PHYSICAL REVIEW VOLUME 151, NUMBER 1 4 NOVEMBER 1966

Characteristic X-Ray Production in Atomic L and M Subshells*

G. S. KHANDELWAL† AND E. MERZBACHER
University of North Carolina, Chapel Hill, North Carolina

(Received 9 May 1966)

Explicit formulas are obtained for atomic form factors describing the energy loss and momentum transfer of a charged particle to electrons in the subshells of the L and M shells. The Bethe-Born approximation is used with hydrogenic wave functions. Application is made to the L_{III} ionization cross section for protons incident on copper in the energy range from 0.5 to 1.7 MeV.

I. INTRODUCTION

THE theory of inner shell ionization and excitation of targets by heavy ions such as protons or α particles dates back to Bethe's[1] calculation for the K-shell cross section. Later these calculations were extended to the L shell by Walske,[2] and experimental and theoretical results were reviewed by Merzbacher and Lewis.[3] Recently these calculations were further extended to the M shell by Khandelwal and Merzbacher.[4] All these calculations assume that the incident and the scattered heavy ion is described by plane waves and the ejected electron by hydrogenic wave functions. Furthermore, in all of these calculations outer electron screening is taken into account by introducing into the calculations an average ionization potential appropriate to the full atomic shell.

TABLE I. L_{III} ionization cross section for protons of energy E incident on Cu ($Z=29$).

	$\sigma_{L_{\text{III}}}$ (cm^2)		
E (MeV)	Experimental[a]	Theoretical	$\sigma_{L_{\text{III}}}$(Theor.)/$\sigma_{L_{\text{III}}}$(Expt.)
0.5	7.8–21[b]	8.20 –20	10.5
0.7	1.3–20	1.08 –19	8.31
0.9	1.6–20	1.25 –19	7.79
1.1	1.9–20	1.35 –19	7.09
1.3	2.4–20	1.41 –19	5.86
1.5	2.6–20	1.436–19	5.52
1.7	2.8–20	1.444–19	5.16

[a] Reference 5.
[b] For 7.8–21 read 7.8×10^{-21} cm^2.

Recently some measurements have been made for the subshells of the L and M shells by Khan *et al.*[5] It thus becomes pertinent to make theoretical estimates of the contributions of the various subshells to the cross section. Since there is an appreciable difference in the measured ionization potentials for different subshells, the cross sections will be affected by these differences as well as by the differences in the form factors.

In this paper we present calculations for the form factors for the subshells of the L and M shells. The method is similar to that employed for the full shells in the earlier papers.

II. CALCULATION OF THE CROSS SECTION

We will follow the notations and the definitions of Ref. 3. The total cross section for ionization (and excitation) from a subshell labeled by s can be written as

$$\sigma_s=\frac{8\pi z^2}{Z_s^4\eta_s}a_0^2\int_{\theta_s/s^2}^{\infty} I(\eta_s,W)dW\,, \tag{1}$$

with

$$I(\eta_s,W)=\int_{W^2/4\eta_s}^{\infty}\frac{dQ}{Q^2}|F_{Ws}(Q)|^2. \tag{2}$$

The form factors $|F_{Ws}(Q)|^2$ for various subshells have been calculated to be

$$|F_{WL_{\text{I}}}(Q)|^2=A_L(Q,k)\left[Q^3-\left(\frac{7}{6}+\frac{5}{3}k^2\right)Q^2+\left(\frac{19}{48}+\frac{2}{3}k^2+\frac{1}{3}k^4\right)Q+\left(\frac{1}{3}k^6+\frac{1}{2}k^4+\frac{3}{16}k^2+\frac{1}{48}\right)\right],$$

$$|F_{WL_{\text{II}}}(Q)|^2=A_L(Q,k)\frac{1}{3}\left[\frac{1}{4}Q^2+\left(\frac{23}{24}+\frac{5}{6}k^2\right)Q+\left(\frac{1}{4}k^4+\frac{7}{24}k^2+\frac{11}{192}\right)\right],$$

and

$$|F_{WL_{\text{III}}}(Q)|^2=2|F_{WL_{\text{II}}}(Q)|^2,$$

---

* Work done under the auspices of the U. S. Atomic Energy Commission and supported in part by a grant from the University Research Council, University of North Carolina at Chapel Hill.

† Now at Department of Physics, Old Dominion College, Norfolk, Virginia.

[1] H. Bethe, Ann. Phys. (Paris) **5**, 325 (1930).

[2] M. C. Walske, Phys. Rev. **101**, 940 (1956).

[3] E. Merzbacher and H. W. Lewis, in *Encyclopedia of Physics*, edited by S. Flügge (Springer-Verlag, Berlin, 1958), Vol. 34, p. 166.

[4] G. S. Khandelwal and E. Merzbacher, Phys. Rev. **144**, 349 (1966).

[5] J. M. Khan, D. L. Potter, and R. D. Worley, Phys. Rev. **136**, A108 (1964); **145**, 23 (1966).

where

$$A_L(Q,k)=\frac{2^4Q\exp[-(2/k)\arctan(k/Q-k^2+\frac{1}{4})]}{[1-e^{-2\pi/k}][(Q-k^2+\frac{1}{4})^2+k^2]^4};\quad W=k^2+\tfrac{1}{4}.$$

The form factors for the subshells of the *M* shell are given by

$$|F_{WM_{\mathrm{I}}}(Q)|^2=A_M(Q,k)\bigg[Q^5+\left(-\frac{17}{9}-\frac{11}{3}k^2\right)Q^4+\left(\frac{98}{81}+\frac{380}{81}k^2+\frac{14}{3}k^4\right)Q^3-\left(\frac{542}{2187}+\frac{3794}{2187}k^2+\frac{254}{81}k^4+2k^6\right)Q^2$$
$$+\left(\frac{311}{19683}+\frac{2612}{19683}k^2+\frac{530}{2187}k^4-\frac{20}{81}k^6-\frac{1}{3}k^8\right)Q+\bigg(\frac{49}{177147}+\frac{1309}{177147}k^2+\frac{1418}{19683}k^4$$
$$+\frac{682}{2187}k^6+\frac{47}{81}k^8+\frac{1}{3}k^{10}\bigg)\bigg],$$

$$|F_{WM_{\mathrm{II}}}(Q)|^2=A_M(Q,k)\frac{8}{81}\bigg[Q^4+\left(\frac{28}{9}+\frac{4}{3}k^2\right)Q^3-\left(\frac{4}{3}+\frac{194}{27}k^2+\frac{14}{3}k^4\right)Q^2$$
$$+\left(\frac{100}{729}+\frac{272}{243}k^2+\frac{8}{3}k^4+\frac{4}{3}k^6\right)Q+\left(\frac{19}{6561}+\frac{146}{2187}k^2+\frac{124}{243}k^4+\frac{38}{27}k^6+k^8\right)\bigg],$$

$$|F_{WM\mathrm{III}}(Q)|^2=2|F_{WM_{\mathrm{II}}}(Q)|^2,$$

$$|F_{WM_{\mathrm{V}}}(Q)|^2=A_M(Q,k)\frac{16}{729}\bigg[(1+k^2)Q^2+\left(\frac{368}{225}+\frac{358}{45}k^2+\frac{158}{25}k^4\right)Q+\left(\frac{493}{14175}-\frac{61}{405}k^2+\frac{149}{225}k^4+\frac{89}{105}k^6\right)\bigg],$$

and

$$|F_{WM_{\mathrm{IV}}}(Q)|^2=\tfrac{2}{3}|F_{WM_{\mathrm{V}}}(Q)|^2,$$

where

$$A_M(Q,k)=\frac{2^7}{3^3}\frac{Q}{1-e^{-2\pi/k}}\frac{\exp[-(2/k)\arctan(\frac{2}{3}k/Q-k^2+\frac{1}{9})]}{[(Q-k^2+\frac{1}{9})^2+(4/9)k^2]^5};\quad W=k^2+\tfrac{1}{9}.$$

III. RESULTS AND CONCLUSIONS

We have computed the L_{III} ionization cross section[6] for protons incident on Cu ($Z=29$) in the energy range between 0.5 and 1.7 MeV. Table I gives the resulting cross sections for energy spacings of 200 keV as well as measured experimental values. This shows that the Born approximation gives estimates of the cross section in excess of the experimental values, with the largest discrepancies in the low-energy region, where the Coulomb deflection of the projectile plays an important role and is expected to lower the theoretical values. The use of better electron wave functions than hydrogenic ones may further improve the theoretical results.

ACKNOWLEDGMENT

We thank G. Basbas for checking some of the calculations for the *M* shell.

---

[6] E. Merzbacher and G. S. Khandelwal, Bull. Am. Phys. Soc. **10**, 262 (1965).