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RELATIVISTIC MODEL DIRAC-FOCK APPROACH TO STUDYING Fe PLASMA EMISSION SPECTRA IN A LOW INDUCTIVE VACUUM SPARK

There are presented the results of theoretical calculation for transition probabilities of the Fe plasma Li-like satellite lines on the basis of the relativistic perturbation theory (PT) with the Dirac-Fock model zeroth approximation and accounting for correlation and radiative corrections. With using the calculated values for relation of intensities of the dielectronic satellites lines and resonant lines of He-like ions, it is carried out an estimate of the plasma electron temperature and density.

At present time a great attention is turned to problems of experimental and theoretical study of high temperature multi-charged ions plasma and developing the new diagnostics methods (c.f. [1-12]). Similar interest is also stimulated by importance of carrying out the approaches to determination of the characteristics for multi-charged ions plasma in thermonuclear (tokamak) reactors, searching new mediums for X-ray range lasers. The X-ray laser problem has stimulated a great number of papers devoting to development of theoretical methods for the modelling the elementary processes in a collisionally pumped plasma. The current trend is to study high Z (Z is a charge of a nucleus of ions). There is a hope to find lasing effects on the transitions in plasma of the Li-, Ne-, Ni-like ions. Very shocking example is a scheme for accomplishing tabletop x-ray lasing in Li-like ion of Ne at 98 Å in an optically ionized plasma during recombination in the transient regime. At the same time, low temperature plasma sources are more efficient and less expensive devices. They show promise for producing lasing in the vacuum ultraviolet and soft X-ray region. Preliminary investigations of capillary spark discharge were made (c.f.[5-9]), which show the possibility of their use as effective plasma sources for the generation of a soft-X-ray or extreme ultraviolet amplified spontaneous emission. A great progress in development of laser technique, tokamak and accelerator experiments resulted to a new class of problems in the plasma physics and correspondingly diagnostics of their parameters. The electron temperatures and particle confinement times in tokamak plasmas permit the ionization of the heavy impurity elements up to the helium-like (eventually hydrogen-like) charge state. High resolution spectroscopy of the line emission of these ions has become a powerful technique for determining the electron and ion temperatures T_e and T_i ,the macroscopic plasma movement and dynamics of the plasma impurity transport. Experimental measurements have beer carried out at several large tokamaks: Ti^{20+} and Fe^{24+} (Princeton Large Torus), Cr^{22+} (tokamak de Fontenau-aux-Roses=TFR) etc. The TFR measurements of the plasma parameters and wavelengths, atomic characteristics of satellite spectrum of the He-like ions from Ar^{16+} to Mn^{23} (Ar, Sc, V,Cr, Mn) are accurately carried out and presented in ref. [3].

In ref. [1-3] a new, effective relativistic version of the PT for calculations of the spectroscopic characteristics of the multicharged ions in plasma have been developed It is based on the fundamental formalism of the QED perturbation theory [10-14]. It has been used for developing

high resolution theoretical spectroscopy schemes for sensing and diagnostics the tokamak plasma parameters [1]. We carried put the estimates of the tokamak plasma parameters (electron temperature etc.) and presented the calculation results for wavelengths and other atomic characteristics of satellite spectrum of the He-like ions from Ar^{16+} to Mn^{23} [4]. However some theoretical non-consistency remained because of the non-account so-called QED corrections in theoretical scheme. For ions of the Ar^{16+} , Sc^{+21} there is got a good agreement with the tokamak de Fontenau-aux-Roses (TFR) and other measurements [5-9], but it is obvious that this scheme must be significantly improved for a case of plasma of more heavy elements. Here we present the results of theoretical calculation of the Fe plasma Li-like satellite lines on the basis of the relativistic perturbation theory with account for correlation and radiative corrections. With using the calculated values for relation of intensities of the dielectronic satellites lines and resonant lines of He-like ions, it is carried out an estimate of the plasma electron temperature which is equal 2,4keV under electron density of $10^{23}sm^3$.

Now we describe the key moments of our theoretical scheme. The details of the whole consistent QED version for studying and spectroscopic characteristics of the multicharged ions in plasma have been earlier presented in refs. [2,3] and based on the gauge invariant QED energy approach [1,10-12] and correct account of the finite nuclear size and QED effects (the Lamb shift, including self-energy part and vacuum polarization part).

The wave functions zeroth basis is found from the Dirac equation solution with potential, which includes core ab initio potential, electric, polarization potentials of nucleus (gaussian form for charge distribution in the nucleus is accepted). All correlation corrections of the PT second and high orders (electrons screening, particle-hole interaction etc.) are accounted for. The nuclear potential is provided by choice of charge distribution in the nucleus. The Coulomb potential for spherically symmetric density $\rho(r|R)$ is:

$$V_{nucl}(r|R) = -((1/r)\int_0^r dr' r'^2 \rho(r'|R) + \int_r^\infty dr' r' \rho(r'|R)$$

Let us consider the Li-like ion as example. One can write the DF-like equations for a three-electron system $1s^2nl$j. Formally they fall into one-electron Dirac equations for the orbitals *1s,nlj* with potential:

$$V(r)=2V(r|1s)+V(r|nlj)+V_{ex}+V(r|R).$$

This potential includes the electrical and polarization potentials of the nucleus. The part V_{ex} accounts for exchange inter-electron interaction. The main exchange effect will be taken into account if in the equation for the *1s* orbital we assume $V(r)=V(r|1s)+V(r|nlj)$ and in the equation for the *nlj* orbital $V(r)=2V(r|1s)$. The rest of the exchange-correlation effects are accounted for in the first two PT orders by the total inter-electron interaction. The core electron density is defined by iteration algorithm within gauge invariant QED procedure [12]. Other details of the calculation procedure, including definition of the matrix elements of the QED PT with effective account of the exchange-correlation effects can be found in refs. [1,10-12]. The details of calculational procedure are described in ref. [1-3]. Here we only note the following: in order to construct the optimal PT zeroth approximation we use ab initio quantum electrodynamics (QED) procedure [12]. The lowest order multielectron effects contribution, in particular, the gauge dependent radiative contribution for the certain class of the photon propagator calibration is minimized. Such a minimization results in the construction of the optimal one-electron basis.

In the Fe plasma in full similarity with the K, Cu plasma in a law inductive vacuum spark [2,7] one could observe the resonant lines $1snp\text{-}1s^2$ of the He- like ions with ground quantum number n from 3 to 6. The satellite lines $1s^22l\text{-}1s2lnl$ with n=3,4 are situated nearly.

In [2,4] we present the measured values of wavelengths (in Å) of the *Li*-like lines dielectronic satellites to $1s^{21}S_0\text{-}1s3p^1P_1$ emission line in the K plasma in a law inductive vacuum spark. We also present theoretical data on wavelengths, obtained on the basis of calculation within different theoretical approaches: PT on the 1/Z, relativistic PT with model zeroth approximation for three-quasiparticle atomic systems with effective

Transitions	Probability			Wavelength			Wave-length [7]
	B	C	D	B	C	D	
$1s^2 2p^2 P_{3/2} - 1s2p3p^2 D_{5/2}$	61,26	59,65	59,70	1,5933	1,5932	1,5934	1,5930± 0,0005
$1s^2 2p^2 P_{1/2} - 1s2p3p^2 D_{3/2}$	33,76	27,39	26,60	1,5931	1,5929	1,5935	
$1s^2 2p^2 P_{3/2} - 1s2p3p^4 S_{3/2}$	4,88	7,56	14,68	1,5947	1,5945	1,5948	
$1s^2 2p^2 P_{3/2} - 1s2p3p^4 P_{3/2}$	-----	5,48	-----	-----	1,5953	---	
$1s^2 2p^2 P_{3/2} - 1s2p3p^4 D_{5/2}$	-----	7,57	-----	-----	1,5952	---	

Table 1. The transitions probabilities (P, in 10^{13} s^{-1}) for Li-like lines of dielectronic satellites to $1s^{21}S_0$-$1s3p^1P_1$ emission line in the Fe plasma: (B)- PT on 1/Z, C- relativistic PT with model "0"-approximation for 3-quasi-particle atomic systems with effective account for correlation and radiative corrections (present work), D-method AUTOJOLS [2,7].

account for correlation and radiative QED corrections, method AUTOJOLS, optimized Dirac-Fock method with account QED corrections [2,7]. Table 1 lists the theoretical data on energies and transitions probabilities (in 10^{13} s^{-1}), which are corresponding Li-like lines of dielectronic satellites to $1s^{21}S_0$-$1s3p^1P_1$ emission line in the Fe plasma.

As in a case of calculating dielectronic satellites to emission line $1s^{21}S_0$-$1s3p^1P_1$ for K plasma in a low inductive vacuum spark [2,7], theoretical and experimental values of wavelengths for satellite lines in a whole are sufficiently well agreed with each other. However, values for the transition probabilities, calculated by different theoretical methods, are significantly disagreed with each other. Our work has shown that new ab initio version of the relativistic PT with correct account of correlation, relativistic and radiative effects for three-particle atomic systems is to be waited for a powerful theoretical tool for studying complex spectra and spectral characteristics of the plasma emission as in a law inductive vacuum spark as other plasma sources. It should be noted also that our approach is in a great degree oriented on the classical tasks of spectroscopy of free multicharged ions and spectroscopy of plasma. The last fact is especially valuable from the point of view of the realizing spectroscopic diagnostics of the hot plasma etc.

To define the electron density and temperature of a plasma one needs the correct data on the intensities of dielectronic satellites to resonant lines and the corresponding set of atomic constants (coefficients of dielectronic recombination, velocities of impact excitation, probabilities of radiation decay and autoionization etc. [2-7,13-17]. In our case the plasma electron temperature and its electron density can be defined using the relationship between the dielectronic satellites intensities, say, *j,k,* and resonant line. The intensity of resonant line of the He- like ion is defined as follows (c.f. [2,7]):

$$I_R = N_e < v\sigma >_{1s-2p} \int_0^{\tau} N_{He} dt$$

where N_{He} is a concentration of the He-like ions, $<vs>$ is an averaged cross-section of the impact excitation *1s-2p*; *t* is a time of the hot plasma. The relationship between the resonant lines satellites intensities of the He- like ions, say, Fe, Cl ions, is as follows:

$$W = I_{R_{Cl}} / I_{R\,Fe} = < v\sigma >_{1s-2p} \int_0^{\tau} N_{He_{Cl}} dt \{ < v\sigma >_{1s-2p} \int_0^{\tau} N_{He_{Fe}} dt \}^{-1}$$

With using the method of ref. [7], theoretical data of present paper, it is possible to evaluate the value of *W* in dependence upon the electronic temperature for given electron density: N_e=10^{23} cm^3. In result we predict the electron temperature 2400 eV that is in an reasonable agreement with experimental data [7]. The presented theory has to be very effective tool in treating the atomic (multicharged ions) spectroscopic characteristics in the laser-produced plasma, where studying of the elementary atomic processes is of a great interest and importance (see, for example, [18,19]).

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Abstract. There are presented the results of theoretical calculation for transition probabilities of the Fe plasma Li-like satellite lines on the basis of the relativistic perturbation theory with the Dirac-Fock model zeroth approximation and accounting for correlation and radiative corrections. With using the calculated values for relation of intensities of the dielectronic satellites lines and resonant lines of He-like ions, it is carried out an estimate of the plasma electron temperature and density.

Key words: Fe plasma Li-like satellite lines, relativistic perturbation theory

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РЕЛЯТИВИСТСКИЙ МОДЕЛЬНЫЙ ПОДХОД ДИРАКА-ФОКА К ИЗУЧЕНИЮСПЕКТРА ИЗЛУЧЕНИЯ ПЛАЗМЫ Fe В МАЛОИНДУКТИВНОЙ ВАКУУМНОЙ ИСКРЕ

Резюме. Проведено изучение параметров Li-подобных сателлитных линий плазмы Fe на основе расчета методом релятивистской теории возмущений с дирак-фоковским модельным нулевым приближением и учетом корреляционных и радиационных поправок. С использованием рассчитанных значений отношения интенсивностей диэлектронных и резонансных линий He- подобных ионов получена оценка величин электронной температуры и плотности плазмы.

Ключевые слова: Li-подобные сателлитные линии, плазма Fe, релятивистская теория возмущений

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РЕЛЯТИВІСТСЬКИЙ МОДЕЛЬНИЙ ПІДХІД ДІРАКА-ФОКА ДО ВИВЧЕННЯ СПЕКТР ВИПРОМІНЮВАННЯ ПЛАЗМИ Fe У МАЛОІНДУКТИВНІЙ ВАКУУМНІЙ ІСКРІ

Резюме. Виконано вивчення параметрів Li-подібних сателітних ліній плазми Fe на основі розрахунку методом релятивістської теорії збурень з дірак-фоківським модельним нульовим наближенням і урахуванням кореляційних та радіаційних поправок. З використанням розрахованих значень відношення інтенсивностей діелектронних й резонансних ліній He- подібних іонів виконано оцінку величини електронної температури та густини плазми.

Ключові слова: Li-подібні сателітні лінії, плазма Fe, релятивістська теорія збурень