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Electron impact ionization of tungsten ions in statistical model

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The statistical model for calculations of the electron impact ionization cross sections of multielectron ions is developed for the first time. The model is based on the idea of collective excitations of atomic electrons with the local plasma frequency, while the Thomas–Fermi model is used for atomic electrons density distribution. The electron impact ionization cross sections and related ionization rates of tungsten ions from W^+ up to W^{63+} are calculated and then compared with the vast collection of modern experimental and modeling results. The reasonable correspondence between experimental and theoretical data demonstrates the universal nature of statistical approach to the description of atomic processes in multielectron systems.

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This study is initiated by the significant interest to the ionization of multielectron tungsten ions in the modern thermonuclear plasma research. This is due to application of tungsten as a material for the plasma facing components of the thermonuclear reactor ITER [1]. The electron impact ionization of tungsten ions is of general interest for atomic physics as practically important example of interaction of the electron projectiles with multielectron targets. The description of this process is connected as with the complicated atomic structure of tungsten ions, as with the variety of channels, related to the excitation-autoionization and the standard direct ionization to continuum [2, 3]. These difficulties result in essential scatter of the data obtained by different numerical codes [4, 5]. In the present paper these problems are seemed to be overcome within the developed statistical model, used for the first time to provide the electron impact ionization cross sections of multielectron ions. The efficiency of the proposed rather simple modeling is demonstrated by comparison with the conventional collection of experimental results.

The statistical approach is applied to the calculations of plasma radiative losses on the tungsten impurity [6] and based on an idea of collective oscillations of atomic electrons similar to the condensed media. In this approach the ground state of an atom is described by the standard Thomas–Fermi (TF) theory [7] and the ionization of multielectron system can be also considered in terms of excitations of collective modes with plasma frequencies determined by the local TF electron density due to well known relation $\omega_p(r) = \sqrt{4\pi e^2 n(r)/m}$, according to the local plasma frequency (LPF) model [8].

The interactions of plasma electrons with tungsten ions are considered using the method of equivalent photons (EQP) given by Fermi [9]. In this method the action of electric field of plasma electrons on the tungsten impurity ions is described as the photoabsorption of equivalent photons flux. Its intensity is determined by Fourier transform of the electric field of the plasma electron, moving along the classical trajectory in the TF ion potential. Thus the moving plasma electrons produce the electromagnetic field, which is absorbed by atomic electrons at the frequencies, related to the atomic plasma oscillations, while the EQP approach makes it possible to express the electron impact ionization in terms of photoionization cross section. Moreover, the cross section of any elementary process due to the multielectron ion interactions with plasma charged particles may be represented in the dipole approximation in terms of cross sections of photo-processes with EQP. Thus the flux of EQP number $\frac{dN(\omega)}{d\omega}$ with the frequency ω per unit frequency interval $d\omega$ for the given energy of electrons E could be written in the form

$$\frac{dN(\omega)}{d\omega} = \left(\frac{c\hbar}{e^2}\right) \cdot \frac{1}{2\sqrt{3}} \cdot \frac{\omega_a}{\omega} \times$$

$$\times \left(\frac{Ry}{E}\right) \cdot g\left(z_i \cdot \left(\frac{Ry}{E}\right)^{3/2} \cdot \frac{\omega}{\omega_a}; Z\right), \qquad (1)$$

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where $g(x)$ is the Gaunt-factor, that describes the curvature of electron trajectory in given potential of ion with the charge z_i and the charge of nuclei Z [8], $\hbar\omega_a = 2Ry$.

In accordance with the statistical model [6] the electron impact ionization cross section is given in terms of the photoionization cross section at the frequency ω, which satisfies the resonance condition [8]

$$\omega = \omega_p, \quad \omega = \sqrt{4\pi e^2 n(r_\omega)/m}, \tag{2}$$

which determines the effective absorption radius r_ω being the solution of the equation above.

The plasma electron trajectory in the TF ion potential could be described in the Coulomb approximation by the effective charge Z_{eff}, determined by the resonance condition (2)

$$Z_{\text{eff}} = Z\left[\chi(r_\omega;\, q) + qr_\omega/r_0\right], \tag{3}$$

where $\chi(r_\omega;\, q)$ is the standard screening function in the TF model, $r_0(Z,\, q)$ is the TF ion radius, determined during the solution of the TF equation for given $q = z_i/Z$.

The conventional dimensionless frequency $s = \hbar\omega/2RyZ$ satisfies the local resonance condition (2) via the implicit dependence of the reduced distance from the nuclear $x_s = r_s/r_{\text{TF}}$ on the variable s ($r_{\text{TF}} = a_0 \cdot (9\pi^2/128)^{1/3} \cdot Z^{-1/3}$, a_0 is the Bohr radius, r_{TF} is the TF radius [7])

$$S = (128/9\pi^2)^{1/2} \cdot [\chi(x_s)/x_s]^{3/4}. \tag{4}$$

Then multiplying the number of equivalent photons (1) by the photoionization cross section and integrating over all EQP dimensionless frequencies s from the reduced ionization potential $I_i/Z \cdot 2Ry$ up to the reduced energy of electron projectile $E/Z \cdot 2Ry$, we arrive to the following expression for electron impact ionization cross section

$$\sigma_i(E_e)/a_0^2 = \frac{\pi^4\sqrt{3}}{32} \cdot \frac{Ry}{E_e} \times$$
$$\times \int\limits_{I_i/(2RyZ)}^{E/(2RyZ)} ds \frac{x_s^2 \chi(x_s,\, q)}{|\chi'(x_s,\, q) - \chi(x_s,\, q)/x_s|} \times$$
$$\times\, g\left[Z_{\text{eff}} Z \left(\frac{Ry}{E_e}\right)^{3/2} \cdot s\right]. \tag{5}$$

The result (5) depends on the electron energy, specific ion and nuclear charges as well as on ionization potentials.

The ionization potentials used in the formula (5) are taken in the TF form in order to make the theory self-consistent: $I_i/2RyZ = (128/9\pi^2)^{1/3} q Z^{1/3}/x_0(Z, q)$ [7]. The Eq. (5) is used below for calculations of ionization cross sections for the large set of tungsten ions.

The statistical method, described above, was applied for the calculations of ionization cross sections for different ionization stages of tungsten ions W^{k+}, where $k = 1, 2, ..., 10, 17, 22, 45, 63$, and presented below in comparison with some experimental data [10–13] in the Fig. 1, as well as with the calculations by the configuration averaged distorted waves (CADW) method [2, 3].

The uncertainties of these experimental data are designated in the Fig. 1 by the vertical error bars. They depend on the energy range and differ for various experimental measurements. In the case, when these error bars are not seen the variation of experimental data do not exceed the size of graphical designations of experimental points.

The agreement between the developed statistical theory and the data of measurements [10–13], as well as with the CADW calculations [2, 3] seen in the Fig. 1 is quite satisfactory. The discrepancies with experimental data are less for the ions with the larger number of bound electrons (and smaller z_i) that is obviously due to the better applicability of statistical theory with the increasing number of atomic electrons. This seems to be quite clear since the precision of statistical methods decreases with the decrease of the atomic electron number. For large enough energies of projectiles the deviation of the statistical theory results from the CADW modeling ones is obviously due to the contribution of excitation-autoionization channels, which could not be explicitly addressed in the present formulation of the statistical approach.

In the Fig. 1 all of the analyzed experimental data for the electron impact ionization cross sections relate to relatively low electron energies in the vicinity of 1 keV, where the cross sections are large enough. In order to test the statistical approach predictions for higher energies the calculations of electron impact ionization rates were performed for the following set of tungsten ions W^{k+}, where $k = 28, 33, 38, 41, 44, 46, 51, 56$ in a wide range of the electron temperatures variation typical for upcoming reactor-size tokamaks, for instance, ITER [1]. These ionization rates are obtained by the average of Eq. (5) over the Maxwellian energy distribution of plasma electrons. The obtained results are compared in the Fig. 2 with the corresponding modeling data of the CADW approach [14]. The agreement between both data collections in the Fig. 2 is quite satisfactory too. As it follows from this comparison the discrepancies between the statistical theory and the CADW method are less pronounced for the ionization rates than in the case of the electron impact ionization cross sections.

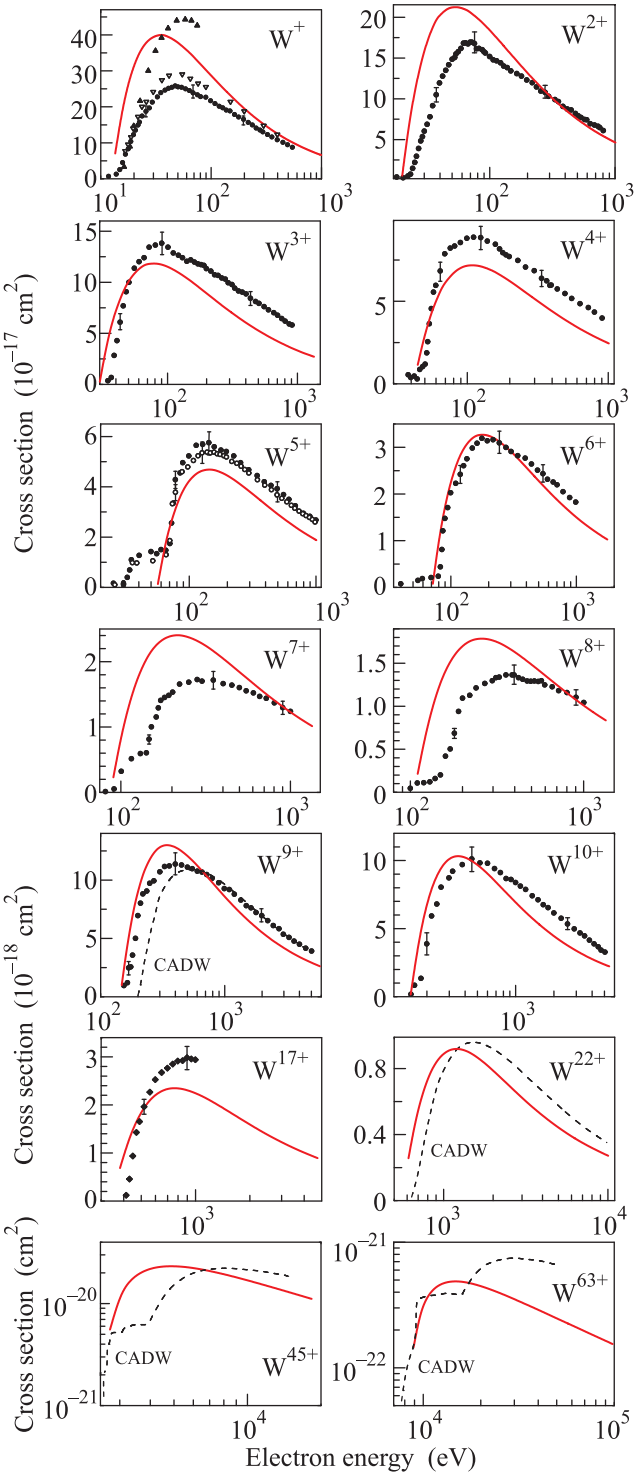

Fig. 1. Comparison of theoretical electron impact ionization cross sections with experimental data for various tungsten ions W^{k+} with $k = 1, 2, ..., 10, 17, 22, 45, 63$: solid curves – present statistical model; black points – [10]; open triangles – [11]; full triangles – CADW data [2]; open circles [12]; full squares – [13]; dashed curves signed CADW – [3]

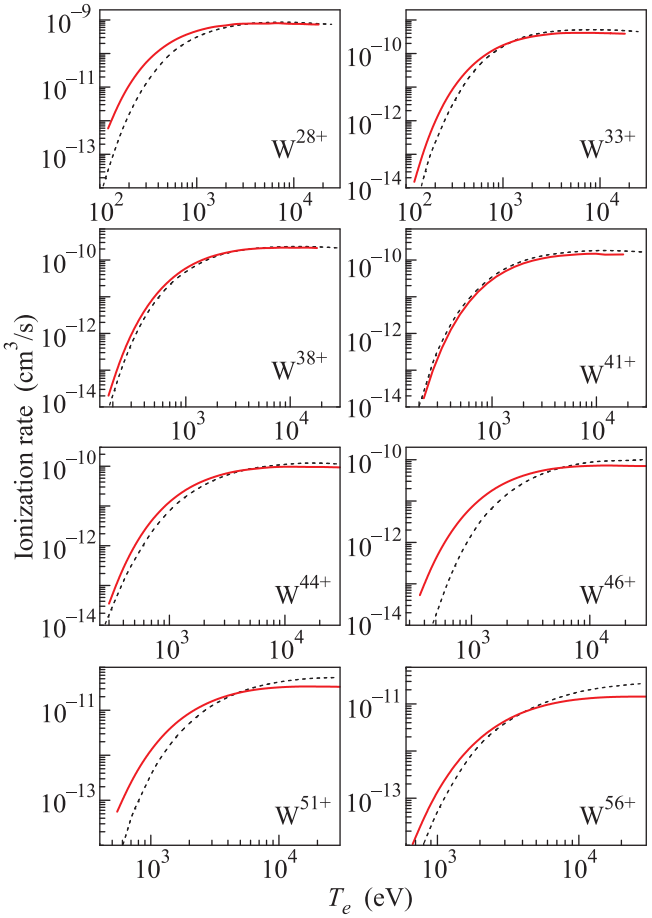

Fig. 2. Comparison of electron impact ionization rates for different tungsten ions W^{k+} with $k = 28, 33, 38, 41, 44, 46, 51, 56$ calculated in the present work and in [14]: solid curves – present statistical model; dashed curves – CADW modeling data [14]

Thus in the present work the electron impact ionization cross sections of tungsten ions from W^+ up to W^{63+} were calculated by the statistical theory methods and tested by the direct comparison with the experimental data [10–13], obtained using different methods of measurements, and the results, provided by the conventional complex approaches like CADW modeling [2, 3, 14]. The additional test was realized via comparison of the ionization rates, calculated in the present statistical approach and using the data of CADW modeling [14]. The modeling data shown above for tungsten ions demonstrates the efficiency of statistical model for calculations of the electron impact ionization cross sections and the corresponding ionization rates, which are in close agreement with the available experimental data [10–13] and the results of conventional complex codes [2, 3, 14]. Some discrepancies relate to the systems with relatively small number of atomic electrons (highly ion-

ized species) which is typical for statistical theories. The correspondence of statistical model with the experimental data on the electron impact ionization cross sections for tungsten ions seems to be due to rather satisfactory implicit description of significant contribution of the excitation-autoionization cascades to the ionization processes. These channels seem to be partly taken into account in the statistical model because of the collective nature of ionization processes in the statistical model.

The present analysis and results for the electron impact ionization cross sections and ionization rates for the large collection of tungsten ions allow us to conclude that the developed statistical approach could be successfully used for estimation of ionization processes in electron-ion collisions. The obtained results demonstrate the universal nature of statistical approach in the description of atomic processes with multielectron ions.

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1. M. Groth, S. Brezinsek, P. Belo, M. N. A. Beurskens, M. Brix, M. Clever, J. W. Coenen, C. Corrigan, T. Eich, J. Flanagan, C. Guillemaut, C. Giroud, D. Harting, A. Huber, S. Jachmich, U. Kruezi, K. D. Lawson, M. Lehnen, C. Lowry, C. F. Maggi, S. Marsen, A. G. Meigs, R. A. Pitts, G. Sergienko, B. Sieglin, C. Silva, A. Sirinelli, M. F. Stamp, G. J. van Rooij, S. Wiesen, and the JET-EFDA Contributors, Nuclear Fusion **53**, 093016 (2013).
2. M. S. Pindzola and D. C. Griffin, Phys. Rev. A **46**, 2486 (1992).
3. S. D. Loch, J. A. Ludlow, M. S. Pindzola, A. D. Whiteford, and D. C. Griffin, Phys. Rev. A **72**, 052716 (2005).
4. L. A. Vainshtein, I. I. Sobelman, and E. A. Yukov, *Excitation of Atoms and Broadening of Spectral Lines*, Springer, N.Y. (2002).
5. B. Tsipinyuk, A. Bekkerman, and E. Kolodney, Inter. J. Mass Spectr. **328–329**, 2 (2012).
6. A. V. Demura, M. B. Kadomtsev, V. S. Lisitsa, and V. A. Shurygin, JETP Lett. **98**, 786 (2013).
7. P. Gombas, *Die Statistische Theorie der Atoms und ihre Anwendungen*, Springer, Wien (1949).
8. W. Brandt and S. Lundqvist, Phys. Rev. **139**, 612 (1965).
9. E. Fermi, Zeitschrift fur Physik **29**, 315 (1924).
10. M. Stenke, K. Aichele, D. Harthiramani, G. Hofmann, M. Steidl, R. Volpel, and E. Salzborn, J. Phys. B: At. Mol. Opt. Phys. **28**, 2711 (1995).
11. M. Stenke, K. Aichele, D Hathiramani, G. Hofmann, M. Steidl, R. Volpel, V. P. Shevelko, H. Tawara, and E. Salzborn, J. Phys. B: At. Mol. Opt. Phys. **28**, 4853 (1995).
12. K. Spruck, A. Becker, A. Borovik, M. F. Gharaibeh, J. Rausch, S. Schippers, and A. Müller, J. Phys.: Conf. Ser. **488**, 062026 (2014).
13. J. Rausch, A. Becker, K. Spruck, J. Hellhund, A. Borovik, K. Huber, S. Schippers, and A. Müller, J. Phys. B: At. Mol. Opt. Phys. **44**, 165202 (2011).
14. T. Putterich, R. Neu, R. Dux, A. D. Whiteford, M. G. O'Mullane and ASDEX Upgrade Team, Plasma Phys. Control. Fusion **50**, 085016 (2008).