CLOSING OF COSTER–KRONIG TRANSITIONS AND VARIATION OF FLUORESCENCE AND AUGER YIELDS IN ISONUCLEAR SEQUENCE OF TUNGSTEN

S. Kučas and R. Karazija

Institute of Theoretical Physics and Astronomy of Vilnius University, A. Goštauto 12, LT-01108 Vilnius, Lithuania
E-mail: sigitas.kucas@tfai.vu.lt

The dependence of Auger yields, partial and total Auger widths of levels, total radiative widths, and fluorescence yields on the ionisation degree is considered for ions of tungsten. The calculations are performed for the N_i subshells in the single configuration quasirelativistic approximation. The intervals of ionisation stages at which the Coster–Kronig transitions are energetically possible or partially possible are determined. It is shown that the partially possible Coster–Kronig transitions between overlapping initial and final configurations can take place in several neighbouring ions successively. According to our calculation results, the nonradiative decay of vacancies in N_i subshells becomes impossible from ionisation stage $q = 21$. The total Auger width depends weakly on ionisation degree up to its values $q = 8$–11, but for higher ions changes non-monotonically due to closing of Coster–Kronig transitions. The fluorescence yield shows the similar dependence on q.

Keywords: Coster–Kronig transitions, Coster–Kronig yield, fluorescence yield, Auger width, tungsten ions

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1. Introduction

Systematic calculations of Auger transitions are mainly restricted by atoms with a single vacancy in an inner shell [1, 2]. Extensive tables of Coster–Kronig and fluorescence yields, Auger and total natural level widths are published and their regularities are established [3–7]. For investigations of Auger cascades after production of inner vacancy and of the rearrangement of electronic shells after atom–ion collisions, required fluorescence and Auger yields for ions are usually derived from the available rates for the single vacancy atoms [8, 9]. For this purpose the scaling procedure for the total Auger transition rates [10] is used. These quantities are expressed in terms of a coefficient containing all the dependence on numbers of electrons in shells or subshells and a reduced transition rate depending only on radial wave functions and quantum numbers of electrons involved in the transitions. The total rate for a higher ionisation degree is calculated by taking the other numbers of electrons in the shells and supposing the second factor is constant or by linearly extrapolating the latter. However, the closing of some low energy Auger transitions can substantially change the fluorescence and Auger yields [11]. It is checked usually from the average energy calculations for considered configurations. This method does not take into account the partial overlap of energy level spectra of initial and final configuration as well as the strong dependence of the radial integrals on the Auger electron energy.

Nowadays the extensive investigations of astrophysical and laboratory plasma, of Auger cascades in atoms require the consideration of Auger transition regularities in multi-charged ions. Such data are necessary also for the interpretation of emission spectra of ions. Radiative and nonradiative transitions are tightly related as competitive, interdependent processes, their relative role is determined by the value of fluorescence yield. In the spontaneous decay of ion states with vacancies the nonradiative Auger transitions often dominate and they give the main contribution to the natural level widths, which are necessary for the calculation of radiative transitions intensities.

The ions of tungsten have been selected as an exemplary object for investigation of Auger transitions regularities in isonuclear sequence due to interest in its spectroscopic properties. This element is used as a first wall material in the last generation tokamaks. However, some quantities of tungsten are sputtered from the divertor surface and migrate into the region of discharge.

The multi-electron ions present in tokamak plasma can cause large radiation power loss [12]. We will consider the Auger transitions, mainly the most probable Coster–Kronig (CK) and super-Coster–Kronig (sCK) transitions, from the initial states with vacancies in the shells with the principal quantum number $n = 4$. Such vacancies are effectively produced at the conditions in tokamak plasma [13]. We suppose that the case of tungsten can reveal some general regularities of CK and fluorescence yields variation in isonuclear sequence.

2. Method of calculation

The calculations have been performed in the quasi-relativistic approximation [14], which is widely used for the investigation of spectral characteristics of tungsten ions [15, 16]. The average quantities depend less than the characteristics of separate transitions on the accuracy of the approximation used, thus in our work such quantities were calculated in a single configuration approximation. The radial integrals were not diminished by scaling factors, because their recommended values vary with q nonmonotonically and that would distort the dependence of considered quantities on the ionisation degree.

For outer and subvalent shells of considered ions the quasirelativistic single configuration approximation is preferable over the relativistic one, because the former takes into account main relativistic corrections and also includes interaction among relativistic nlj-configurations, corresponding to the same nl-configuration. On the other hand, the partitioning of shells into subshells enables one to obtain the average characteristics of subshells or of transitions between subshels, thus such scheme is more appropriate and habitual in inner-shell physics. For configurations with single vacancies in the closed shells it is possible to reconcile the advantages of both schemes: to perform calculations for nl-configurations, but afterwards to distinguish the groups of levels corresponding to nlj-configurations. For vacancies in inner shells such groups can be separated energetically. Even for partially overlapping energy level spectra with different values of total angular momentum of vacancy such separation can be performed by classification of states according to the largest weight in the expansion of the wave functions in jj coupling scheme. However, such attribution becomes invalid at strong mixing of wave functions, when nlj-configurations strongly overlap.

We attempted to preserve jj classification where it was possible. For this purpose the energy matrices were calculated and the wave functions classified in this scheme. The traditional for inner-shell physics notations of subshells with the principle quantum number $n = 4$ (N_i) are used.

The ground configurations of tungsten ions were taken from the latest revised data [17], they coincide with configurations obtained in single configuration quasirelativistic approximation, except $q = 12$, where the calculation gives the lowest level corresponding to a $4f^{13}5s^25p$ configuration instead of a $4f^{14}5s^2$ configuration following from experimental data.

During CK transitions the free electron escapes with a small energy, thus the rates of such transitions can depend strongly on the free electron energy ε. The example of very strong dependence of radial integrals of Auger transitions on the ε value can be sCK transition N_2–$N_3\,N_{6,7}$: values of integrals $R^2(4p4f,\,4p\varepsilon f)$ and $R^2(4p4f,\,\varepsilon f4p)$ increase twice in the interval of spectrum equal to about 20 eV. These integrals also show an unusual dependence on ε. The oscillation of free electron wave function $P_{\varepsilon l}(r)$ increases with ε, thus the absolute value of Auger radial integrals R^k usually tends to decrease. However, for some transitions the absolute value of R^k can increase within some interval of small values of ε; the reason of such behaviour is the varying overlap between wave functions of electrons contained in this integral. Then the usual tendency manifests itself only at larger values of ε. Such is the indicated case.

In order to take into account the dependence of transition rates on the energy of Auger electron, we used the following procedure. The Auger transition integrals were calculated for seven equidistant values of ε within its interval for one channel of considered Auger transitions. Then the contribution to total Auger transition rate [18] was calculated for these values of ε and the average energy of Auger electron determined as follows:

$$\varepsilon_{\mathrm{av}} = \frac{\sum_i \varepsilon_i A_i}{\sum_i A_i}, \tag{1}$$

where A_i is the total transition rate for the ith value of ε and i runs from 1 to 7. Subsequently all contributions to total transition rates were recalculated with this one $\varepsilon_{\mathrm{av}}$ value.

In the case of overlapping initial and final configurations the detailed level-by-level calculations for energetically allowed Auger transitions were performed, taking the radial integrals calculated at the middle value of the allowed energy interval.

Table 1. Intervals of ionisation stages of tungsten ions, where $N_i N_j X$ Coster–Kronig and $N_i N_j N$, super-Coster–Kronig transitions are possible (p) or partially possible (pp)

Final vacancy state	Initial vacancy state										
	N_1		N_2		N_3		N_4		N_5		$N_{6,7}$
	p	pp	p	pp	p	pp	p	pp	p	pp	
$N_{2,3} N_{2,3}$	–	–	–	–	–	–	–	–	–	–	–
$N_{2,3} N_{4,5}$	–	–	–	–	–	–	–	–	–	–	–
$N_2 N_{6,7}$	1–3	4	–	–	–	–	–	–	–	–	–
$N_2 O_1$	–	1–2	–	–	–	–	–	–	–	–	–
$N_2 O_{2,3}$	1–2	3–5	–	–	–	–	–	–	–	–	–
$N_2 O_{4,5}$	1–6	–	–	–	–	–	–	–	–	–	–
$N_2 P_1$	1–2	–	–	–	–	–	–	–	–	–	–
$N_3 N_{6,7}$	1–7	8–9	–	1–3	–	–	–	–	–	–	–
$N_3 O_1$	1–6	–	–	–	–	–	–	–	–	–	–
$N_3 O_{2,3}$	1–7	8–10	–	1–3	–	–	–	–	–	–	–
$N_3 O_{4,5}$	1–6	–	–	1–4	–	–	–	–	–	–	–
$N_3 P_1$	1–2	–	–	1–2	–	–	–	–	–	–	–
$N_{4,5} N_{4,5}$	1–3	4–6	–	–	–	–	–	–	–	–	–
$N_4 N_{6,7}$	1–13	14–15	1–9	10–12	1–7	8–9	–	–	–	–	–
$N_4 O_1$	1–13	14–15	1–8	9–11	1–5	–	–	–	–	–	–
$N_4 O_{2,3}$	1–12	–	1–10	11–12	1–7	8–9	–	–	–	–	–
$N_4 O_{4,5}$	1–6	–	1–6	–	1–6	–	–	–	–	–	–
$N_4 P_1$	1–2	–	1–2	–	1–2	–	–	–	–	–	–
$N_5 N_{6,7}$	1–14	15–16	1–9	10–12	1–7	8–10	–	–	–	–	–
$N_5 O_1$	1–14	15–16	1–8	9–12	1–6	–	–	–	–	–	–
$N_5 O_{2,3}$	1–12	–	1–11	12	1–7	8–10	–	–	–	–	–
$N_5 O_{4,5}$	1–6	–	1–6	–	1–6	–	–	1	–	–	–
$N_5 P_1$	1–2	–	1–2	–	1–2	–	–	1	–	–	–
$N_{6,7} N_{6,7}$	1–19	20–21	1–17	18–19	1–14	15–17	1–8	9–12	1–8	9–11	–
$N_{6,7} O_1$	1–17	–	1–17	–	1–15	16–17	1–7	8–10	1–7	8–10	–
$N_{6,7} O_{2,3}$	1–12	–	1–12	–	1–12	–	1–9	10–12	1–9	10–12	–
$N_{6,7} O_{4,5}$	1–6	–	1–6	–	1–6	–	1–6	–	1–6	–	–
$N_{6,7} P_1$	1–2	–	1–2	–	1–2	–	1–2	–	1–2	–	–

3. Results and discussion

The energy level spectra of configurations with vacancies in N_i subshells and outer open shells extend up to several tens of eV. Thus the case of overlapping initial and final configurations is rather frequent. The intervals of ionisation stages at which the CK transitions are energetically possible or partially possible are indicated in Table 1. The partially possible transitions between some levels of overlapping configurations can extend in the sequence of ions even up to 4 successive values of q. It is necessary to note that the interval of CK spectrum, where intensities of lines obtain practically significant values, can be noticeably narrower than the interval of energetically possible transitions.

With increasing the ionisation degree the transitions become impossible due to the absence of electrons in the shells involved in the transitions. Additionally, the CK transitions with a small energy of Auger electron can become energetically forbidden with increasing atomic number of an element. The same regularity manifests itself with increasing the ionisation degree q. It follows from the expression for the energy of Auger transition in terms of binding energies of three electrons involved in the transition. The sum of binding energies of two such electrons present in the initial configuration of CK transition can be changed to a larger extent than the binding energy of the electron present in the final configuration. The nonradiative decay of $N_{2,3}$ vacancy states becomes impossible from ionisation stage 19 and of N_1 states from $q = 21$.

CK yield $S_{i,j}$ is defined as the probability that a vacancy in the subshell X_i is shifted to the subshell X_j during the CK transition, while the other vacancy is produced in the same or other subshell:

$$S_{i,j} = \frac{\sum_k A_{\mathrm{CK}}(X_i - X_j X_k)[1 + \delta(j,k)]}{A_{\mathrm{tot}}(X_i)}, \quad (2)$$

where A_{CK} is the CK transition rate and A_{tot} is the total Auger and radiative transitions rate for the state with initial vacancy. The last multiplier in the nominator takes into account the possibility for both vacancies

Table 2. Coster–Kronig N_i yields for tungsten ions

Ionisation degree	$S_{1,2}$	$S_{1,3}$	$S_{1,4}$	$S_{1,5}$	$S_{1,67}$	$S_{2,3}$	$S_{2,4}$	$S_{2,5}$	$S_{2,67}$	$S_{3,4}$	$S_{3,5}$	$S_{3,67}$	$S_{4,67}$	$S_{5,67}$
1 [7]	0.19	0.56	0.062	0.092	0.59	0.114	0.67	0.10	0.79	0.14	0.73	0.82	1.7	1.73
1	0.187	0.538	0.068	0.102	0.521	0.068	0.715	0.107	0.803	0.122	0.719	0.646	1.662	1.620
2	0.186	0.538	0.073	0.100	0.522	0.017	0.757	0.112	0.804	0.122	0.720	0.650	1.664	1.622
3	0.186	0.544	0.068	0.101	0.527	0.006	0.765	0.114	0.811	0.123	0.718	0.650	1.666	1.624
4	0.149	0.566	0.072	0.107	0.554	0.005	0.765	0.114	0.814	0.122	0.717	0.654	1.679	1.641
5	0.032	0.643	0.084	0.125	0.614		0.768	0.116	0.822	0.123	0.715	0.664	1.692	1.652
6	0.018	0.658	0.089	0.132	0.637		0.768	0.116	0.823	0.110	0.723	0.680	1.713	1.678
7		0.642			0.722		0.767	0.118	0.835	0.120	0.696	0.753	1.736	1.699
8		0.340			0.596		0.760	0.122	0.809	0.083	0.633	0.662	1.696	1.672
9		0.005			0.840		0.761	0.141	0.878	0.009	0.315	0.831	1.825	1.837
10					0.866		0.770	0.140	0.946			1.260	1.898	1.804
11					0.893		0.484	0.272	0.939			1.330	1.043	0.994
12					0.854		0.031	0.112	1.233			1.297	0.702	0.556
13					0.970				1.783			1.643		1.620
14					0.937				1.756			1.605		
15					1.169				1.727			1.564		
16					1.350				1.689			1.282		
17					1.546				1.816			1.000		
18					2.000									
19					2.000									
20					2.000									
21					2.000									

to appear in the same X_j subshell by sCK transitions $X_i - X_j^2$. Thus in the presence of such transitions the yield $S_{i,j}$ can obtain a value greater than 1. The values of these quantities for various subshells are presented in Table 2. Only for single ions our results can be compared with the values of previous calculations [19] obtained in nonrelativistic approximations [20] (recently published data [7] employ the same results [19] fitted to polynomials as a function of atomic number). The differences of nonrelativistic and quasirelativistic calculations for single ions are not significant.

Nonradiative transitions dominate in the decay of vacancies in the N_i subshells of tungsten, thus the Auger width is practically equal to the natural width $\Gamma(N_i)$. For low ionisation degrees the calculated values for N_1, $N_{2,3}$, and $N_{4,5}$ vacancy states amount to several eV and even exceed 10 eV (Fig. 1). In the sequence of ions the Auger width almost does not depend on ionisation degree q while Auger transitions remain energetically possible. At ionisation stages $q = 6$–11 the sudden decrease of Auger width takes place due to energetic interdiction of the CK transitions.

The calculated widths can be compared with experimental values as well as with results of calculations in various approximations, compiled for single ions in [6] (Table 3). Our results correspond better to experimental values than those calculated by relativistic Dirac–Fock–Slater [21] or nonrelativistic Hartree–
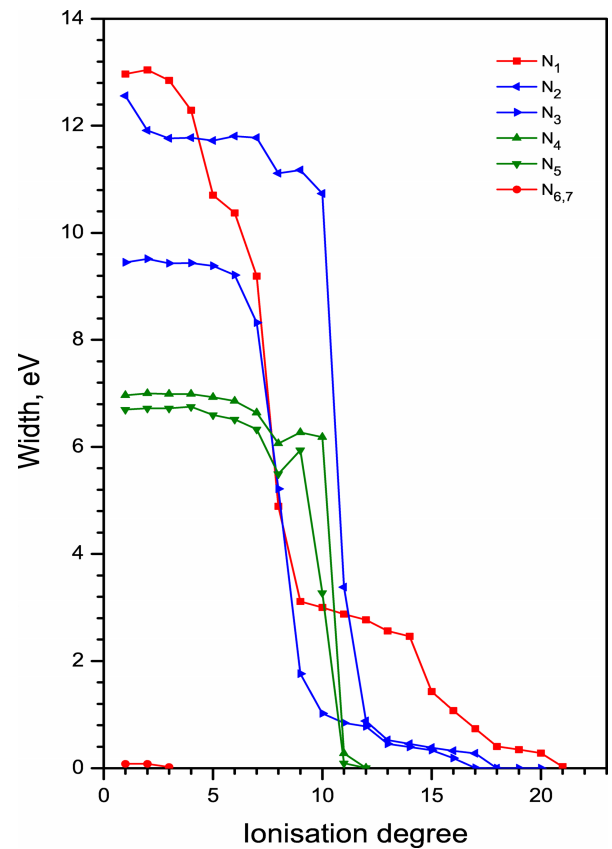

Fig. 1. Dependence of N_1, N_2, N_3, N_4, N_5 and $N_{6,7}$ Auger widths on ionisation degree.

Table 3. Auger widths for tungsten atom with one vacancy. Comparison of results, calculated in quasirelativistic (RHF) approximation with the values obtained in Dirac–Fock–Slater (DFS), Hartree–Fock–Slater (HFS), many-body-perturbation theory (MBPT) approximations and experimental data.

Subshell	Exp [6]	DFS [21]	HFS [19]	MBPT [22]	RHF This work
N_1	7.4±1.6	14.5	15		12.97
N_2	5.4±0.7	13.6	13.8		12.56
N_3	4.7±0.8	10	12.3		9.45
N_4	2.9±0.6	7.3	7.89	3.41	7.14
	5.0±0.7			4.61	
N_5	3.1–5.0	6.9	7.72	3.41	6.70
N_6	0.16–0.09		0.07		} 0.08
N_7	0.11–0.19				

Fock–Slater [19] methods. However, for all shells, except $N_{6,7}$, single configuration calculation significantly overestimates experimental data. Good correspondence was obtained by application of many-body perturbation theory [22], but such results were given only for N_4 and N_5 subshells. It indicates the essential role of correlation effects for CK transitions, which significantly contribute to Auger width. However, the separation of rela-

tivistic configurations tends to increase with q and configuration interaction effects often become weaker for ions (with exceptions of some intersecting configurations). Thus a better correspondence of calculated and experimental results for higher ions can be supposed.

The near-independence of partial Auger width on q and on the outer passive shell is clearly expressed up to the ionisation stages, when corresponding Auger transitions become energetically forbidden (Figs. 2 and 3). The decay of N_i ($i = 1$–5) vacancy states is dominated by transitions involving 4f electrons. The largest contribution to $\Gamma(N_1)$ width is given by N_1–$N_3 N_{6,7}$ transitions, but also N_1–$N_3 O_{2,3}$ and N_1–$N_{4,5} O_{2,3}$ transitions play a significant role. For $\Gamma(N_3)$ almost half of the width is given by transitions to $N_5 N_{6,7}$, while transitions to $N_4 N_{6,7}$ dominate more in deexcitation of N_2 vacancy state. In the case of $\Gamma(N_4)$ and $\Gamma(N_5)$ widths the contribution of transitions to $N_{6,7}^2$ amounts already to about 2/3 of the total width.

The total radial width $\Gamma_{\mathrm{rad}}(N_i)$ varies slowly at low ionisation degrees, when the outer shells are ionised (Fig. 4). The reason of a sudden decrease of this quantity at $q = 16$ for N_2 and N_3 vacancy states is
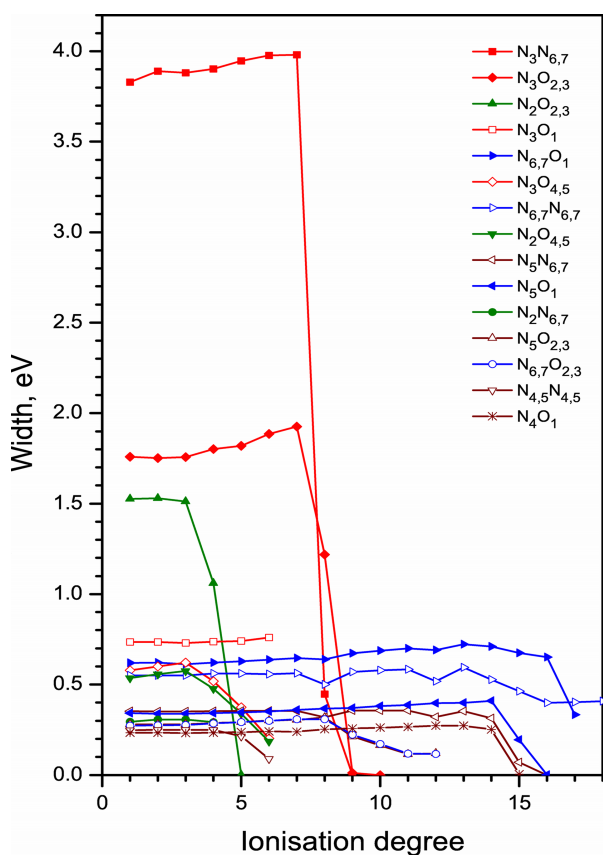

Fig. 2. Contributions of Coster–Kronig transitions to N_1 Auger width at various ionisation degrees. Transitions which contribute less than 0.23 eV for the first ion of sequence are not indicated.
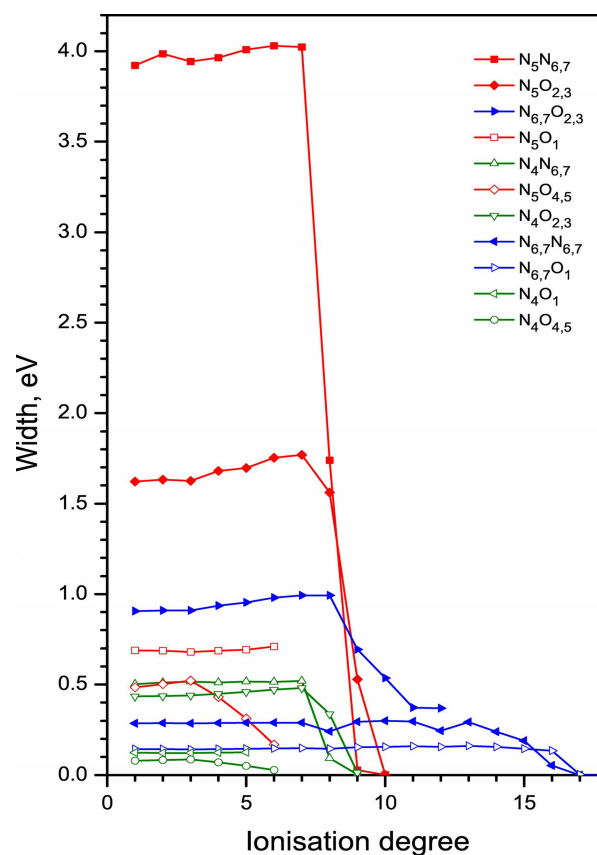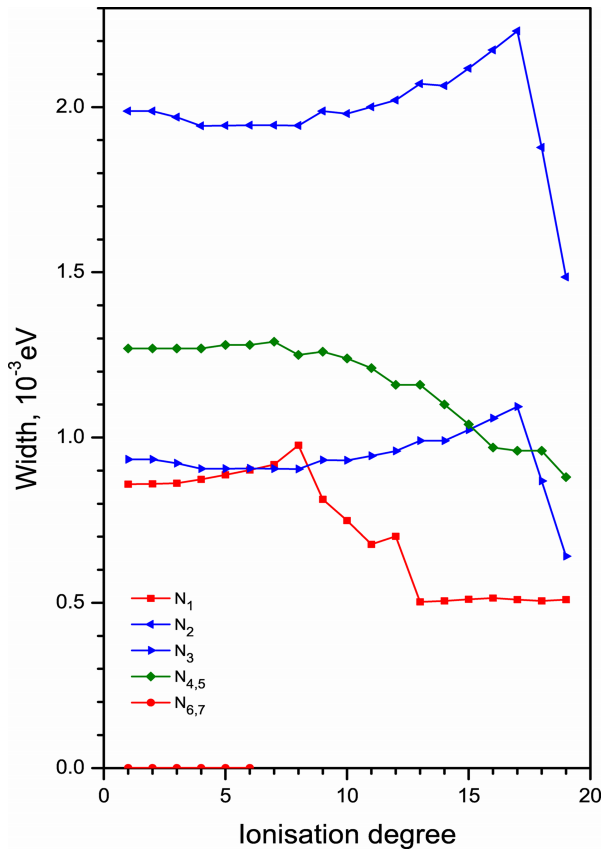

Fig. 3. Contributions of Coster–Kronig transitions to N_3 Auger width at various ionisation degrees. Transitions which contribute less than 0.075 eV for the first ion of sequence are not indicated.

Fig. 4. Dependence of N_1, N_2, N_3, $N_{4,5}$, and $N_{6,7}$ radiative widths on ionisation degree.

Fig. 5. Dependence of ω_1, ω_2, ω_3, $\omega_{4,5}$, and $\omega_{6,7}$ fluorescence yields on ionisation degree.

the disappearance of electrons in 5s shell. The similar two downfalls in the variation of $\Gamma_{\rm rad}(N_1)$ width are caused by the beginning ionisation of the $5p^N$ shell and its full ionisation. Only the $\Gamma_{\rm rad}(N_{4,5})$ width changes almost monotonically, because the main contribution to this quantity is given by transitions from the $4f^N$ shell containing a large number of electrons ($N = 14$ or 13).

The N_i fluorescence yield ω_i for tungsten ions up to W^{16+} is of order of 10^{-5}–10^{-2} (Fig. 5). Its values for $i = 1$–5 remain almost constant at small ionisation stages. At $q = 1$ our values of ω_i, as well as the Auger yields S_{ij}, approximately correspond to calculation results given in [19]. It is necessary to note that later published data [7], obtained by fitting with polynomials the results of [19], essentially differ from the latter for the very elements the data of which were used, including tungsten.

4. Conclusions

We have determined the intervals of ionisation degrees in which the CK transitions for the vacancy states in N_i subshells of tungsten are possible or partially possible.
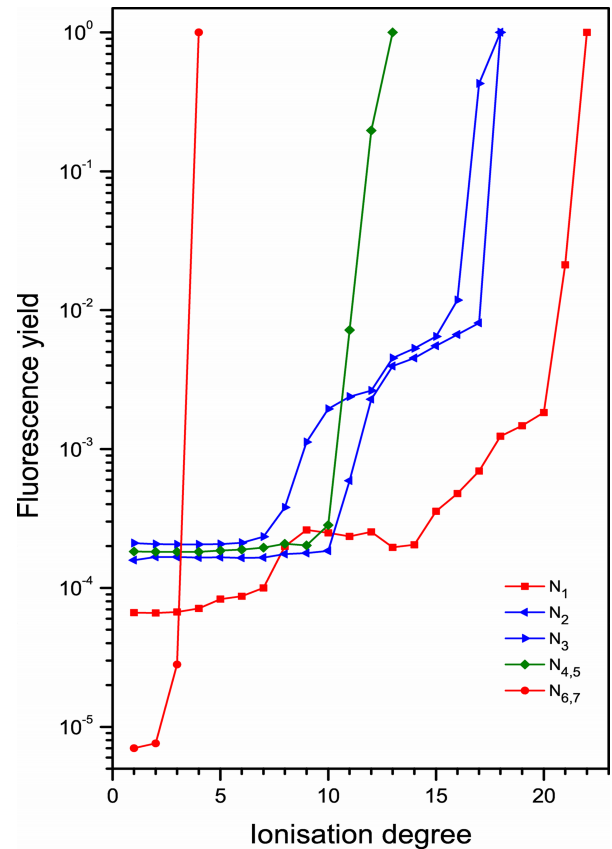
The energy level spectra of configurations with such vacancies and outer open shells extend up to several tens of eV, thus the case of overlapping initial and final configurations is rather frequent and the partially possible Coster–Kronig transitions can take place in several ions successively. At small ionisation degrees various CK and sCK transitions are permitted and the Auger width as well as the practically equal to it total natural width obtains a rather large value; but at ionisation stages from about 7 a sudden decrease of width takes place due to energetic interdiction of the most probable Auger transitions. The ω_1–ω_5 fluorescence yields have very small, almost constant value, approximately equal to 10^{-4}, at ionisation degrees up to 7–10; for higher ions its value significantly increases.

Only the calculated natural widths for single ions can be compared with experimental values as well as with results of calculations in other approximations. Our results correspond better to experimental values than the ones calculated by relativistic Dirac–Fock–Slater [21] or nonrelativistic Hartree–Fock–Slater [18] methods. However, for all shells except $N_{6,7}$, the single configuration calculation significantly overestimates experimental data. The configuration interaction effects tend

to become weaker with ionisation degree, thus a better correspondence of calculated and experimental results for higher ions can be supposed.

The indicated regularities of Coster–Kronig and fluorescence yields variation in isonuclear sequence can be characteristic also for the ions of other elements.

Acknowledgements

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COSTERIO IR KRONIGO ŠUOLIŲ DRAUDIMAS IR FLUORESCENCIJOS BEI AUGER IŠEIGOS VOLFRAMO IZOBRANDUOLINĖJE SEKOJE

S. Kučas, R. Karazija

Vilniaus universiteto Teorinės fizikos ir astronomijos institutas, Vilnius, Lietuva

Santrauka

Auger šuoliai yra plačiai nagrinėti eksperimentiškai ir teoriškai atomams su vidine vakansija. Tuo tarpu duomenų jonams yra labai mažai, nėra tirti šių šuolių kitimo dėsningumai izobranduolinėse sekose. Darbe toks nagrinėjimas atliktas volframui, kurio spektriniai tyrimai yra aktualūs dėl šio elemento naudojimo termobranduolinės sintezės reaktoriaus – tokamako konstrukcijose. Atlikti sistemingi Auger ir fluorescencijos išeigų, lygmenų Auger bei radiacinių plo-čių skaičiavimai volframo jonams su $4l^{-1}$ (l = s, p, d, f) vakansija iki jonizacijos laipsnių, kuriems esant Auger šuoliai tampa nebegalimi. Šios charakteristikos stipriai priklauso nuo labiausiai tikėtinų Costerio ir Kronigo šuolių, todėl nustatyti jonizacijos laipsnių intervalai, kuriuose šie šuoliai yra galimi energetiškai. Nustatyta ir aptarta Auger šuolių pagrindinių charakteristikų priklausomybė nuo jonizacijos laipsnio ir vakansijos tipo.