K-shell x-ray production cross sections for 1.0–4.4-MeV α particles on selected thin targets of Z = 22-34

C. G. Soares,* R. D. Lear, J. T. Sanders, and H. A. Van Rinsvelt Department of Physics and Astronomy, University of Florida, Gainesville, Florida 32611

(Received 28 October 1975)

K-shell x-ray production cross sections for 1.0-4.4 MeV α particles have been measured. The elements selected were Ti, V, Mn, Fe, Co, Ni, Cu, Zn, Ge, and Se, and all data were for thin targets evaporated onto thin carbon backings. The measured cross sections are compared with predictions of the plane-wave Born approximation (PWBA), the PWBA with binding-energy and trajectory corrections, and the binary-encounter approximation. It is found that the PWBA with both corrections fits the data best for all elements and energies considered.

I. INTRODUCTION

A large amount of recent literature has been devoted to the measurement of x-ray production cross sections¹⁻³ and to the descriptions of the various theoretical models which are applicable to the results. The research reported here has been motivated by an interest in the use of these cross sections as applied to trace element analysis in environmental and biomedical samples. The use of xray production cross sections for quantitative analysis work has become more important in recent years,⁴ and it is hoped that with the availability of reliable x-ray cross-section measurements, this very sensitive and inclusive method can be extended to do accurate quantitative studies routinely.

The energy range used in such analysis work is that commonly available from low-energy particle accelerators, i.e., 1-5 MeV. α particles have been chosen since there is already a wealth of data for protons in this energy range^{1-3, 5-12} and since α particles are also being used for x-ray trace-element emission studies.¹³ The values measured here are compared with overlapping earlier measurements,^{2,14-16} and also with results predicted by several theoretical models. These include the plane-wave Born approximation (PWBA) with various corrections, and the binary-encounter approximation (BEA).

II. EXPERIMENTAL PROCEDURE AND DATA REDUCTION

Well-collimated (2.5 mm diameter) beams of ⁴He ions were obtained from the University of Florida's 4-MV Van de Graaff accelerator. The normal to the targets was oriented at 22.5° with respect to the incident beam, and the beam was monitored using a Faraday cup. The targets of $3-30 \ \mu g/cm^2$ thickness were evaporated onto $10-30-\mu g/cm^2$ -thick carbon backings. The various target thicknesses are shown in Table I. Target thicknesses were determined using Rutherford scattering measured at 135° relative to the beam axis, in the vertical plane. The scattered particles were detected by a silicon surface barrier detector collimated to 1.5×10^{-3} sr, as measured with a calibrated ²⁴¹Am α source.

The x rays produced were detected by a KEVEX Si(Li) detector with an 80 mm² active area, located at 135° to the beam direction in the horizontal plane. The collimated beam of x-rays passed through the 0.025-mm-thick Mylar window of the scattering chamber, a short (<5 mm) air path, and into the detector through a 0.025-mm-thick beryllium window.

Pulses from both detectors were amplified and then stored and analyzed by an 1830 General Automation on-line computing facility, which was also used for the analysis of the data. Beam current was kept low (<60 nA) so that dead-time corrections were less than 1%.

The number of x rays, N_x , under the peaks of

TABLE I. T	arget thicknesses,	determined usin	ıg
Rutherford sca	attering measured a	at 135° relative t	o the
beam axis, in	the vertical plane.		

Element	Target thickness (µg/cm ²)		
Ti	5.8 ± 0.6		
V	3.8 ± 0.4		
Mn	4.5 ± 0.5		
Fe	2.6 ± 0.3		
Co	25 ± 3		
Ni	9.8 ± 1.0		
Cu	30 ± 3		
Zn	12 ± 1		
Ge	28±3		
Se	6.9 ± 0.7		

13

953

interest for a particular run is given by

$$N_{x} = N_{p} N_{t} \epsilon \sigma_{x}, \qquad (1)$$

where N_p is the number of the incident particles, N_t is the number of target atoms per unit area, ϵ is the absolute detector efficiency corrected for solid angle and absorption, and σ_x is the K-shell x-ray production cross section. The absolute detector efficiency was determined in the standard manner^{17,18} using calibrated radioactive sources of ⁵¹Cr, ⁵⁷Co, ⁶⁵Zn, and ²⁴¹Am, located at the actual beam-spot position. The target thickness N_t was determined by the elastic scattering as given by

$$N_t = \frac{N_c}{\left(d\sigma / d\Omega \right) N_p \Omega} . \tag{2}$$

Here, N_c is the number of particles scattered in the particle detector, $d\sigma/d\Omega$ is the differential scattering cross section, and Ω is the solid angle of the particle detector. Substitution of Eq. (2) into Eq. (1) gives the following expression for the xray production cross section:

$$\sigma_x = \frac{N_x}{N_c} \frac{\Omega}{\epsilon} \frac{d\sigma}{d\Omega} .$$
(3)

If x-ray and charged-particle data are taken simultaneously, σ_x is independent of the actual projectile number. This eliminates the need for corrections due to the equilibrium charge state of the beam.

All theories given predict the ionization cross section (σ_I), while the experimentally measured quantity is the x-ray production cross section (σ_x). For K-shell measurements, these two quantities are related to the K-shell fluorescence yield (ω_k) by the relation

$$\sigma_I = \sigma_x / \omega_k$$
.

The values of McGuire¹⁹ as tabulated by Bambynek *et al*.²⁰ are used to calculate the x-ray production cross sections for the various models. All calculations shown in this work were performed with the computer code $XCODE^{21}$ which includes data tables cited in these references.

The spectra obtained were very clean, with low background, and were easily summed to give spectral-line intensities. The number of counts in the peaks was always such as to give 1% statistics in the raw sum, and 3% accuracy was estimated in all background subtractions. Further contributions to the uncertainty in the measured cross sections were from errors in the Rutherford cross section due to geometrical uncertainties and possible projectile charge effects, as a nucleus-nucleus interaction with no screening effect was assumed for the Rutherford cross section calculation. Also, an 8% uncertainty in the strengths of calibrated sources used in this experiment contributed to an over-all 10% error in the efficiency curve. Thus, combining these errors, the total uncertainty in the cross sections was estimated to be of the order of 15%.

III. THEORY

Several theories were used to compare to the data. The plane-wave Born approximation (PWBA)²²⁻²⁶ is a quantum-mechanical treatment of the inner-shell ionization problem using first-or-der perturbation theory. Projectiles are assumed to be point charges traveling at high velocities which leads to the use of plane waves to describe the projectiles. The interaction is assumed to be Coulombic in nature, with initial- and final-state wave functions taken to be those of bound atomic states and initial bound states with one electron in the continuum, respectively. The projectile is assumed to be far from the electron when ionization occurs; so nonrelativistic hydrogenic wave func-tions may be used for bound states.

Two major corrections have been applied to the above PWBA calculations which apply to the energy range considered in this work (1.0-4.4 MeV). The major effect arises from the increased binding of the inner-shell electrons owing to the presence of the projectile charge within the electron orbital radius.²⁷⁻³⁰ The other correction is due to the Coulomb deflection of the incident particle caused by the target nucleus, as first developed in the semiclassical approach by Bang, Hansteen, and Mosebekk.^{31,32} A quantum-mechanical treatment²⁸ shows that the correction is more important for low-energy projectiles and high-Z targets. In the range Z = 22 - 34 and projectile energy 1.0-4.4 MeV, the trajectory correction is always much less than the binding-energy correction. The corresponding theory, when both corrections are applied, is denoted by PWBABC.

The binary-encounter approximation (BEA) is a semiclassical treatment of the inner-shell ionization problem.^{33,34} The mechanism is a Coulombic interaction between two free particles with the electron velocity determined by the interaction with the nucleus and electrons of its atom. The cross section is then an average of the free-particle ionization cross sections over all possible energy exchanges and all possible electron velocities, where the velocity distribution is given by the square of the momentum-space wave function for the particular atomic state.³⁵⁻³⁷

No consideration was given to multiple ionization effects, although such effects have been shown to be present.³⁸ These may affect the cross sections and especially the fluorescent yields; however in-

clusion of such effects must await further theoretical developments.

IV. DISCUSSION OF RESULTS

The measured K-shell x-ray production cross sections from this experiment are tabulated in Table II and plotted in Figs. 1 and 2. Also shown in these figures are the predictions of the PWBA, the BEA, and the PWBA with binding energy and trajectory corrections (PWBABC). In addition, results of available earlier measurements are plotted. These include a partial use of measurements from Ref. 15 which cover energies up to 2.5 MeV over a wide range of targets as well as the results of the measurements from Ref. 14 for Ni, Cu, Fe, and Co and those of Ref. 2 for Ti, Mn, Zn, and Se. Finally, thin-target ionization cross sections for 1-5-MeV ⁴He bombardment of Fe and Cu as given in Ref. 16 have been converted to x-ray production cross sections using the fluorescent yields previously cited. As is seen, all previous results except those of Ref. 2 agree within the experimental error. The reproducibility of measurements of

this kind is very encouraging, particularly if we consider the wide range of targets and projectile energies covered by the data. While all theories appear to reproduce the general shape of the data, all but the PWBABC overpredict the cross section for all targets and energies reported here. It is also noted that the PWBABC seems to underpredict the data at low energy for all targets, while tending to overpredict the higher energies for the higher-Z elements. It has been suggested³⁹ that relativistic effects in the K-shell electron velocity could be important for the higher-Z elements; however, it has been noted that including relativistic wave functions³⁹ in the theory will only tend to raise the predicted cross sections. These effects have yet to be formally applied to the theory.

In conclusion, although minor discrepancies still remain, the Born approximation with binding-energy and Coulomb-deflection corrections is the most successful model for predicting experimental thin-target x-ray production cross sections. These results give one enough confidence to attempt using these values for trace-element analysis applications.

TABLE II. K-shell x-ray production cross sections (in barns).

E_{α} (MeV)	Ti Z = 22	V Z=23	Mn Z = 25	Fe $Z = 26$	Co Z = 27	Ni Z=28	Cu Z=29	Zn Z=30	Ge Z= 32	Se Z = 34
1.0	2.63	1.21	0.814	0.453	0.399	0.207	0.201	0.104	0.0676	0.0303
1.1	3.37	•••	1.02	•••	0.619	•••	0.270	•••	0.0908	0.0482
1.3	5.43	• • •	1.66	•••	0.975	•••	0.464	•••	0.161	0.0736
1.5	7.80	•••	2.50	•••	1.47	•••	0.709	•••	0.262	0.121
1.7	11.5	•••	3.54	• • •	2.12	•••	1.02	• • •	0.389	0.186
1.9	18.3	• • •	6.27	•••	3.39	•••	1.85	•••	0.630	0.295
2.1	22.8	• • •	•••	•••	•••	•••	2.81	•••	1.05	0.386
2.2	30.6	19.7	10.8	7.48	5.31	3.95	3.02	2.11	1.11	0.665
2.3	34.9	22.6	12.3	8.66	6.00	4.52	3.38	2.38	1.30	0.801
2.4	40.2	25.9	13.5	9.86	6.80	4.97	3.74	2.68	1.48	0.887
2.5	45.1	29.6	16.1	11.0	7.83	5.80	4.22	3.05	1.66	0.943
2.6	46.7	29.6	15.9	11.7	9.69	6.66	4.70	3.39	1.83	1.12
2.7	56.7	37.0	19.8	14.1	9.86	7.32	5.45	3.94	2.17	1.30
2.8	63.8	41.5	22.2	15.9	11.1	8.21	6.12	4.44	2.42	1.48
2.9	70.1	45.4	24.7	17.9	12.3	9.08	6.84	5.01	2.73	1.62
3.0	77.5	50.0	28.8	19.3	13.6	10.2	7.67	5.58	2.96	1.76
3.1	84.6	55.1	30.1	21.5	14.8	11.0	8.32	6.24	3.28	1.89
3.2	90.8	59.3	31.9	23.4	16.2	12.0	8.99	6.42	3.68	2.11
3.3	100	64.6	35.3	26.5	17.9	13.4	9.80	7.11	4.08	2.62
3.4	111	68.6	38.4	29.9	19.7	14.6	10.8	7.74	4.54	3.15
3.5	119	77.1	42.5	33.3	21.6	16.1	12.1	8.44	5.17	2.84
3.6	123	83.7	46.0	35.9	23.1	17.6	13.5	9.42	5.56	3.41
3.7	134	90.1	49.4	38.9	25.2	19.2	14.6	10.4	5.91	3.56
3.8	146	97.0	54.3	41.4	27.2	20.9	15.9	11.3	6.49	3.87
3.9	158	105	55.7	47.7	29.5	21.7	16.7	11.4	6.92	4.26
4.0	169	112	62.0	49.4	32.2	24.3	18.5	12.3	7.59	4.92
4.1	175	111	67.4	52.1	34.0	26.1	19.7	14.3	8.04	5.08
4.2	190	125	71.9	56.6	36.9	28.1	21.5	15.4	8.72	5.90
4.3	204	136	77.6	60.0	39.2	29.7	22.7	16.5	9.17	5.76
4.4	203	138	83.6	61.2	43.5	32.4	25.7	18.1	10.0	5.81



FIG. 1. Measured K-shell x-ray production cross sections and predictions of the PWBA, PWBABC, and BEA for α -particle bombardment of Fe, Ge, Co, and Se.

ACKNOWLEDGMENTS

We would like to thank Professor Tom Gray and his associates at North Texas State University for making data available to us prior to their publication and also for the loan of some calibrated radioactive sources. Also we would like to thank Dr. G. Pepper for use of the computer code XCODE to carry out the theoretical calculations used in this work, and Dr. Louis Brown for the loan of some of the target materials.



FIG. 2. Measured K-shell x-ray production cross sections and predictions of the PWBA, PWBABC, and BEA for α -particle bombardment of Ti, Ni, V, Cu, Mn, and Zn.

¹J. D. Garcia, R. J. Fortner, and T. M. Kavanagh, Rev. Mod. Phys. 45, 111 (1973).

^{*}Present address: National Bureau of Standards, Washington, D. C. 20234.

- ²J. Lin, J. L. Duggan, and R. F. Carlton, in Proceedings of the International Conference on Inner-Shell Ionization Phenomena and Future Applications, Atlanta, Georgia, 1972, edited by R. W. Fink, S. T. Manson, J. M. Palms, and P. V. Rao, CONF-720404 (Natl. Tech. Information Service, Dept. of Commerce, Springfield, Va., 1973), p. 998.
- ³C. H. Rutledge and R. L. Watson, At. Data Nucl. Data Tables <u>12</u>, 195 (1973).
- ⁴T. B. Johansson, R. E. Van Grieken, J. W. Nelson, and J. W. Winchester, Anal. Chem. <u>47</u>, 855 (1975).
- ⁵R. C. Bearse, D. A. Close, J. J. Malanify, and C. J. Umbarger, Phys. Rev. A 7, 1269 (1973).
- ⁶G. A. Bissinger, J. M. Joyce, E. J. Ludwig, W. S. Mc-Ever, and S. M. Shafroth, Phys. Rev. A 1, 841 (1970).
- ⁷G. A. Bissinger, S. M. Shafroth, and A. W. Waltner, Phys. Rev. A <u>5</u>, 2046 (1972).
- ⁸T. L. Criswell and T. J. Gray, Phys. Rev. A <u>10</u>, 1145 (1974).
- ⁹D. V. Ferree, thesis (University of Tennessee, 1972) (unpublished).
- ¹⁰N. A. Khelil and T. J. Gray, Phys. Rev. A <u>11</u>, 893 (1975).
- ¹¹R. Lear and T. J. Gray, Phys. Rev. A 8, 2469 (1973).
- ¹²L. M. Winters, J. R. McDonald, M. D. Brown, L. D. Ellsworth, and T. Chiao, Phys. Rev. A 7, 1276 (1973).
- ¹³H. A. Van Rinsvelt, F. E. Dunnam, J. P. Russell, and W. E. Bolch, in *Proceedings of the Third Conference* on the Use of Small Accelerators in Research, Teaching, and Industrial Applications, Denton, Texas, 1974, edited by J. L. Duggan and I. L. Morgan, CONF-741040 (ERDA, Oak Ridge, Tenn., 1975), Vol. 1, p. 148.
- ¹⁴R. F. Carlton, J. L. Duggan, J. Lin, K. Eger, M. T. Lu, M. J. Kelly, J. R. Dunning, and H. D. Fetzer, Bull. Am. Phys. Soc. <u>17</u>, 89 (1972).
- ¹⁵F. D. McDaniel, T. J. Gray, and R. K. Gardner, Phys. Rev. A 11, 1607 (1975).
- ¹⁶R. H. McKnight, S. T. Thornton, and R. R. Karlowicz, Phys. Rev. A <u>9</u>, 267 (1974).
- ¹⁷R. J. Gehrke and R. A. Lokken, Nucl. Instrum. Methods 97, 219 (1971).
- ¹⁸J. S. Hansen, J. C. McGeorge, D. Nix, W. D. Schmidt-Ott, I. Unus, and R. W. Fink, Nucl. Instrum. Methods

106, 365 (1973).

- ¹⁹E. J. McGuire, Phys. Rev. <u>185</u>, 1 (1969); Phys. Rev. A <u>2</u>, 273 (1970).
- ²⁰W. Bambynek, B. Crasemann, R. W. Fink, H. U. Freund, H. Mark, C. D. Swift, R. E. Price, and P. V. Rao, Rev. Mod. Phys. <u>44</u>, 716 (1972).
- ²¹G. H. Pepper, thesis (North Texas State University, 1974) (unpublished).
- ²²E. Merzbacher and H. W. Lewis, in *Handbuch der Physik*, edited by S. Flügge (Springer, Berlin, 1958), Vol. 34, p. 166.
- ²³G. S. Khandelwal and E. Merzbacher, Phys. Rev. <u>151</u>, 12 (1966).
- ²⁴G. S. Khandelwal, B. -H. Choi, and E. Merzbacher, At. Data 1, 103 (1969).
- ²⁵B.-H. Choi and E. Merzbacher, Phys. Rev. <u>177</u>, 233 (1969).
- ²⁶B.-H. Choi, E. Merzbacher, and G. S. Khandelwal, At. Data <u>5</u>, 291 (1973).
- ²⁷W. Brandt, R. Laubert, and I. Sellin, Phys. Rev. <u>151</u>, 56 (1966).
- ²⁸G. Basbas, W. Brandt, and R. H. Ritchie, Phys. Rev. A 7, 1971 (1973).
- ²⁹G. Basbas, W. Brandt, and R. Laubert, Phys. Rev. A 7, 983 (1973).
- ³⁰W. Brandt and G. Lapicki, Phys. Rev. A <u>10</u>, 474 (1974).
- ³¹J. Bang and J. M. Hansteen, K. Dan. Vedensk. Selsk. Mat.-Fys. Medd. <u>31</u>, No. 13 (1959).
- ³²J. M. Hansteen and O. P. Mosebekk, Z. Phys. <u>234</u>, 284 (1970).
- ³³J. S. Hansen, Phys. Rev. A <u>8</u>, 822 (1973).
- ³⁴J. H. McGuire and P. Richard, Phys. Rev. A <u>8</u>, 1374 (1973).
- ³⁵J. D. Garcia, E. Gerjuoy, and J. E. Welker, Phys. Rev. 165, 66 (1968).
- ³⁶J. D. Garcia, Phys. Rev. A <u>1</u>, 280 (1970); <u>1</u>, 1402 (1970); <u>4</u>, 955 (1971).
- ³⁷J. H. McGuire and K. Omidvar, Phys. Rev. A <u>10</u>, 182 (1974).
- ³⁸T. K. Li, R. L. Watson, and J. S. Hansen, Phys. Rev. A 8, 1258 (1973).
- ³⁹B.-H. Choi, Phys. Rev. A <u>4</u>, 1002 (1971).