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Parameterization of Proton Induced M_i (I=1-5) sub-shell X-ray Production Cross Sections

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***Abstract*— The cross sections for production of the M_i (i=1-5) sub-shell X-rays by proton impact have been calculated for different elements with 67≤Z≤92 at energies 0.4-2.0 MeV using the Dirac-Hartree-Slater (DHS) model [2] and the ECPSSR model [3] based proton ionization cross sections, X-ray emission rates based on the Dirac-Fock model [6], the fluorescence yields and Coster-Kronig transition probabilities based on the Dirac-Hartree-Slater model [9]. These XRP cross sections have been fitted to polynomials in Z as, $\sigma_{Mi}^{X} = \sum_n a_n Z^n$. These fitting Coefficients help to reduce the required database parameters and can be used in different software to interpolate the XRP cross sections for required element.**

***Index Terms*—X-ray production cross sections, proton ionization cross sections.**

I. Introduction

The M_i (i=1-5) sub-shell vacancy created by an incident proton can decay through either radiative or non-radiative transition. The radiative vacancy decay results in characteristic emission spectrum comprising several M X-ray lines. Accurate knowledge of the M_i (i=1-5) sub-shell X-ray production (XRP) cross sections and relative intensities for different elements at various incident proton energies is important for ion-beam applications including the quantitative elemental analysis of different types of samples employing proton induced X-ray emission (PIXE) technique. Besides, such data are useful for testing the theories governing the proton-atom collisions. The relative X-ray line intensities can be calculated from the XRP cross sections which, in turn, are evaluated using theoretical data on different physical parameters, namely, the proton ionization cross sections, X-ray emission rates, fluorescence yields and Coster-Kronig (CK) transition probabilities. A literature search indicated lack of systematic tabulation of the theoretical proton induced M_i (i=1-5) sub-shell XRP cross sections.

II. Physical parameters

Proton ionization cross sections

In literature, two approaches are available to calculate the proton ionization cross sections. The first approach is based on the plane wave Born approximation (PWBA) employing screened hydrogenic wave functions including the corrections for polarization and binding effects in the Perturbed Stationary State (PSS), relativistic effects (R), energy loss (E) and Coulomb deflection (C) and is generally referred to as the ECPSSR model calculations [1]. The second approach is based on the plane wave Born approximation (PWBA) employing more realistic Dirac-Hartree-Slater (DHS) wave functions including consistent incorporation of relativity and corrections due to binding, polarization and Coulomb deflection effects. The DHS model based M_i (i=1-5) sub-shell ionization cross sections are tabulated only for fifteen elements with 54≤Z≤92 at different incident proton energies ranging 0.06 MeV to 2.0 MeV [2]. However, a computer code "ISICS" has been made available by Liu and Cipolla [3] to obtain the ECPSSR model based K, L and M shell ionization cross sections for various target projectile combinations.

X-ray emission rates

The M-shell X-ray emission rates based on the DHS model [4] were tabulated for only six elements with 48≤Z≤93 and those based on the DF model [5] were tabulated for only ten elements with 48≤Z≤92. The complete sets of emission rates based on both, the DHS and the DF models generated for elements with 65≤Z≤92 by logarithmic interpolation from the available limited data were reported by us [6]. It is pertinent to mentioned that experimental data on relative intensity ratios for different M X-ray groups is desirable to check the reliability of these two sets of emission rates.

Fluorescence yields and Coster-Kronig transition probabilities

The M_i (i=1-3) sub-shell fluorescence (ω_i) and CK (f_{ij}) yields based on the DHS model were available for ten elements in the atomic region 67≤Z≤95 [7], and in case of the M_i (i=4, 5) sub-shells these values were available for eight elements in the atomic region 70≤Z≤100 [8]. Recently, a complete set of the DHS model based ω_i and f_{ij} yields for elements with 67≤Z≤92 evaluated considering the cutoff/onset of different M_i sub-shell Coster-Kronig transitions have been reported by Chauhan and Puri [9]. A second set of the M_i (i=1-5) sub-shell fluorescence yields calculated using the DF model based X-ray emission rates have also been given in this reference. The tabulation of theoretical M-shell Auger and CK transition rates are not available in literature.

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III. PRESENT WORK

In the present work two sets of the total M XRP cross sections have been calculated for elements 67≤Z≤92 for 0.4-2.0 MeV proton impact using the using the X-ray emission rates based on the Dirac-Fock (DF) model [6], fluorescence yields and the Coster-Kronig transition probabilities based on the DHS model [9] and two sets of the proton ionization cross sections based on the Dirac-Hartree-Slater (DHS) model employing more realistic wave functions [2] and the ECPSSR model [3]. Further, the present calculated two sets of the total M XRP cross sections have been fitted to polynomials in Z as, $\sigma_{Mi}^{X} = \sum_n a_n Z^n$; Z represents the atomic number of the element.

Basic Formalism and Computational Procedure

The total M shell X-ray production cross sections, at a given incident proton energy can be evaluated using the equations

$$\sigma_M^X = \sum_{i=1}^{5} \sigma_{M_i}^{\tau} \omega_i \quad (1)$$

Where, ω_i represents the M_i (i = 1 - 5) sub-shell fluorescence yields. The $\sigma_{M_i}^{\tau}$ denote the total number of vacancies in the M_i (i = 1 - 5) sub-shell including those transferred through the Coster-Kronig (CK) transitions and can be calculated using the equation

$$\sigma_{M_i}^{\tau} = \sigma_{M_i}^{P} + \sum_{k<i} \sigma_{M_k}^{\tau} f_{ki} \quad (2)$$

Where, $\sigma_{M_i}^{P}$ represents the M_i sub-shell proton ionization cross section for a given element at the incident proton energy, E_P.

In the present work, the total M-shell XRP cross sections have been evaluated using Eqns. (1-2). In these evaluations, the proton ionization cross sections based on the DHS model [2] and ECPSSR model [3], the X-ray emission rates based on the Dirac-Fock (DF) model [6], the fluorescence yields and Coster-Kronig transition probabilities based on the DHS model [9] have been used. It may be noted that an inner-shell vacancy can be created through direct ionization by the incident proton or following the decay (radiative / Auger) of the inner-shell vacancy. The incident proton of specific energy simultaneously creates K/L/M shell/sub-shell vacancies in proportion to the ionization cross section of that shell/sub-shell for a given element at that proton energy. The contribution to the production of different Mi (i=1-5) sub-shell vacancies created following decay of the primary K-shell / Li (i=1-3) sub-shell vacancies were found to be <1%.

Two sets of present calculated total M XRP cross sections for 0.4, 1.0 and 2.0 MeV proton impact have been plotted as a function of atomic number (Z) in Fig. 1. These cross sections are found to vary smoothly with the atomic number. These two sets are compared with each other by plotting the ratios of these cross sections, $\boldsymbol{\sigma_{Mtotal}^{ECPSSR}/\sigma_{Mtotal}^{DHS}}$, as a function atomic number (Z) for 0.4, 1.0 and 2.0 MeV proton energies in Fig. 2. The differences between these two sets of the M XRP cross sections for elements with 67≤Z≤92 are found to be ~4-13%.

Recently, Deghfel et al [10] reported semi-empirical values of the total M XRP cross sections for elements with 60≤Z≤92 deduced from the measured cross sections reported up to 2009 by adjusting these to the corresponding values calculated using the ECPSSR model [1] based proton ionization cross sections. The measured total M XRP cross sections reported by different groups considered by Deghfel et al [10] were found to be substantially scattered and also differ significantly from the theoretical XRP cross sections. The present calculated DHS model [2] and ECPSSR model [3] based total M XRP cross sections for some heavy elements are found to differ from those given by Deghfel et al [10] by up to 20% and 32% at energies above 0.6 MeV and the difference increased up to 95% and 75% at energies below 0.6 MeV, respectively.

The total M-shell XRP cross sections based on DHS and ECPSSR have been fitted to polynomials in Z as

$$\sigma_M^X = \sum_n a_n Z^n$$

The fitting Coefficients of the total M XRP cross sections deduced from present calculated DHS model [2] and ECPSSR model [3] based XRP cross sections for incident proton energies ranging 0.4 MeV to 2.0 MeV are given in Tables 1-2. The error in fitting coefficient is <1%.

TABLE I
FITTING COEFFICIENTS FOR TOTAL M-SHELL X-RAY PRODUCTION CROSS SECTIONS

Energy (MeV)	a_0	a_1	a_2	a_3
0.4	13946.9	-441.677	4.73715	-0.01717
0.5	17681.86	-552.047	5.84474	-0.02093
0.6	21637.05	-671.295	7.07466	-0.02525
0.7	24283.49	-741.978	7.70893	-0.02714
0.8	26372.12	-793.199	8.1192	-0.02819
0.9	27599.17	-814.989	8.19692	-0.02799
1.0	28189.4	-814.658	8.0187	-0.0268
1.25	603.3134	247.3718	-5.30712	0.02814
1.5	24990.07	-622.73	5.18657	-0.01431
1.75	22884.39	-527.648	3.97801	-0.00957
2.0	18866.28	-368.89	2.04207	-0.00198

TABLE 2
FITTING COEFFICIENTS FOR TOTAL M-SHELL X-RAY PRODUCTION CROSS SECTIONS BASED ON ECPSSR MODEL

Energy (MeV)	a_0	a_1	a_2	a_3	a_4
0.4	23577.67	-962.128	15.2881	-0.11175	3.15E-04
0.5	31885.69	-1303.2	20.75481	-0.15193	4.29E-04
0.6	18487.34	-545.073	5.45116	-0.01846	
0.7	20648.06	-595.418	5.81665	-0.01921	
0.8	21622.21	-603.26	5.67842	-0.01798	
0.9	21614.96	-577.24	5.15326	-0.01529	
1	20842.67	-525.875	4.35031	-0.01159	
1.25	16925.23	-337.594	1.75428	-4.44E-04	
1.5	11856.67	-124.018	-0.97706	0.01066	
1.75	6773.046	76.90374	-3.42899	0.02025	
2	-6042.53	566.7068	-9.49137	0.04488	

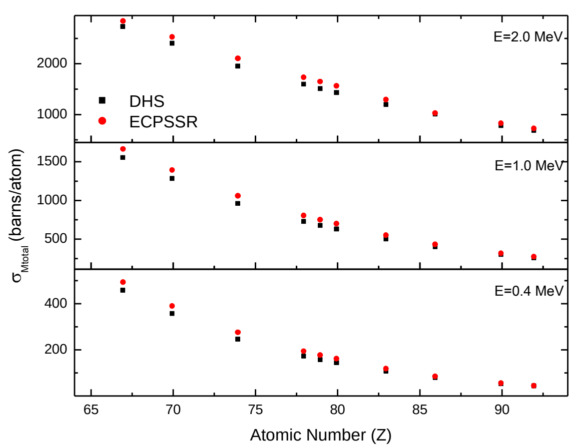

Fig. 1: A typical plot of DHS and ECPSSR model based total M-shell X-ray production cross sections as a function of atomic number (Z).

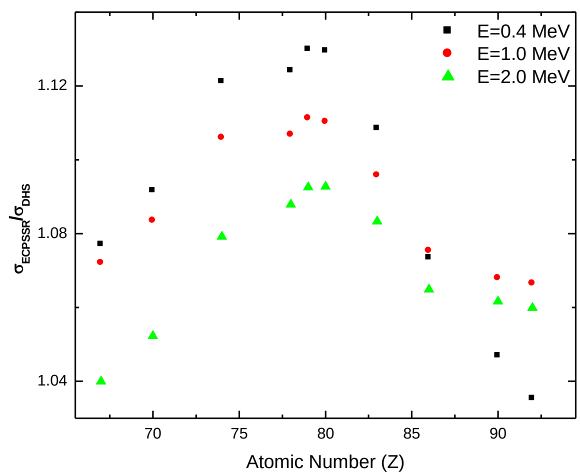

Fig. 2: A typical plot of ratios of $\boldsymbol{\sigma^{ECPSSR}_{Mtotal}}$/ $\boldsymbol{\sigma^{DHS}_{Mtotal}}$ at energy 0.4, 1.0 and 2.0 MeV as a function of atomic number (Z).

REFERENCES

[1] D.D. Cohen and M. Harrigan. (1985, Sept.). *At. Data and Nucl. Data Tables* [online]. *33(2)*, pp. 255-343 Available: http://www.sciencedirect.com/science/article/pii/0092640X8590004X.

[2] M.H. Chen and B. Crasemann. (1985, Sept.). *At. Data and Nucl. Data Tables* [online]. *33(2)*, pp. 217- 233 Available: http://www.sciencedirect.com/science/article/pii/0092640X85900026; *ibid* (1989, March) *41(2)*, pp. 257-285. Available: http://www.sciencedirect.com/science/article/pii/0092640X8990020X.

[3] Z. Liu, S. Cipolla, (1996, Sept.). *Comput. Phys. Communi.* [online] *97(3)*, pp. 315-330 Available: http://www.sciencedirect.com/science/article/pii/0010465596000689 ; S. Cipolla, (2007, Jan.) *Comput. Phys. Communi.* [online] *176(2)*, pp. 157-159 Available: http://www.sciencedirect.com/science/article/pii/S0010465506003195 ; (2009, Sept.)*180(9)*, pp. 1716-1717 Available: http://www.sciencedirect.com/science/article/pii/S0010465509001337 ; (2011, Nov.) *182(11)*, pp. 2439-2440 Available: http://www.sciencedirect.com/science/article/pii/S0010465511002141.

[4] C.P. Bhalla, (1970, Nov.). *J. Phys. B* [online]. *3(7)*, pp. 916-924 Available: http://iopscience.iop.org/article/10.1088/0022-3700/3/7/004/meta

[5] M.H. Chen and B. Crasemann, (1984, July). *Phys. Rev. A* [online]. *30(1)*, pp. 170-176 Available: https://doi.org/10.1103/PhysRevA.30.170

[6] Sanjiv Puri. (2007, Sept.). *At. Data and Nucl. Data Tables* [online]. *93(5)*, pp. 730-741 Available: http://www.sciencedirect.com/science/article/pii/S0092640X07000277.

[7] M.H. Chen, B. Crasemann and H. Mark, (1983, June). *Phys. Rev. A* [online] *27(6)*, pp. 2989-2994 Available: https://doi.org/10.1103/PhysRevA.27.2989

[8] M.H. Chen, B. Crasemann and H. Mark, (1980, Feb.). *Phys. Rev. A* [online] *21(2)*, pp. 449-453 ; https://doi.org/10.1103/PhysRevA.21.449

[9] Y. Chauhan and Sanjiv Puri. (2008, Jan.). *At. Data and Nucl. Data Tables* [online] *94(1)*, pp. 38-49 Available: http://www.sciencedirect.com/science/article/pii/S0092640X07000538.

[10] B. Deghfel, A. Kahoul, S. Kerai, M. Saadaoui, S. Dechoucha, M. Nekkab, (2013, Nov.). *Radiat. Phys. and Chem.* [online] *92,* pp. 32-36 Available: http://dx.doi.org/10.1016/j.radphyschem.2013.06.021 ; *ibid:* (2013, April). *85*, pp. 89-94 Available: http://dx.doi.org/10.1016/j.radphyschem.2013.06.021