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L shell fluorescence yields and total ionization and x-ray production cross sections for elements with $40 \leq Z \leq 92$

A. Bendjedi [a,b], B. Deghfel [a,b,*], A. Kahoul [c,d], I. Derradj [a,b], F. Khalfallah [c,d], Y. Sahnoune [c,d], A. Bentabet [e], M. Nekkab [a,f]

[a] Laboratory of Materials Physics and Their Applications, Physics Department, Faculty of Sciences, University of Mohamed Boudiaf, 28000 M'sila, Algeria
[b] Department of Physics, Faculty of Sciences, University of Mohamed Boudiaf, 28000 M'sila, Algeria
[c] Department of Materials Science, Faculty of Sciences and Technology, Mohamed El Bachir El Ibrahimi University, Bordj-Bou-Arreridj 34030, Algeria
[d] LPMRN Laboratory, Department of Materials Science, Faculty of Sciences and Technology, University of Mohamed El Bachir El Ibrahimi, Bordj-Bou-Arreridj 34030, Algeria
[e] Laboratory of Characterization and Valuation of Natural Resources, University of Mohamed El Bachir El Ibrahimi, Bordj-Bou-Arreridj 34030, Algeria
[f] LESIMS Laboratory, Physics Department, Faculty of Sciences, Ferhat Abbas University, Setif 19000, Algeria

HIGHLIGHTS

- L shell cross sections are deduced from updated experimental data (till 2014).
- Derive a new values of average fluorescence yield from L shell cross sections.
- The obtained results are compared with others works for elements with $40 \leq Z \leq 92$.
- Good agreement was obtained by comparing our result with other works.

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ABSTRACT

Existing experimental compilation (till 2014) for a wide range of elements ($40 \leq Z \leq 92$) by proton impact (up to 10.0 MeV) is used to deduce empirical ionization and x-ray production cross sections. The reliability of the obtained cross sections is then exploited to derive new values of L shell average fluorescence yield. This was based on the fact that ratio of ionization to x-ray production cross sections is independent of the excitation energy of proton ranging from 0.02 to 10.0 MeV, for a given element. The obtained values are compared with earlier theoretical and experimental results, where a good agreement is observed for all elements under investigation.

1. Introduction

The average fluorescence yield connects the ionization cross-section and the subsequent x-ray production one by filling of vacancies created in the corresponding shell. Accurate values of average fluorescence yield are important in many uses of inner shell ionization and related phenomena such as PIXE analysis that uses the inner shell fluorescence yields to predict or compare theoretical x-ray cross sections with those measured experimentally (Cohen, 1987; Oz et al., 1999; Hubbel et al., 1994; Küçükönder et al., 2004). The collected database consists of 991 and 5266 experimental points for total ionization and x-ray production cross sections, respectively, from existing compilation (Miranda and Lapicki, 2014) and other experimental data extracted from curves (Miranda et al., 2013; Zhou et al., 2013; Batyrbekov et al., 2014; Bertol et al., 2014; Mohan et al., 2014). Sometimes a remarkable dispersion is pointed out in both theoretical (Cohen, 1987; Mitchell and Barfoot, 1981; Hubbell et al.,1994; Oz et al., 1999) and experimental values (Singh et al., 1990; Simsek et al., 1999; Garg et al., 1992; Ertugrul, 2002; Apaydın and Tırasoglu, 2012). This situation motivates the need to a consistent and reliable new set of

* Corresponding author at: Laboratory of Materials Physics and Their Applications, Physics Department, Faculty of Sciences, University of Mohamed Boudiaf, 28000 M'sila, Algeria. Fax: +213 035666599.
E-mail address: b_deghfel@yahoo.fr (B. Deghfel).

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average L shell fluorescence yields. For this purpose, we adopt a criterion of dispersion of the existing experimental data, which are considerably scattered, from their corresponding calculated using the most advanced theoretical model (Smit and Lapicki, 2014).

The present contribution is organized as follows. In the first part, the available experimental compilation, (Miranda et al., 2013; Zhou et al., 2013; Batyrbekov et al., 2014; Bertol et al., 2014; Mohan et al., 2014; Miranda and Lapicki, 2014), for a wide range of elements ($40 \leq Z \leq 92$) by proton impact (0.02 to 10.0 MeV) are used to deduce empirical ionization and x-ray production cross sections. These cross sections are then exploited, in the second part, to derive a new values of average fluorescence yield. Finally, the obtained results are compared with other theoretical and experimental values.

2. Summary of experimental database

Table 1 displays the number of the available experimental points of L shell total ionization and x-ray production cross sections for elements in the range $40 \leq Z \leq 92$ by proton impact (0.02–10.0 MeV) from compilation of Miranda and Lapicki (Miranda and Lapicki, 2014) and other experimental data extracted from curves (Miranda et al., 2013; Zhou et al., 2013; Batyrbekov et al., 2014; Bertol, et al., 2014; Mohan et al., 2014). To produce a consistent and reliable set of average L shell fluorescence yields and enhance the quality of interpolation in the next section, we introduce the dispersion criterion, fixed within the interval [0.5–1.5], of the existing experimental data for both ionization and x-ray production cross sections from their corresponding calculated using ECPSSR model (Brandt and Lapicki, 1981; Liu and Cipolla, 1996.; Deghfel et al., 2013b) with correct exact integration limits (noted as eCPSSR by Smit and Lapicki, 2014). In such model Smit and Lapicki indicated that it would be wrong to evaluate the exact limits for momentum transfers of integration in calculating form factors (Q_{min} and Q_{max}) by replacing η_s with η_S^R ($\eta_S^R = m_S^R \eta_S$), where η_S^R is the reduced ion energy and m_S^R is the relativistic correction functions (Brandt and Lapicki, 1981). As a solution of this problem, they proposed that the factor m_S^R should multiply electron rest mass m wherever it occurs. This led to the correct integration limits given by Eq. (14) from reference of Smit and Lapicki (2014) given as

$$Q_{\substack{\min \\ \max}} = \left(\frac{M}{m_S^R m}\right)^2 \eta_S^R \left(1 \mp \sqrt{1 - m_S^R m W / \eta_S^R M}\right)^2 \tag{1}$$

where W is the transferred energy from projectile to the ejected electron and Q is the square of the transferred momentum of the projectile.

Also, the eCPSSR model is distinguished from the original ECPSSR theory of Brandt and Lapicki (1981) developed from *PWBA* theory by including f_S-functions to account for the energy loss (E), the perturbed stationary state (PSS), Coulomb deflection (C) effects of the projectile and relativistic (R) nature of the target's inner-shell. These effects are included in the PWBA cross section (Liu and Cipolla, 1996; Reis and Jesus, 1996) by changing θ_S to $\zeta_s \theta_S$, where ζ_S accounts for the changes in binding energy and multiplying the PWBA cross section by Coulomb deflection factor C_S and m by the relativistic correction functions $m_S^R(\xi_S)$, where ξ_S is the scaled projectile velocity. Then, the rejected experimental data are also incorporated in Table 1. This criterion is applied by several authors (Paul, 1982; Paul and Muhr, 1986; Rodriguez-Fernandez et al., 1993; Orlic, 1994; Deghfel et al., 2013a) and has no much influence on the present calculation of the cross section; 121 (448) data are removed for ionization (x-ray production) cross section, which represents about 12.21% (08.50%) from the total number of experimental data.

Table 1
Number of available (rejected) experimental data of ionization, $N^I(N_R^I)$, and x-ray production, $N^X(N_R^X)$, cross sections for elements with atomic number $40 \leq Z \leq 92$ by proton impact.

Z	N^I	N_R^I	N^X	N_R^X	Z	N^I	N_R^I	N^X	N_R^X
40	30	22	75	03	64	27	02	146	12
41	30	19	68	27	65	24	00	115	01
42	–	–	99	12	66	53	00	198	23
44	–	–	09	00	67	30	04	156	15
45	–	–	60	09	68	13	00	148	17
46	–	–	101	34	69	–	–	67	00
47	30	00	250	86	70	29	01	181	30
48	13	01	109	13	71	15	00	62	00
49	29	00	138	06	72	15	00	71	09
50	35	02	191	32	73	37	17	185	05
51	16	00	75	02	74	47	00	173	08
52	16	00	112	06	75	–	–	19	00
53	26	00	82	01	76	06	00	26	00
54	–	–	08	04	77	20	00	57	00
55	–	–	79	01	78	18	00	113	00
56	–	–	103	05	79	176	32	445	14
57	–	–	166	11	80	15	00	58	00
58	04	00	130	01	81	–	–	33	01
59	07	00	123	06	82	59	01	277	01
60	17	00	179	11	83	58	19	200	06
62	12	00	126	22	90	33	00	61	02
63	17	01	93	07	92	34	00	99	05

3. Total ionization and x-ray production cross sections

Measured L-shell total ionization and x-ray production cross sections, reported from the compilation of Miranda and Lapicki (Miranda and Lapicki, 2014) and other extracted data from curves (Miranda, et al., 2013; Zhou, et al., 2013; Batyrbekov, et al., 2014; Bertol, et al., 2014; Mohan, et al., 2014), are found to be universal when plotted, in a logarithmic scale, as a function of the scaled velocity ξ_L given as

$$\xi_L = (\xi_{L_1} + \xi_{L_2} + 2\xi_{L_3})/4 \tag{2}$$

where, $\xi_s = 2\, v_1/\theta_s v_s$ ($s = L_1$, L_2 and L_3).

This is shown in Fig. 1 for selected elements with $40 \leq Z \leq 92$ by proton impact. Universal character of L-shell for both ionization and x-ray production cross sections allows us to derive an empirical cross section for each elements; the set of the experimental data, following its evolution, is interpolated by a first order exponential decay function as

$$\ln \sigma_{emp} = r_0 + r_1 \exp(-r \ln \xi_M) \tag{3}$$

The result of interpolation is shown in Fig. 1 with a full line for both ionization and x-ray production cross sections.

The root-mean-square error (ε_{rms}) is considered as a criterion of the quality of the calculated empirical cross section. This error is expressed as the total deviation of the experimental cross sections ($\sigma_{\exp}$) from their corresponding empirical ($\sigma_{\exp}$) values (Deghfel et al., 2013a). The interpolation coefficients (r_0, r_1 and r) with the values of ε_{rms} for both x -ray production and ionization empirical cross sections, are listed in Table 2.

From this table, it can be seen that the empirical method, described in the previous section, gives the better representation of the experimental data for both ionization and x-ray production cross sections. Generally, the values of ε_{rms} vary within an acceptable ranges:from 0.08% to 3.91% for the first cross section and from 0.05% to 6.70% for the second one. This allows us to use them as reliable cross sections to deduce new values of the average