Empirical approximation for Lα production cross sections

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The production cross sections for Lα X-ray lines of the elements Z=47-92 induced with protons are given by a simple semi-empirical expression suitable for thick target PIXE applications..

Keywords: L-shells, Lα line, proton-induced cross sections.

INTRODUCTION

For L-shells, the reference cross sections induced by protons equivalent to those for the K shell are not available. The L X-ray production cross sections were published by Orlić and Sow [1], though the averaged ionization cross sections remained unpublished; it was only by personal communication that these values are used in the GUPIX data-base [2]. Averaged L X-ray production cross sections were also published by Reis and Jesus [3]. Since this is still the most complete calculation of the mean L X-ray production cross sections, we make these values more accessible for applications in PIXE algorithms by fitting them to an analytical expression. We shall limit our attention to Lα line only since it is strongest and composed of only two sub lines, and thus most widely used in PIXE analyses.

THE FITTING PROCEDURE

Our approach was from the user's view: the expression should be simple, though accurate and should not necessarily reflect the physical processes beyond ionization and photon emission. The energy range should extend from the lowest energies (occasionally met in thick target integrations) to several MeV; in our case we cut the high energy boundary at 4 MeV. The lowest energies were limited by the values given in [3]. Within this range, the Lα cross sections span over several orders of magnitude, implying that $\ln \sigma_{L\alpha}$ should be fitted as a function of $\ln E_p$. However, such a function did not appear smooth enough to be fitted by a polynomial approximation. By several trials we find that $\ln \sigma_{L\alpha}$ can be well approximated with a rational function of the type
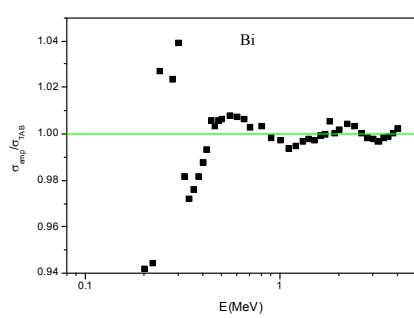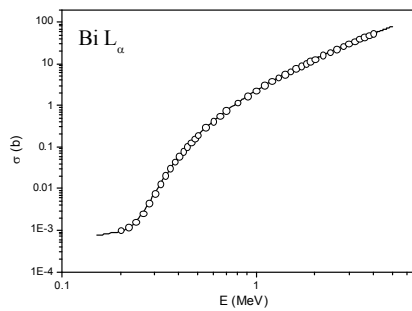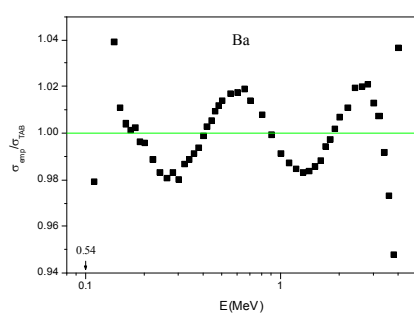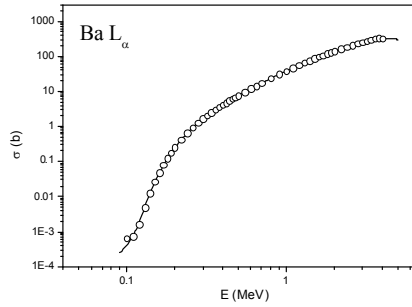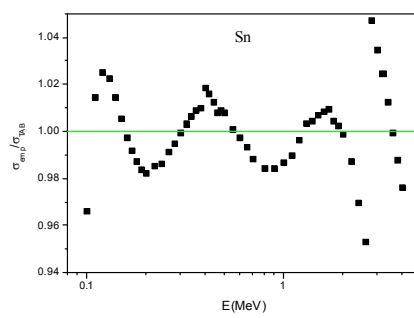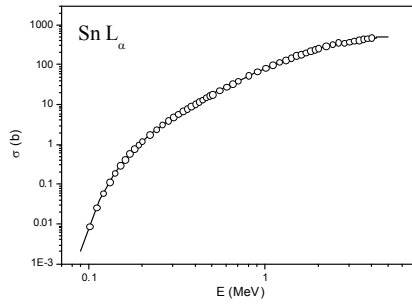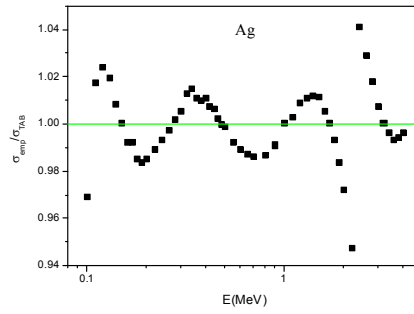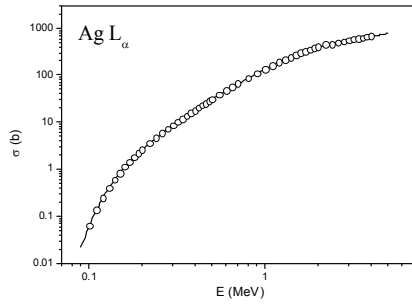
$$\ln \sigma_{L\alpha} = \frac{a_1 + a_2 x + a_3 x^2 + a_4 x^3 + a_5 x^4}{1 + a_6 x + a_7 x^2 + a_8 x^3}$$

$$x = \ln E_p \qquad (1)$$

For the determination of parameters a_1-a_8, eq.(1) was rewritten as a polynomial of x and the coefficients were calculated by the linear least squares procedure. It was also required that the resulting function (1) has a positive derivative at the energy E_m; thus, unreasonably large values that are encountered at low energies required by integration algorithms are avoided. A positive derivative at E_m was not ever obtained. We have therefore forced the positive derivative at E_m by extrapolating one more low-energy point from 2-4 lowest energy data. The evaluated coefficients a_1-a_8 are listed in Table 1.

THE Lα CROSS SECTIONS

The original Lα cross sections and their empirical approximations are shown in Fig. 1 for selected elements. It can be seen that function (1) describes the Lα cross sections well in medium as well as high Z elements. Values for the energies below E_m were calculated by the power approximation $\sigma_{L\alpha} = A E^p$; the parameters A and p were calculated by matching the values and first derivatives at the energy E_m.

FIGURE 1. Mean Lα production cross sections [3] (symbols) and their empirical approximation (this work; line).

FIGURE 2. The ratios between empirical (this work) and tabulated mean [3] Lα cross sections.

The accuracy of the empirical approximation can be inspected in Fig.2, showing the ratio between the empirical and original [3] cross sections. Medium Z elements show an apparent discontinuity of several percent at certain energies; this is a drawback of the original averaging procedure [3] and probably resulted from inefficient matching of cross sections obtained in neighboring energy regions. The empirical cross sections smooth the discontinuity jumps [3] and we believe they contribute to more realistic estimates of the cross section values at these energies.

In general we can state that the accuracy of the fitted values themselves is within several percent and therefore smaller than the uncertainty of the averaged cross sections for the L shells. At the lowest energies of high Z elements, the accuracy of the fit is within 10-20%; however this difference is unimportant in comparison with the cross section uncertainties in this energy region.

COMPARISON WITH THEORY

The reliability of the mean [3] and empirical cross sections can be examined further by comparison with theory. The Lα production cross sections were obtained from the expression
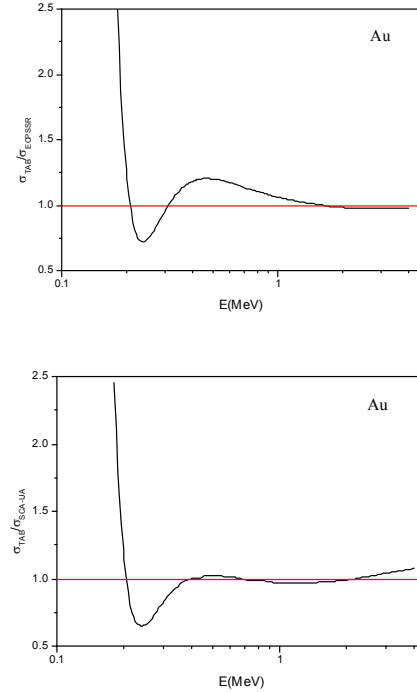
$$\sigma_{L\alpha} = \omega_3 \frac{\Gamma_{L\alpha}}{\Gamma_L}\left(\sigma_{L_3} + f_{23}\sigma_{L_2} + (f_{12}f_{23} + f_{13})\sigma_{L_1}\right) \quad (2)$$

where the Coster-Kronig transition probabilities, fluorescence yields and emission rates were taken from [4,5]. The ionization cross sections for particular subshells were calculated by the ECPSSR theory and for Au (Fig. 3) also by the semiclassical method in the united atom approximation, using screened hydrogenic relativistic wave functions [6]. The impact energies were corrected for projectile motion through the cloud of atomic electrons. The intershell transitions were not considered, as they are generally small for the L_3 subshell, yet the Z_1/Z_2 ratio for proton bombardment of gold is small, i.e. the Coulomb perturbation is weak.

As we see from Fig. 3, the ratios between the mean [3] and theoretical values are rather similar for both theories. The semiclassical method underestimates the experimental values at high energies, as the united atom approximation is no more realistic in this energy range. However, at medium energies it reproduces the experimental values better, probably due to relativistic wave functions. At lowest energies, both theories largely underestimate the experimental data. As the semiclassical approximation reproduces the K shell ionization cross sections at adiabatic collisions quite well, it seems likely that the mean (and therefore empirical) cross sections for the lowest energies are overestimated.

Fig.2 reveals that the differences between empirical and mean [3] cross sections exhibit oscillatory behavior. Inspecting both sets of data normalized to the ECPSSR values, we found that oscillations are generated by the data [3], most probably as a result of the averaging procedure.

FIGURE 3. Comparison of the mean cross sections [3] for gold with the values calculated by the ECPSSR theory and semiclassical approximation.

CONCLUSION

The empirical cross sections reproduce the averaged values [3] within ±5% in the high energy region and within ±10-20% for low energies below 200 keV. The data are currently used in the differential PIXE applications at J. Stefan Institute. The empirical cross sections can be obtained from the authors in a form of Pascal module.

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Z	E_m	a_1	a_2	a_3	a_4	a_5	a_6	a_7	a_8
47	0.10	4.898503	3.547527E-01	-3.721500E-01	7.732714E-01	1.670241E-01	-3.203234E-01	1.304118E-01	1.218532E-01
48	0.10	4.752109	6.182991E-01	-3.501462E-01	6.843359E-01	1.381783E-01	-2.830375E-01	1.170225E-01	1.126196E-01
49	0.10	4.607631	1.523669	2.630126E-01	7.018801E-01	9.830487E-02	-1.039133E-01	1.778827E-01	1.099986E-01
50	0.10	4.404419	1.362241	-3.032861E-01	3.925085E-01	5.880445E-02	-1.349800E-01	6.316011E-02	7.506961E-02
51	0.10	4.277624	2.276331	-3.672454E-01	-1.096579E-01	-2.440566E-02	7.070853E-02	-4.747590E-02	1.422895E-02
52	0.10	4.148919	3.048404	-5.157218E-01	-6.439041E-01	-1.040291E-01	2.569495E-01	-1.755723E-01	-5.153612E-02
53	0.10	4.017226	3.279529	-6.109841E-01	-8.745083E-01	-1.369658E-01	3.177048E-01	-2.377566E-01	-8.062063E-02
54	0.10	3.887220	3.330671	-1.820855E-01	-6.289307E-01	-1.397739E-01	3.281807E-01	-1.514658E-01	-5.680211E-02
55	0.10	3.767396	3.175614	-6.429971E-01	-8.999458E-01	-1.459589E-01	2.977319E-01	-2.577276E-01	-8.698145E-02
56	0.10	3.639672	3.308349	-3.565256E-01	-7.878564E-01	-1.495422E-01	3.371391E-01	-2.143711E-01	-7.945519E-02
57	0.20	3.539067	5.100246	1.979739	-8.103348E-03	-9.869021E-02	8.384513E-01	1.517252E-01	-1.458032E-02
58	0.20	3.430015	5.078417	2.026523	-6.300955E-04	-1.047996E-01	8.507710E-01	1.552468E-01	-1.616818E-02
59	0.10	3.322042	6.661996	4.301454	7.772842E-01	-8.119332E-02	1.336313	5.233733E-01	4.670094E-02
60	0.10	3.215719	5.261464	2.466313	1.529103E-01	-1.073505E-01	9.463775E-01	2.234878E-01	-6.981335E-03
61	0.10	2.914744	6.430212	4.543802	9.340272E-01	-6.466147E-02	1.393707	5.691921E-01	5.612831E-02
62	0.10	2.989290	4.966970	2.227109	4.546878E-02	-1.310937E-01	9.050406E-01	1.748073E-01	-2.241477E-02
63	0.10	2.886583	5.079330	2.503707	1.531510E-01	-1.300709E-01	9.669167E-01	2.213198E-01	-1.560356E-02
64	0.10	2.728258	3.956074	8.665189E-01	-4.106764E-01	-1.306744E-01	5.829586E-01	-4.091989E-02	-5.163234E-02
65	0.11	2.626637	3.808569	6.498583E-01	-5.178067E-01	-1.329489E-01	5.410167E-01	-8.917854E-02	-6.208447E-02
66	0.12	2.529727	3.936101	9.287917E-01	-4.169241E-01	-1.389463E-01	6.005896E-01	-4.354374E-02	-5.661350E-02
67	0.13	2.420205	3.731062	6.042610E-01	-5.751007E-01	-1.421938E-01	5.344407E-01	-1.141200E-01	-7.140403E-02
68	0.13	2.321323	3.757475	7.264955E-01	-5.277411E-01	-1.508801E-01	5.575353E-01	-9.525407E-02	-7.089181E-02
69	0.13	2.217725	3.958994	1.154219	-3.655305E-01	-1.378590E-01	6.591456E-01	-2.122017E-02	-5.725989E-02
70	0.14	2.110463	4.432132	2.141861	-4.342804E-03	-1.351812E-01	8.981112E-01	1.496797E-01	-3.096775E-02
71	0.14	2.011636	3.830094	1.054452	-4.345751E-01	-1.525820E-01	6.390103E-01	-5.278480E-02	-6.901826E-02
72	0.15	1.908833	3.770910	1.010948	-4.582106E-01	-1.540977E-01	6.301268E-01	-6.586978E-02	-7.364605E-02
73	0.15	1.806299	4.126691	1.881340	-7.459184E-02	-1.303425E-01	8.382727E-01	1.049638E-01	-4.061338E-02
74	0.16	1.712144	3.770396	1.162287	-4.126735E-01	-1.531179E-01	6.698087E-01	-4.641149E-02	-7.386025E-02
75	0.16	1.619135	3.823604	1.399038	-3.050731E-01	-1.567534E-01	7.259849E-01	-2.287164E-03	-6.883879E-02
76	0.16	1.521691	3.927993	1.806856	-1.070850E-01	-1.536836E-01	8.255575E-01	7.977208E-02	-5.615646E-02
77	0.17	1.441201	3.579448	9.093106E-01	-5.828814E-01	-1.478096E-01	6.165066E-01	-1.216337E-01	-9.291344E-02
78	0.17	1.326967	4.115541	2.708425	3.962304E-01	-1.206399E-01	1.053398	2.844008E-01	-1.739988E-02
79	0.18	1.230686	4.079444	2.816018	4.711355E-01	-1.103350E-01	1.086876	3.131279E-01	-1.208092E-02
80	0.18	1.130741	4.086305	3.102865	6.537172E-01	-9.399960E-02	1.166311	3.868644E-01	2.738898E-03
81	0.19	1.042860	2.337357	-3.109484	-3.185670	-5.509299E-01	-4.194552E-01	-1.211543	-3.923109E-01
82	0.19	9.274851E-01	4.051863	3.601433	1.008399	-2.659340E-02	1.315627	5.347715E-01	4.172059E-02
83	0.20	8.259017E-01	3.870061	3.215495	7.804260E-01	-6.265270E-02	1.224079	4.389870E-01	1.432686E-02
84	0.20	7.243114E-01	3.737436	2.967037	6.245814E-01	-7.442007E-02	1.167692	3.763433E-01	-1.598897E-03
85	0.20	6.210497E-01	3.555811	2.339068	1.513570E-01	-1.276779E-01	1.005547	1.872925E-01	-5.198805E-02
86	0.20	5.162365E-01	3.563133	2.797813	5.030461E-01	-5.952276E-02	1.139664	3.361370E-01	-8.930910E-03
87	0.20	3.962714E-01	4.133014	8.477692	4.767858	5.474218E-01	2.771241	2.121718	4.769469E-01
88	0.20	3.048181E-01	3.501932	3.908199	1.413833	9.249525E-02	1.482711	7.194082E-01	9.770978E-02
89	0.20	1.967792E-01	3.389175	3.882432	1.385853	9.628467E-02	1.487961	7.151137E-01	9.671545E-02
90	0.20	8.847940E-02	3.317614	5.038204	2.339789	2.913238E-01	1.854433	1.131822	2.275680E-01
91	0.20	-7.137171E-03	3.171958	4.583033	2.035429	1.894222E-01	1.732239	9.950288E-01	1.748973E-01
92	0.20	-1.056873E-01	3.075308	3.685892	1.276430	8.410639E-02	1.467251	6.826292E-01	8.385065E-02

TABLE 1
Coefficients a_i for the empirical Lα cross sections; E_m (in MeV) limits validity of the fit at lowest energies.