unacceptable values for the power balance and suggesting the unlikely existence of non-Maxwellian electron energy distributions. These problems were resolved with calculations from a new atomic code. It is now possible to perform reliable electron-temperature measurements and to eliminate the uncertainties associated with determinations of non-Maxwellian distributions.

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The theory of the dielectronic satellite spectra of heliumlike ions, which are widely used for the diagnosis of stellar flares, tokamak plasmas, and laser-produced plasmas, has been continuously improved during the past few decades to satisfy the demands for accurate atomic data and to establish a solid base for the development of the theory for more complex ions with more than two electrons. As a result, several numerical codes, which are based on different theoretical approaches and relativistic approximations, are now available. An extensive comparison of the predictions from three widely used codes, the MZ, AUTOLSJ, and YODA codes, with solar flare spectra of heliumlike iron was recently presented by Kato *et al.* [1]. Kato found that the predictions from the three codes for the main satellite lines were to within 20% in agreement with each other and that synthetic spectra constructed from each individual code were in good general agreement with the experimental data. However, it is fair to say that the spectral resolution and statistics of the considered solar flare spectra were insufficient for a detailed comparison with the theoretical predictions, since on the basis of these experimental data it was not possible to make a distinction between the predictions from the different codes or to detect inherent inconsistencies. In particular, the predictions for the numerous dielectronic satellites in the neighborhood of the heliumlike resonance line, which are associated with principal quantum number $n = 3$ and commonly used to infer the existence of non-Maxwellian electron energy distributions in solar flares and tokamaks [2,3], could not be tested. Earlier observations of the Fe XXV satellite spectra in plasmas of the Princeton Large Torus were in good general agreement with theoretical predictions, but we point out that there were deviations between the AUTOSLJ code values and the experimental data for the ratio of the $n = 2$ and $n = 3$ satellites [4]. The $K\beta$ branch of these satellites also plays an important role in the electron density and temperature measurements of inertial confinement fusion plasmas [5].

An experimental investigation of these satellites requires measurements with high-resolution instruments from well-diagnosed plasmas of sufficiently low electron temperature where these features become prominent. Such conditions are now available at the National Spherical Torus Experiment (NSTX) in Ohmically heated plasmas which have electron temperatures in the range from 0.3 to 1.2 keV and ion temperatures below 0.5 keV. This range of temperatures is particularly well suited for investigations of the satellite spectra of heliumlike argon, Ar XVII, which are the subject of this Letter. We note that the temperatures in these Ohmic discharges at NSTX are much lower than those found in typical tokamaks, such as the Joint European Torus, Alcator, or Textor [6], which, unlike NSTX, have a high aspect ratio of the major and the minor plasma radii.

In the following we demonstrate that there are still discrepancies between the existing theory and measurements of Ar XVII satellite spectra from NSTX, which lead to unacceptable uncertainties in the electron-temperature measurements. These discrepancies are resolved by new, more detailed theoretical calculations. A satellite spectrum of Ar XVII, which was observed with the NSTX high-resolution crystal spectrometer [7], is shown in Fig. 1. The spectral data were accumulated from six nearly identical discharges during the time interval of steady-state conditions to reduce the statistical error. The spectrum spans the wavelength range from 3.94 to 4.00 Å and consists of the characteristic heliumlike lines of Ar XVII, i.e., the $1s^2\,{}^1S_0$–$1s2p\,{}^1P_1$ resonance line (w), the intercombination lines $1s^2\,{}^1S_0$–$1s2p\,{}^3P_2$ (x) and

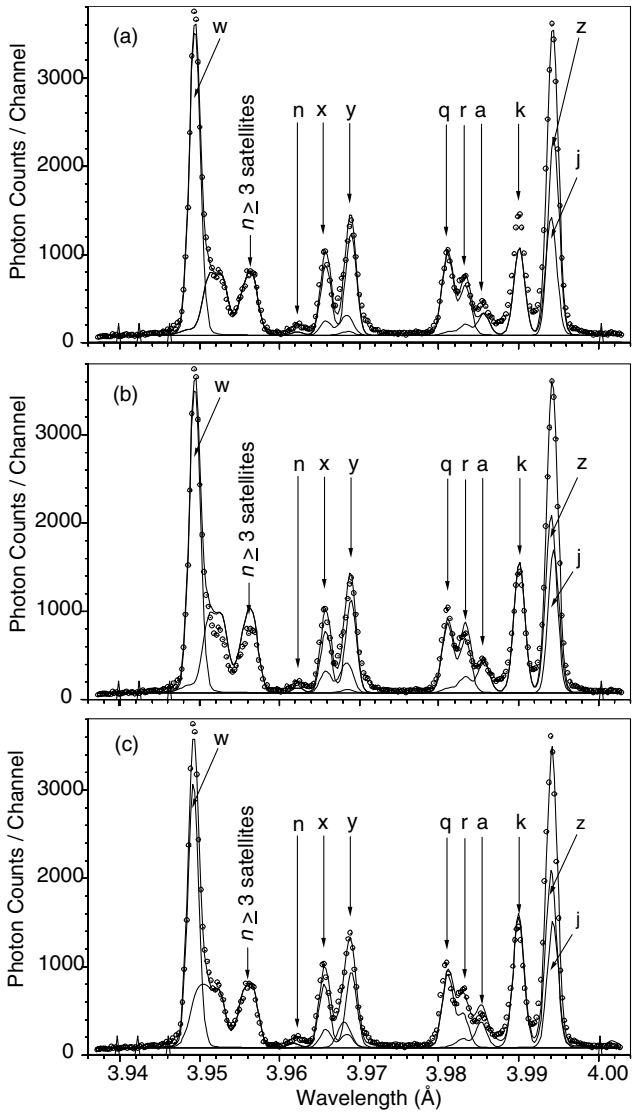

FIG. 1. Least-squares fit comparisons of a satellite spectrum of heliumlike argon, Ar XVII, from Ohmically heated NSTX discharges (#105885–105890) with synthetic spectra constructed from the predictions of the MZ code (a),(b) and the flexible atomic code (c). The data were accumulated during the time interval of steady-state conditions from 0.210 to 0.320 s. The MZ code and the flexible atomic code include the contributions from satellites with $n \leq 6$. The total intensity and dielectronic and inner-shell excited satellite components are shown separately in the synthetic spectra. The fit in (c) employed enhancement factors for the lines x, y, z, and q of 0.67, 1.29, 3.02, and 0.38, respectively. The enhancement factors for x and z are consistent with theoretical expectations for redistribution of the population between the $^3P_2$ and $^3S_1$. The enhancement factor for q is a measure of the relative abundance of Ar XVI and Ar XVII.

$1s^2\,{}^1S_0$–$1s2p\,{}^3P_1$ (y), and the forbidden line $1s^2\,{}^1S_0$–$1s2p\,{}^3S_1$ (z), and numerous lithiumlike satellites due to transitions $1s^2nl$–$1s2pnl$ with $n > 2$. The heliumlike lines and the prominent lithiumlike satellites q, r, a, k, and j with $n = 2$ have been identified with Gabriel's notation [8]. Most of the lithiumlike satellites, with the exception of the $1s^22s$–$1s2s2p$ satellites q and r whose upper levels can be populated by inner-shell excitation from the lithiumlike ground state, are produced in the process of dielectronic recombination of the heliumlike ion by resonant capture of an electron into a doubly excited lithiumlike state $1s2pnl$ [9]. This state can decay by autoionization, the reverse process of resonant electron capture, or by stabilizing radiative transitions, such as $1s2pnl \rightarrow 1s^2nl$ giving rise to an observable satellite line near the resonance line w, or other radiative cascades $1s2pnl \rightarrow 1s2pn'l'$ giving rise to lines in other spectral bands. The intensity of the dielectronic satellites is therefore determined by the electron energy distribution and the branching ratios for radiative and autoionizing transitions. For a Maxwellian distribution, the dielectronic satellite intensities are a function of the electron temperature and are proportional to the electron density and density of the heliumlike ions [10]. With increasing principal quantum number n, the wavelengths of the dielectronic satellites converge to the wavelengths of heliumlike resonance and intercombination lines [10,11]. Additional information on the process of dielectronic recombination may be found in Refs. [8,12].

The electron temperature is usually determined from the intensity ratios of the strong $n = 2$ dielectronic satellites j and k with respect to the heliumlike resonance line w, whose emissivity is given by

$$\varepsilon_w = N_e N_{\mathrm{He}} C(T_e), \tag{1}$$

where N_e and N_{He} are the electron density and density of the heliumlike ions, and $C(T_e)$ is the effective rate coefficient for electron impact excitation. In the Ar XVII spectrum, only k can be used because j is blended with z. However, the high-resolution spectrometers in tokamak experiments, which are designed for Doppler broadening and Doppler shift measurements capable of resolving wavelength shifts of less than 10^{-4} Å, provide spectra in which a substantial part of the $n = 3$ satellites is well resolved from the resonance line w (see Fig. 1). It is therefore possible to determine the electron temperature also from the ratios of the resolved $n = 3$ dielectronic satellites with respect to the resonance line w and from the ratio of the $n = 3$ to $n = 2$ satellites. For a Maxwellian energy distribution one expects to obtain a unique electron-temperature value from these three ratios. Disagreement among the inferred temperature values is generally taken as evidence for the existence of a non-Maxwellian distribution [2,3].

The analysis of the spectral data was performed by a least-squares fit comparison with synthetic spectra constructed from the predictions of the MZ code [13]. The MZ code was chosen since it provides the most accurate wavelengths, which are typically in agreement with the experimental wavelengths to within a few 10^{-4} Å. The results of this comparison are shown Figs. 1(a) and 1(b). We found that the very detailed spectral predictions from

the MZ code were in excellent agreement with the experimental data, but that it was not possible to fit the entire spectrum with a unique value for the electron temperature. In fact, the electron temperatures inferred from the fitted ratios of the $n \geq 3$ satellites [Fig. 1(a)] and the $n = 2$ satellite k [Fig. 1(b)], with respect to the resonance line w, were $T_e = 0.73 \pm 0.01$ keV and $T_e = 0.62 \pm 0.01$ keV, respectively, where the error bars indicate the statistical error. These results suggested the existence of a non-Maxwellian distribution, which, however, is unlikely in steady-state, Ohmically heated NSTX plasmas with central electron densities of 5×10^{13} cm^{-3}. Moreover, the results from the spectral data were in disagreement with independent measurements of the electron temperature by the Thomson scattering system [14] and led to unacceptable assumptions for the energy transport and the values of the power balance of the NSTX plasmas.

The synthetic spectra shown in Figs. 1(a) and 1(b) were constructed in several steps using the procedure outlined in [15] by first determining the electron and ion temperatures from the resonance line and $n \geq 3$ satellite lines in the wavelength range from 3.94 to 3.96 Å, and then extending the fit to the remaining spectral features in the wavelength range from 3.96 to 4.00 Å. In Fig. 1(a) the electron temperature was determined from a fit of the $n \geq 3$ satellites and w, and in Fig. 1(b) the electron temperature was determined from the ratio of k and w. The intensities of the heliumlike lines w, x, y, and z were calculated using the recent rate coefficients for electron impact excitation from Keenan *et al.* [16]. Electron impact excitation is by far the dominant line formation process for w. Empirical enhancement factors, which were determined from a least-squares fit to the experimental data, were applied to lines x, y, and z to account for additional excitation processes which play a strong role for the triplet lines [15]. An expression analog to Eq. (1) was used for the inner-shell excited $1s^2 2s$–$1s2p2s$ satellites, q and r, replacing N_{He} by N_{Li}, the density of the lithiumlike argon ions [8].

The conflicting electron-temperature results inferred from the fits in Figs. 1(a) and 1(b) pointed to possible omissions of radiative branches and levels in the MZ code, and motivated extensive calculations with a new atomic physics code, the flexible atomic code [17], which included all levels and autoionizing and radiative branches, such as the $K\beta$ branch. The main difference between the predictions from the MZ code and the flexible atomic code resides, therefore, in the calculation of the branching ratios, or F_2 line factors (as defined in [10]), for the $n \geq 3$ satellites. The F_2 values obtained from the MZ code are systematically higher than those from the flexible atomic code. A comparison of the obtained F_2 factors for some prominent dielectronic satellites is given in Table I.

A least-squares fit comparison of a synthetic spectrum constructed from the new calculations, by the same procedure as before, with the experimental data is shown in Fig. 1(c). This synthetic spectrum provided, within the experimental uncertainties, a fit of all the spectral features with a unique electron-temperature value of $T_e = 0.58 \pm 0.01$ keV. The value of the ion temperature was $T_i = 0.45 \pm 0.04$ keV. However, like most other codes the flexible atomic code yields less accurate wavelengths than the MZ code. For the construction of the synthetic spectrum shown in Fig. 1(c) we, therefore, adopted only the F_2 line factors from the flexible atomic code, while wavelengths were still taken from the MZcode. In order to confirm the uniqueness of the temperature value, we employed a third way of determining the temperature using the ratio of the resolved $n = 3$ satellites and line k [2]. This ratio does not involve the use of line w and therefore is not sensitive to the tail of the electron energy distribution. From this ratio we obtained $T_e = 0.56 \pm 0.03$ keV, which is in excellent agreement, and therefore indicative of a Maxwellian electron-temperature distribution.

The temperatures inferred from the spectral fits using the flexible atomic code are also in excellent agreement with independent measurements by the Thomson scattering system. A comparison of the time histories of the

TABLE I. Wavelengths and F_2 line factors (as defined in [10]) from the flexible atomic and MZ codes for some prominent dielectronic satellites.

Transition	Flexible atomic code		MZ code	
	λ (Å)	F_2 (10^{13} s^{-1})	λ (Å)	F_2 (10^{13} s^{-1})
$1s2p^2\,{}^2D_{5/2}$–$1s^2\,2p\,{}^2P_{3/2}$ (j)	3.9936	23.1	3.9941	24.4
$1s2p^2\,{}^2D_{3/2}$–$1s^2 2p\,{}^2P_{1/2}$ (k)	3.9896	17.0	3.9901	18.0
$1s2p^2\,{}^2P_{3/2}$–$1s^2 2p\,{}^2P_{3/2}$ (a)	3.9856	3.78	3.9860	4.57
$1s2p3p\,{}^2D_{3/2}$–$1s^2 3p\,{}^2P_{3/2}$	3.9572	15.6	3.9567	18.6
$1s2p3p\,{}^2D_{3/2}$–$1s^2 3p\,{}^2P_{1/2}$	3.9564	9.70	3.9557	11.7
$1s2p3d\,{}^2F_{7/2}$–$1s^2 3d\,{}^2D_{5/2}$	3.9519	8.82	3.9525	13.5
$1s2p4p\,{}^2D_{5/2}$–$1s24p\,{}^2P_{3/2}$	3.9528	5.17	3.9532	7.08
$1s2p4d\,{}^2F_{7/2}$–$1s^2 4d\,{}^2D_{5/2}$	3.9517	4.83	3.9516	6.09
$1s2p4p\,{}^2D_{3/2}$–$1s^2 4p\,{}^2P_{1/2}$	3.9526	3.55	3.9528	5.63

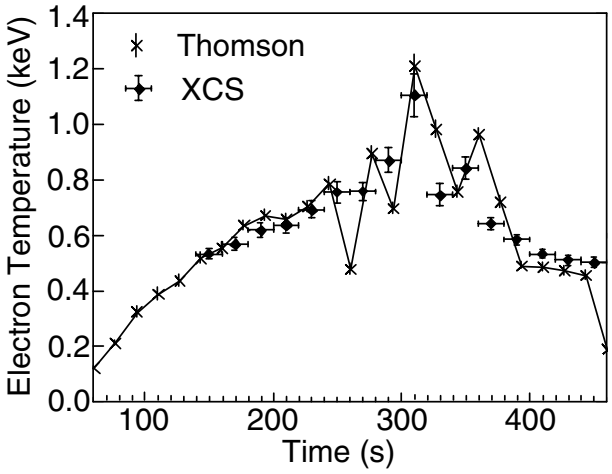

FIG. 2. Comparison of electron temperature results from the crystal spectrometer with the Thomson scattering results for the NSTX discharge #108258. The Thomson scattering data represent three-point averages of the values surrounding and including the maximum of the radial profiles.

peak electron temperature from the Thomson scattering system with the electron-temperature results from the crystal spectrometer is shown in Fig. 2. The data were obtained from a single NSTX discharge with pure Ohmic heating. For this comparison it is important to note that the Thomson data are from instantaneous measurements, which provided a radial electron-temperature profile every 16.6 ms, and that the x-ray spectra were integrated over time intervals of 20 ms. The first argon spectrum with sufficient statistics for electron-temperature measurements was observed during the time interval from 140 to 160 ms, since it takes about 110 to 140 ms to ionize argon to the heliumlike charge state. The somewhat erratic oscillations in the Thomson scattering data during the time interval from 240 to 390 ms are ascribed to the occurrence of a magneto-hydrodynamic instability, which affects the profile of the Ohmic heating current and therefore the electron temperature.

In conclusion, the experiments at NSTX have demonstrated that a new level of accuracy in the atomic data is needed. Especially measurements to infer the existence of non-Maxwellian electron energy distributions are extremely sensitive to small errors in the atomic data for the dielectronic satellites. In order to adequately represent the spectra of heliumlike ions and to correctly utilize their diagnostic potential for determining electron temperatures and non-Maxwellian electron energy distributions, the atomic calculations must include all possible radiative and autoionization transitions. Shortcuts that are commonly used in the calculation of the satellite line strengths may lead to erroneous assumptions of the existence of tails on the electron distribution. Although the present investigations were performed for the satellite spectra of Ar XVII, we believe that our results generally apply to the spectra of heliumlike ions. A forthcoming paper with a detailed description of the codes used for the analysis of the satellite spectra of heliumlike argon from NSTX and TEXTOR tokamak plasma discharges is in preparation.

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