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# Verification of the Atomic Data for the X-Ray Spectroscopy at the Tokamak TEXTOR

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## Abstract

He-like spectra of argon have been intensively studied at the tokamak TEXTOR with the aim to test and thus to improve the data for effective excitation of the lines $1s2l$-$1s^2$ and the dielectronic satellites $1s2lnl'$-$1s^22l$. The effective excitation rates for the He-like lines have been calculated by means of two methods: Coulomb-Born-Exchange and R-matrix. The atomic data for the dielectronic satellites were obtained in the framework of two main approaches based on $Z$-expansion of perturbation theory and multi-configurational wave functions. Other processes, such as the recombination of H-like ions as well as inner-shell ionization of Li-like ions have been also taken into account. The spectra obtained from the tokamak TEXTOR at substantially different plasma conditions have been compared with theoretical ones based on different sets of atomic data. The deviations for the intensities of the lines were shown to be within 10 % for the whole spectral range.

**Keywords:**

He-like spectra, dielectronic satellite, excitation rate

## 1. Introduction

The diagnostic of the hot plasma core is a challenging task for fusion research. The recent development of the x-ray detectors [1] and x-ray imaging systems [2] stimulates the plasma core diagnostics by means of spectroscopy.

The highly charged impurities penetrate up to the plasma core and by emitting the photons in the x-ray region deliver the necessary information on the plasma. The measurements of electron and ion temperatures as well as toroidal plasma velocity belong now to the routine techniques on a number of fusion devices like NSTX, TEXTOR or TORE SUPRA [3-5]. Except for the main plasma parameters, the He-like spectra of highly charged ions carry the unique information on ionization distribution and concentration of neutrals in the plasma [6]. Unlike the fusion devices, these spectra are the only source of information on plasma parameters in solar flares [7].

In a fusion plasma, at the condition of the low-density limit, the electron-ion collisions are the most important mechanism for the population of excited states. Until now, the largest discrepancies in the description of the He-like spectra have been observed for the triplet lines of the He-like system and the intensities of the dielectronic satellites. Despite of the intensive theoretical studies of the He-like spectra for different ions with intermediate Z these discrepancies were still not completely resolved. So, Bitter *et al*. [8] observed the deviations for the triplet lines more than a factor of two for He-like titanium at the tokamak TFTR. Platz *et al*. [9] pointed out to the discrepancies for the forbidden lines at the tokamak TORE SUPRA. Weinheimer *et al*. [10] reported deviations for triplet lines and dielectronic satellites for He-like argon. The more recent report [3] proved the progress in the description of dielectronic satellites $1s2l3l'$ of argon, but nevertheless, did not discuss the problem of excitation for the triplet lines.

## 2. Theoretical description of He-like spectra

The full theoretical description of the He-like spectra for fusion has been presented in number of papers [11,12]. The excitation of the ground state of He-like

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ions is the main process for the population of the excited states. The emission of the photons from the states 1s2l of He-like ions produce the singlet line **w**($^1P_1$-$^1S_0$) and the triplet lines **x**($^3P_2$-$^1S_0$), **y**($^3P_1$-$^1S_0$) and **z**($^3S_1$-$^1S_0$). In addition to the excitation, the recombination of H-like ions contributes to the intensities of these lines too. The inner-shell ionization of Li-like ions also enhances the **z** line.

Except for the main He-like lines, the Li-like dielectronic satellites 1s2*lnl*' - 1s$^2$2*l* fill the interval between **w** and **z** lines, producing the quasi-continuous spectra. The most important satellites for plasma diagnostics are **j**: 1s$^2$2p($^2P_{3/2}$)-1s2p$^2$($^2D_{5/2}$), **k**: 1s$^2$2p($^2P_{1/2}$)-1s2p$^2$($^2D_{3/2}$), **q**: 1s$^2$2s($^2S_{1/2}$)-1s2p2s($^1$P)($^2P_{3/2}$) and **r**: 1s$^2$2s($^2S_{1/2}$)-1s2p2s($^1$P)($^2P_{1/2}$). So, the measurements of the electron temperature are based either on the satellites **k** or **j** or the group of the satellites with $n$ = 3. The measurements of the Li-like charged state depend on the intensities of the satellites **q** and **r**.

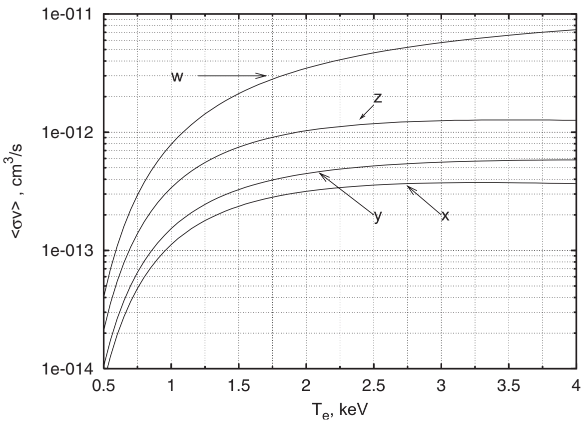


Fig. 1 Effective rates coefficients for the He-like lines, R-matrix calculations.

## 3. Effective excitation rates for He-like lines

The effective excitation rates coefficients have been calculated using two approaches: Coulomb-Born-Exchange (CBE) and R-matrix methods. CBE calculations were carried out by the code ATOM [13]. For the calculations by the R-matrix method we used 31 lowest states of He-like argon. The details of this calculation and comparison of collisional strength with other methods can be found in [14]. For producing the effective rates coefficients we used the radiative data from the AUTOSTRUCTURE program [15]. For the radiative transitions among the $n = 2$ states and the two photon decay to the ground state the data [16] were used. The Fig. 1 demonstrates the effective rates coefficients for the He-like lines of argon. The comparison between two methods is presented in the Fig. 2. For this procedure we introduce the parameter $\epsilon$, defined as follows

$$\epsilon_i = \frac{<\sigma \cdot v>^i_R - <\sigma \cdot v>^i_{CBE}}{<\sigma \cdot v>^i_R}.$$

Here, $i$ is one of the He-like lines, $<\sigma \cdot v>^i_R$ and $<\sigma \cdot v>^i_{CBE}$ are the effective rates calculated using the R-matrix method and the CBE approximation, cm$^3$/s. The discrepancies for the effective rates between the CBE and the R-matrix methods do not exceed 4 % in the electron temperature interval of 0.5...4.0 keV for the **w**, **x** and **y** lines and 10 % for the **z** line.

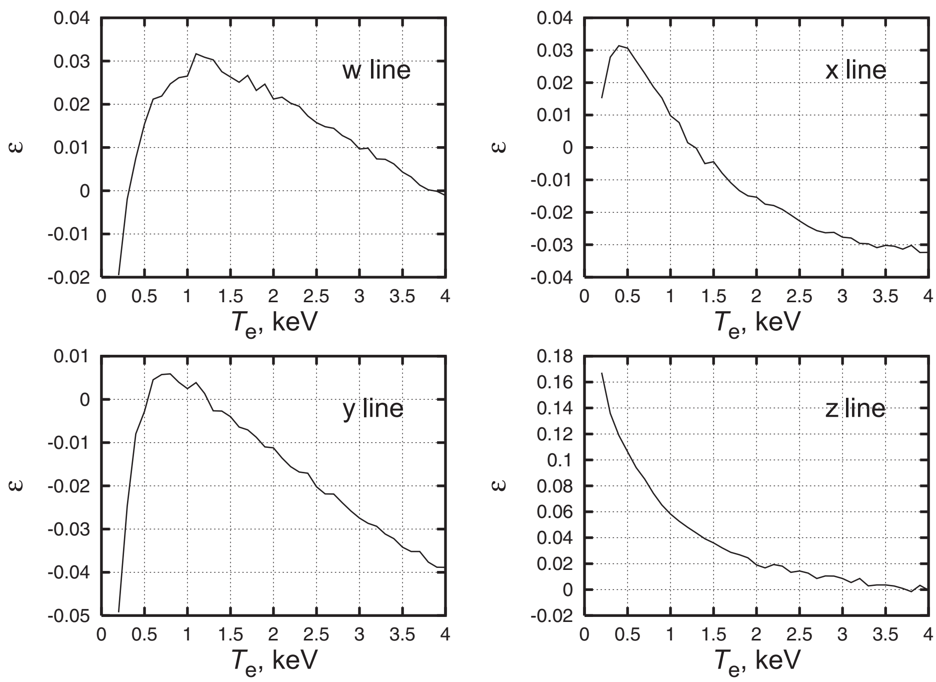


Fig. 2 Comparison between the R-matrix and the CBE calculations for the effective rates coefficients.

Table 1 $F_2$ values in $10^{13}\,s^{-1}$ for Li-like satellites. The correction factor $\gamma$ at the different electron temperatures.

| Key | $F_2$ (AUTOSTR.) | $F_2$ (MZ) | Correction factor, $\gamma$ | | |
|---|---|---|---|---|---|
| | | | $T_e = 1.0\,keV$ | $T_e = 2.0\,keV$ | $T_e = 4.0\,keV$ |
| **j** | 23.0 | 22.9 | 1.01 | 1.01 | 1.01 |
| **k** | 16.7 | 16.7 | 1.01 | 1.01 | 1.01 |
| **q** | 1.25 | 0.73 | 1.84 | 2.10 | 2.26 |
| **k** | 2.68 | 2.23 | 1.17 | 1.23 | 1.26 |

## 4. Dielectronic satellites

A number of different theoretical approaches have been developed for the calculation of the dielectronic satellites 1s2*lnl*'. They utilize either the model potentials (SUPERSTRUCTURE and AUTOLSJ [11]) or the perturbation theory methods (MZ [17]). To resolve the discrepancies between the experiment and theoretical data for the $n = 3$ satellites [3,4] we have studied the cascades between the doubly excited states of Li-like ions. The new $F_2$ values [12], have been obtained using AUTOSTRUCTURE and a modified version of the MZ program. We have found a substantial enhancement of the intensities of the **q** and **r** lines in both approaches [18]. The results are given in the Table 1, where the intensities of the satellites, $F_2$ values, are increased by $\gamma$ factor. This effect has no influence on the intensity of other lines and satellites with $n > 2$.

## 5. Results of the verification and conclusions

The new data of effective excitation rates and dielectronic satellites have been used to simulate the experimental spectra from the tokamak TEXTOR.

The verification of the atomic data was made in the coronal approximation (low-density limit) by the fitting of the synthetic spectra to the measured one. Though the emission of the spectral lines occurs mostly in the plasma core, the profiles of plasma parameters can influence the modelling as well. The assumed radial profiles of electron temperature and density were taken from the measurements of electron cyclotron emission and from the measurements using interferometry, respectively [10]. The radial profiles of argon were based either on the impurity-transport modeling or the coronal distribution in the plasma. In the first case, the diffusion coefficients were determined from the gas puff experiments [19].

The optimization parameters of the model were electron and ion temperatures and relative ionic abundances at the plasma core. The synthetic spectra were constructed using Voigt profiles: the Lorentzian width for each spectral line was determined from the theoretical transition probabilities and the rocking curve of the crystal. The Gaussian width included the Doppler broadening and the contribution from instrumental effects. The optimization was carried out by the iteration procedure minimizing successively the $\chi^2$ values in the vicinity of various lines resolved in the spectra [10]. Measurements of the electron temperature were based on the satellite **k** and **w** line, relative abundances of Li- and H- ions were obtained with the help of the **q** satellite and triplet lines, respectively. The ion temperature was derived from the shape of the **w** line.

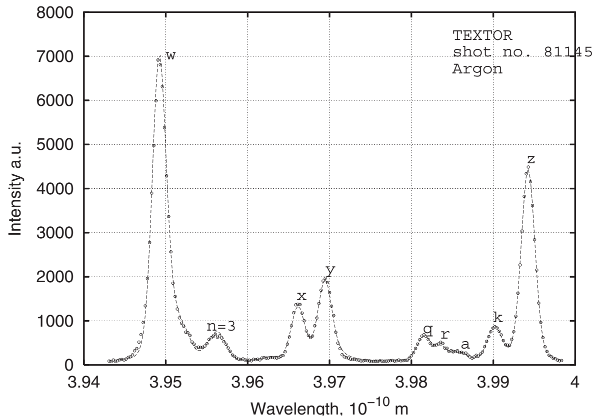


Fig. 3 Spectrum of He-like argon from the tokamak TEXTOR. Experimental spectrum is open circles and theoretical spectrum is dashed line.

The results of the verification are presented in the Fig. 3. The influence of the radial profiles is the most noticeable for the measurements of the ionic abundance. So, the measured density of the Li-like ions in the ohmic heated plasma exceeds coronal values of up to a factor 5 [20]. Our values were found in the agreement with the gas puff experiments within 20 %. These results confirmed the influence of the diffusion and charge-exchange processes on the total ionization balance in the plasma core.

The deviations between the experimental spectra and theoretical fit do not exceed 5 % for the whole spectral interval,except for the **y** line, where it increases up to 7–10 %. The detailed discussion of the fit procedure and the evaluation of the theoretical data will be given in a forthcoming paper.

## References


[1] S.M. Gruner, M.W. Tate and E.F. Eikenberry, Rev. Sci. Instrum. **73**, 2815 (2002).

[2] S. Fraenkel and M. Bitter, Rev. Sci. Instrum. **70**, 296 (1999).

[3] M. Bitter, M.F. Gu, L.A. Vainshtein, P. Beiersdorfer, G. Bertschinger, O. Marchuk, R. Bell, B. Leblanc, K.W. Hill, D. Johnson and L. Roquemore, Phys. Rev. Lett. **91**, 26 (2003).

[4] G. Bertschinger, W. Biel, the TEXTOR-94 Team, O. Herzog, J. Weinheimer, H.-J. Kunze and M. Bitter, Phys. Scr. **T83**, 132 (1999).

[5] P. Platz, J. Ramette, E. Belin, C. Bonelle and A. Gabriel, J. Phys. E: Sci. Instrum. **14**, 448 (1981).

[6] F.B. Rosmej, D. Reiter, V.S. Lisitsa, M. Bitter, O. Herzog, G. Bertschinger and H.-J. Kunze, Plasma Phys. Control. Fusion **41**, 191 (1999).

[7] K.J.H. Phillips, L.K. Harra, F.P. Keenan, D.M. Zarro and M. Wilson, Astron. J. **419**, 426 (1993).

[8] M. Bitter, K.W. Hill, M. Zrnstorff, S. von Goeler, R. Hulse, L.C. Johnson, N.R. Sauthoff, S. Sesnic, and K.M. Young, Phys. Rev. A **32**, 5 3011 (1985).

[9] P. Platz, M. Cornille and J. Dubau, J. Phys. B, At. Mol. Opt. Phys. **29**, 3787 (1996).

[10] J. Weinheimer, I. Ahmad, O. Herzog, H.-J. Kunze, G. Bertschinger, W. Biel, G. Borchert and M. Bitter, Rev. Sci. Instrum. **72**, 6 2566 (2001).

[11] TFR Group, F. Bombarda, F. Bely-Dubau, P. Faucher, M. Cornille, J. Dubau and M. Loulergue, Phys. Rev. A **32**, 4 2374 (1985).

[12] F. Bely-Dubau, J. Dubau, P. Faucher, A.H. Gabriel, M. Loulergue, L. Steenman-Clark, S. Volonte, E. Antoniccu and C.G. Rapley Mon. Not. R. Astron. Soc. **201**, 1155 (1982).

[13] V.P. Shevelko and L.A. Vainshtein, *Atomic physics for hot plasmas* (IOP publishing, 1993).

[14] A.D. Whiteford, N.R. Badnell, C.P. Balance, M.G. O'Mullane, H.P. Summers and A.L. Thomas, J. Phys. B, At. Mol. Opt. Phys. **34**, 3179 (2001).

[15] N.R. Badnell, J. Phys. B, At. Mol. Opt. Phys. **30**, 1 (1997).

[16] H.F. Beyer, H.-J. Kluge and V.P. Shevelko, *X-ray of Highly Charged Ions* (Springer, Berlin, 1997).

[17] L.A. Vainshtein and U. I. Safronova, At. Data Nucl. Data Tables **21**, 49 (1978).

[18] O. Marchuk, G. Bertschinger, H.-J. Kunze, N.R. Badnell and S. Fritzsche, J. Phys. B, At. Mol. Opt. Phys. **37**, 1951 (2004).

[19] Biel W. *et al.*, Proc. 28th EPS Conference on Controlled Fusion and Plasma Physics, Madeira, Portugal (2001).

[20] G. Bertschinger and O. Marchuk, *High-Temperature Plasmas Diagnostics by X-ray Spectroscopy in the Low Density Limit*, R.E.H. Clark, D.H. Reiter (Eds.), *Nuclear Fusion Research, Understanding Plasma-Surface Interactions* (Springer Verlag, 2004) p. 183.