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Measurement of $K\alpha$ and $K\beta$ fluorescence cross sections for elements in the range $44\leqslant Z\leqslant 68$ at 59.5 keV

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The $K\alpha$ and $K\beta$ x-ray fluorescence cross sections have been measured for elements in the range $44\leqslant Z\leqslant 68$ at an excitation energy of 59.5-keV γ ray from ^{241}Am radioisotope with a Si(Li) detector. A reasonable agreement is found between the present experimental results and the theoretically calculated values based on photoionization cross sections by Scofield using Hartree-Slater and Hartree-Fock central potential theory. [S1050-2947(99)03409-5]

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I. INTRODUCTION

Information regarding the experimental values of K x-ray fluorescence (XRF) cross sections for different elements at various photoionization energies is important because of its wide use in atomic, molecular, and radiation physics and in the nondestructive elemental analysis of materials using energy-dispersive x-ray fluorescence. On the other hand, accurate knowledge of cross section data makes XRF very suitable for quantitative elemental analysis.

Several attempts have been made for measuring XRF cross sections and yields. Kraus *et al.* [1] have calculated theoretically K and L XRF cross sections but there have been few reports on experimental measurements of XRF cross sections. Bahn, Chaturvedi, and Nah [2] determined K-shell cross sections for ten elements with $18\leqslant Z\leqslant 48$ at two excitation energies from ^{109}Cd and ^{125}I radioisotopes. Garg *et al.* [3] measured $K\alpha$ and $K\beta$ cross sections at ten excitation energies ranging from 5.9 to 59.54 keV for elements with $20\leqslant Z\leqslant 56$.

In recent years, K-shell fluorescence yields and cross sections for several elements have been measured by many authors [4–10]. Durak *et al.* [6] have measured K-shell fluorescence cross sections for some elements with $40\leqslant Z\leqslant 70$ at 122-keV incident photon energy. Rao, Cesareo, and Gigante [8] have reported some measurements of K XRF cross sections for low-Z elements at low excitation energies. Puri *et al.* [11] have calculated K and L shell x-ray fluorescence cross sections for elements with $13\leqslant Z\leqslant 92$ and $35\leqslant Z\leqslant 92$, respectively, at 1–200-keV incident photon energy range.

In this paper $K\alpha$ and $K\beta$ XRF cross sections are measured for the elements with $44\leqslant Z\leqslant 68$ at the excitation energy 59.537 keV of ^{241}Am radioisotopes. The experimental results are compared with theoretical values.

II. EXPERIMENTAL PROCEDURES

The experimental arrangement and geometry used in the present measurements are shown in Fig. 1. In this arrangement low-energy photon sources of ^{241}Am (100 mCi) were used, and the energy of the primary photons are 59.537 keV for ^{241}Am. Spectroscopically pure (purity better than 99.9%) samples of thickness ranging from 20–55 mg/cm^{-2} have been used for the measurements. The K x-ray spectra from various materials were recorded with the collimated Si(Li) detector with an active area of 12.5 mm^2, sensitive crystal depth of 3.5 cm, and a Be window of 2.5-mm thickness coupled to a 1024 channel ND 66B analyzer through a spectroscope amplifier. The energy resolution of the Si(Li) detector was 190-eV full width at half maximum at 5.9 keV (^{55}Fe). In order to reduce the statistical error in the measurements, three sets of observations were taken for each target for time intervals ranging from 1000–10 000 s. For the overlapped peaks, net peak areas were determined with the method developed in our earlier publication [12]. A typical x-ray spectra of Dy is shown in Fig. 2.

III. DATA ANALYSIS

Calculation of the K XRF cross sections. The theoretical K x-ray fluorescence cross sections σ_{Ki} were calculated using the fundamental parameter equation

$$\sigma_{Ki}=\sigma_K^P(E)\,\omega_K f_{Ki} \quad (i=\alpha,\beta), \tag{1}$$

where $\sigma_K^P(E)$ is the K-shell photoionization cross section for the given elements at excitation energy E, ω_K is the fluorescence yields of the K-shell line, f_{Ki} is the fractional ratio of the Ki x-rays, and $f_{K\alpha}$ and $f_{K\beta}$ are defined as

$$f_{K\alpha}=[1+I_{K\beta}/I_{K\alpha}]^{-1},$$

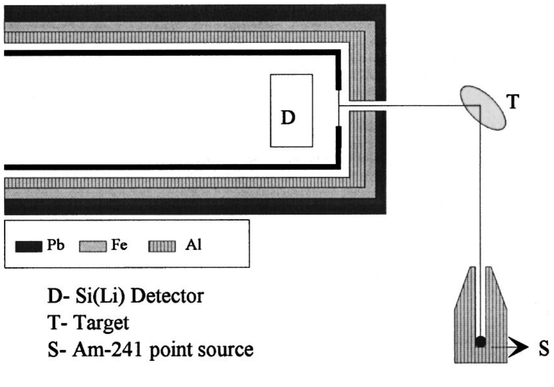

FIG. 1. Experiment setup.

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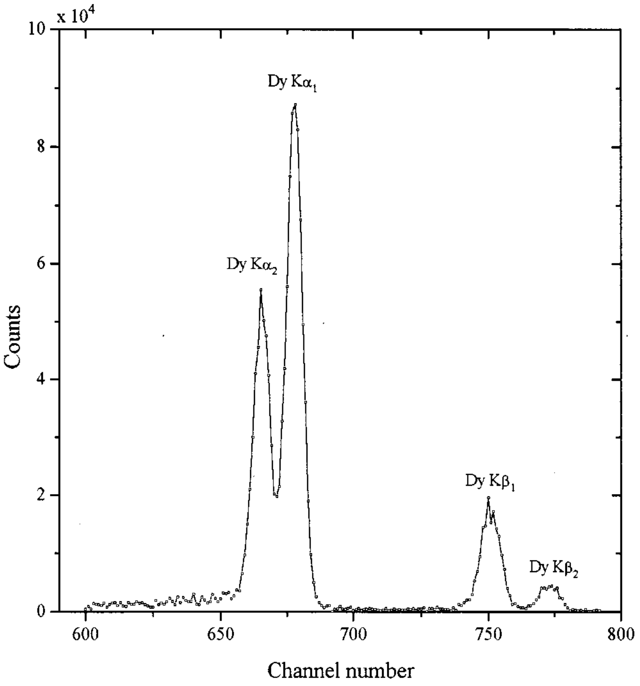

FIG. 2. K x-ray spectrum of Dy excited by 59.537 keV.

$$f_{K\beta}=[1+I_{K\alpha}/I_{K\beta}]^{-1}, \tag{2}$$

where $I_{K\beta}/I_{K\alpha}$ is the $K\beta$ to $K\alpha$ x-ray intensity ratio.

In the present calculations, the values of $\sigma_K^P(E)$ were taken from Scofield [13] based on Hartree-Slater (HS) potential theory and the values of ω_K were taken from an annotated bibliography by Hubbel *et al.* [4]. Two sets of values of $I_{K\beta}/I_{K\alpha}$ intensity ratios were used for the evaluation of theoretical K XRF cross sections, one based on HS theory [14] and the other on Hartree-Fock (HF) theory [15].

Measurement of the K XRF cross sections. The experimental K x-ray fluorescence cross sections σ_{Ki} for a given element were evaluated using the equation

$$\sigma_i=\frac{N_{Ki}}{I_0 G \varepsilon_K \beta_{Ki} t} \quad (i=\alpha,\beta), \tag{3}$$

where N_{Ki} is the number of counts per unit time under Ki x-ray peak of the given elements, I_0G is the intensity of exciting radiation falling on the sample, ε_{Ki} is the detector efficiency for the K x rays, t is the mass in g/cm^{-2} of the element, and β_{Ki} is the target self-absorption correction for both the incident and the emitted characteristic x-rays radia-

TABLE I. $K\alpha$ and $K\beta$ XRF cross sections.

	$\sigma_{K\alpha}$ (barns)				$\sigma_{K\beta}$ (barns)			
Element-Z	Expt.	Fitted	Theor.[a]	Theor.[b]	Expt.	Fitted	Theor.[a]	Theor.[b]
Ru-44	467± 33	469	447		93± 8	90	84	
Rh-45		514	496			102	95	
Pd-46	562± 39	563	545		114±10	114	105	
Ag-47	c	616	596	588	123±11	128	117	125
Cd-48	660± 38	668	650		139±12	142	130	
In-49	739± 54	725	706		162±15	157	143	
Sn-50	773± 56	785	765	755	164±15	172	158	168
Sb-51	846± 63	847	827	816	191±17	189	173	185
Te-52	c	913	891		215±17	206	190	
I-53	994± 73	981	958		231±21	224	208	
Xe-54		1052	1026	1012		243	226	240
Cs-55	1139± 85	1126	1097		268±25	263	246	
Ba-56	1200± 86	1202	1173	1158	291±27	283	267	282
La-57	1258± 91	1282	1251		298±27	304	288	
Ce-58	c	1364	1337		323±30	326	310	
Pr-59	1468± 88	1449	1418		355±32	349	331	
Nd-60	1539± 93	1537	1504	1486	382±35	377	354	378
Pm-61		1628	1592			397	378	
Sm-62	1724±105	1722	1678		414±36	422	401	
Eu-63	c	1818	1774	1753	446±36	448	427	447
Gd-64	1882±112	1917	1869	1847	462±37	475	453	475
Tb-65	2025±118	2019	1968	1946	512±40	503	479	501
Dy-66	2088±120	2124	2063		517±39	531	505	
Ho-67	2278±132	2232	2218		580±43	560	546	
Er-68	c	2342	2301	2276	594±47	590	570	594

[a] Values calculated using $I_{K\beta}/I_{K\alpha}$ based on HS theory [14].

[b] Values calculated using $I_{K\beta}/I_{K\alpha}$ based on HF theory [15].

[c] The $K\alpha$ x rays of these elements were utilized to evaluate the $I_0G\epsilon_K$ values.

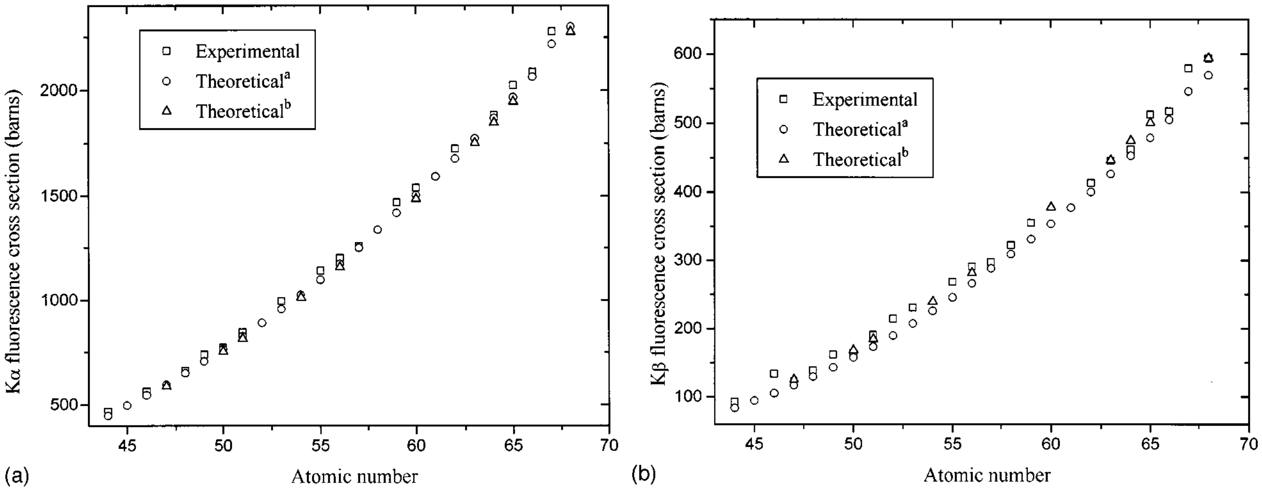

FIG. 3. (a) $K\alpha$ x-ray fluorescence cross sections. (b) $K\beta$ x-ray fluorescence cross sections.

tion. The values of β_{Ki} have been calculated by using the following expression obtained by assuming that the fluorescent x rays have a normal incidence to the detector:

$$\beta_K = \frac{1-\exp[-(\mu_{\mathrm{inc}}/\cos\theta_1+\mu_{\mathrm{emt}}/\cos\theta_2)t]}{(\mu_{\mathrm{inc}}/\cos\theta_1+\mu_{\mathrm{emt}}/\cos\theta_2)t}, \qquad (4)$$

where μ_{inc} and μ_{emt} are the total attenuation coefficients [16] at primary and emitted x-ray photon energies, respectively. $\theta_1(=45)$ and $\theta_2(=45)$ are the angles with the sample normal primary and emitted K x rays. The effective incident photon flux elements $I_0G\varepsilon_K$ was evaluated by measuring the K x-ray fluorescence cross sections from Mo, Ag, Te, Ce, Eu, and Er in the same geometry. The weighted average of the $I_0G\varepsilon_K$ values obtained from different samples was taken. The errors in the efficiency values in this energy are estimated to be less than 3%.

IV. RESULTS AND DISCUSSION

The K x-ray fluorescence cross sections of the elements in the atomic range $44 \leqslant Z \leqslant 68$ are listed in Table I. They are plotted as a function of the atomic number in Fig. 3. It can be seen from Table I and Fig. 3 that the present values are in good agreement within the experimental uncertainties with theoretical values calculated using emission rates (f_{Ki}) based on HF theory and HS potential theory. In addition, these experimental values were fitted to a second-order polynomial and are listed in Table I found values for the fluorescence cross sections. The overall error in the measured $K\alpha$ and $K\beta$ XRF cross sections are estimated to be less than 7% and 9%, respectively. These errors are attributed to the uncertainties in the different parameters using the Eq. (2). The error in the evaluation of area under the $K\alpha$ and $K\beta$ x-ray peak is about 1% and 3%, respectively [12]; the error in $I_0G\varepsilon_K$ is less than 3%, the error in the target thickness measurements is on the order of 2%, and the error in the absorption correction β is less than 2%. The uncertainty in the area of the K x-ray peak was evaluated by the weighted average method.

As a result, the present agreement between the theoretical and the present experimental values leads to the conclusion that the data presented here will benefit those using radioisotope XRF technique for elemental analysis.

[1] M. O. Krause, C. W. Jr. Nestor, C. J. Jr. Sparks, and E. Ricci, Oak Ridge National Laboratory Report No. ORNL-5399, 1978 (unpublished).
[2] C. Bahn, S. N. Chaturvedi, and N. Nah, X-Ray Spectrom. **10**, 128 (1981).
[3] M. L. Garg, D. Matha, S. Kumar, P. C. Mangal, and P. N. Trehan, X-Ray Spectrom. **14**, 165 (1985).
[4] J. H. Hubbell, P. N. Trehan, N. Singh, B. Chand, D. Metha, M. L. Garg, R. R. Garg, S. Singh, and S. Puri, J. Phys. Chem. Ref. Data **23**, 339 (1994).
[5] R. Durak, Phys. Scr. **58**, 111 (1998).
[6] R. Durak, S. Erzeneoğlu, Y. Kurucu, and Y. Sahin, Radiat. Phys. Chem. **51**, 45 (1998).
[7] Ö. Şimşek, Phys. Scr. **58**, 235 (1998).
[8] D. V. Rao, R. Cesareo, and G. E. Gigante, X-Ray Spectrom. **22**, 406 (1993).
[9] R. Durak and Y. Şahin, Phys. Rev. A **57**, 2578 (1998).
[10] E. Casnati, C. Baraldi, and A. Tartari, Phys. Rev. A **44**, 1699 (1991).
[11] S. Puri, B. Chand, T. D. Mehta, M. L. Garg, N. Singh, and P. N. Trehan, At. Data Nucl. Data Tables **61**, 289 (1995).
[12] Y. Şahin, A. Karabulut, and G. Budak, Appl. Spectrosc. Rev. **31**, 333 (1996).
[13] J. H. Scofield, Lawrence Livermore Laboratory Report No. UCRL-51326, 1973 (unpublished).
[14] J. H. Scofield, At. Data Nucl. Data Tables **14**, 121 (1974).
[15] J. H. Scofield, Phys. Rev. A **9**, 1041 (1974).
[16] J. H. Hubbell and S. M. Seltzer, National Institute of Standards and Technology Center for Radiation Research, Document No. NISTIR 5632 (1995) (unpublished).