Semiempirical analysis of electron-induced K-shell ionization*

C. A. Quarles
Texas Christian University, Fort Worth, Texas 76129
(Received 21 July 1975)

We report the results of an analysis of the available experimental data on electron-induced K-shell ionization which show that the data can be described by the Bethe theory of ionization corrected for relativistic energies by a classical correction. This analysis, which extends over five orders of magnitude in the ratio of bombarding energy to ionization potential, appears to be superior to the available theoretical treatments, and suggests where further work would be useful.

There is now a fairly extensive amount of data available on the total cross section for K-shell ionization by electron bombardment.[1-18,30] A variety of theoretical treatments, beginning with that of Bethe, have been made in an attempt to describe this process.[19-29] While each treatment appears to have some region of validity, none has been fully successful in describing the process over a wide range of atomic number (or ionization potential) or bombarding energy. The more complex quantum-mechanical[20,21,22,27,28] calculations in the Born approximation have the most restricted regions of validity. The classical calculation of Gryzinski[23] works rather well at lower bombarding energy, while the calculation of Kolbensvedt[12,25] is most successful at higher bombarding energy. While the classical calculation involves no adjustable parameters, the Kolbensvedt calculation does involve the adjustment of at least one parameter for each atomic number and so is in the nature of a semiempirical treatment.

Because of the difficulty of obtaining a good theoretical treatment of the ionization problem in general, a variety of empirical analyses have been made.[30-34] Until now, however, none has attempted to look at all data over the entire measured range of energy and atomic number. We began this analysis with the observation that data for low to medium atomic numbers and bombarding energy less than about 500 keV appeared to be well described within experimental errors by the simple functional form suggested by the Bethe theory of ionization[19,26]: $\sigma \propto (1/UI^2)\ln U$, where U is the ratio of bombarding energy E to ionization potential I. When σUI^2 was plotted vs $\ln U$, a straight line appeared to give a reasonable fit to the data. Data at higher bombarding energy or higher atomic number, however, deviated quite significantly from this apparent linear behavior.

In what we expected to be only a first attempt to extend the region of validity of this analysis, it seemed plausible to correct the experimental data by the relativistic correction factor R suggested by the classical calculation[23]

$$R=\left(\frac{2+I}{2+E}\right)\left(\frac{1+E}{1+I}\right)^2\left(\frac{(I+E)(2+E)(1+I)^2}{E(2+E)(1+I)^2+I(2+I)}\right)^{3/2};$$

I and E are in rest-mass units. This correction was made to the data, and in Fig. 1 we have plotted $\sigma UI^2/(R\ln U)$ vs U. The surprising result is that the data, so plotted, can be described very well by a straight line with zero slope. It should be noted that the atomic numbers of the data range from 2 to 83 and the variable U extends over five orders of magnitude. The unweighted-average intercept is 854×10^{-16} cm^2 eV^2 for 195 data points. Data from Refs. 16, 17, and 18 were not included in the present analysis, but inclusion of this data is not expected to alter the conclusions.

In order to estimate the accuracy of the fit to a straight line we have associated with each data point an error of 15%. This is reasonable as a first approximation, since the typical systematic error in the various experiments, where quoted, appear to range from 10 to 20%. The major exception to this seems to be the single high-energy experiment where a 6% error is typical. With a 15% error, we obtain a minimum value of χ^2 of 143 for 174 data points for an intercept of $(828\pm13)\times10^{-16}$ cm^2 eV^2. The error represents a one-standard-deviation range. In this estimate we have omitted 21 data points from consideration whose inclusion would have about tripled this value of χ^2. This seems reasonable, since all but one were lower-energy data points which, especially for the higher atomic numbers, should probably be corrected for multiple scattering. The other point omitted is the unusually low cross-section datum for $Z=57$ of Ref. 14.

Clearly the fit is very good and consistent with an average error per point somewhat less than 15%. Certainly if the error in the high-energy data were taken at 6%, the value of χ^2 would increase substantially. What we are really saying here, then, is that to within a 15% error all of the data available except for a few points at low U are fitted well by a straight line of zero slope. Of course, if additional high-energy data become available, the conclusion may need to be altered somewhat, perhaps to include a small nonzero slope to improve the fit.

In Fig. 1, we have also plotted the predictions of the calculations of Gryzinski and Kolbensvedt. The Gryzinski calculation is parameter-free and gives a value of χ^2 of 141.3 for 142 degrees of freedom for U less than 400. The calculation obviously does not fit for U greater than 400. The simple straight-line fit described above gives a χ^2 of 112.7 for the same data and is thus a somewhat better fit. The Kolbensvedt calculation depends on the choice of two parameters which vary with the atom ionized. We have plotted the case for $Z=29$ with $I=0.017\,57$ and $I_0=0.0224$. Variations of these parameters over their reasonable physical range does not change the curve very much, as must be the case if the calculation is to describe the data. For U greater than about 10, the Kolbensvedt calculation appears to be a reasonable fit to the data and a minimum value of χ^2 could be obtained by adjusting I and I_0 in the Kolbensvedt formula; however, there does not seem to be much point to this exercise, since the simple formula does so well. The range of validity of the more complex quantum-mechanical calculations is too limited to make any comparison very interesting.

The analysis presented here suggests several areas for further study. First, as more data become available on the other atomic shells, particularly the L shell, it will be very interesting to see if the same formula with perhaps the same constant (per electron) will describe this data. The small amount of L-shell data presently available[5,13,35,36] appears to be consistent with the formula presented here. Second, there is need for accurate K-shell data at low values of U for medium to high atomic numbers to test whether the simple linear behavior suggested here is really preferred over the curvature suggested by the classical calculation. Third, there is need

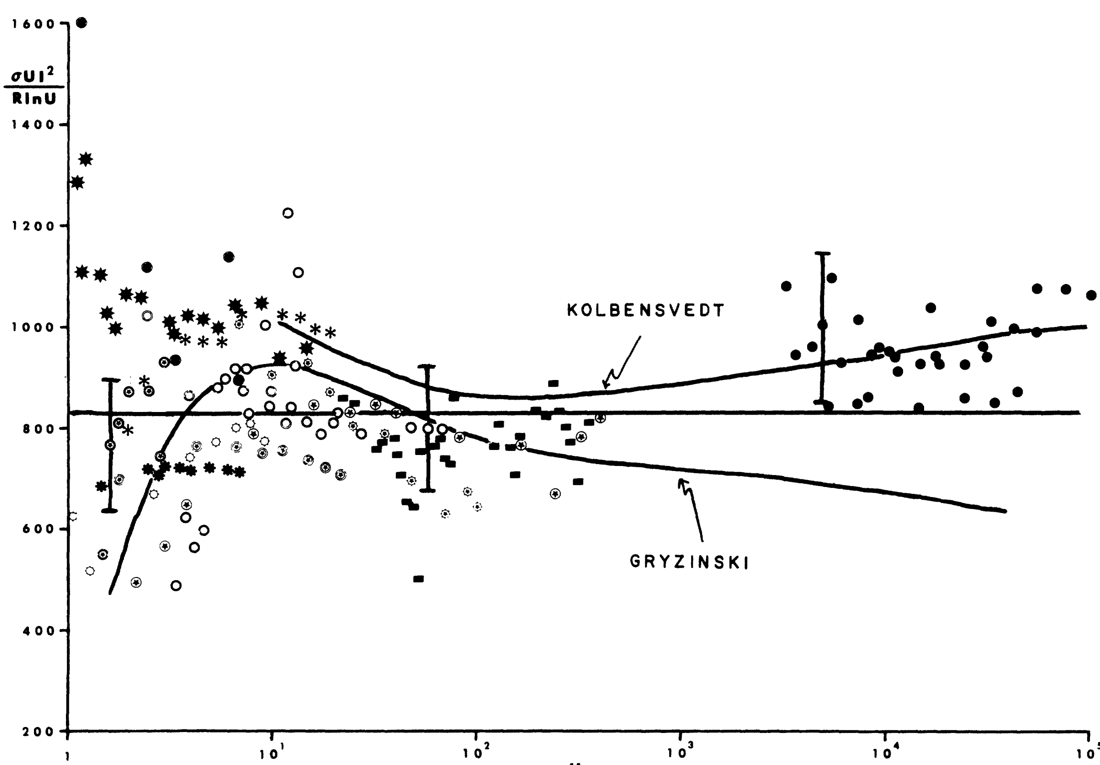

FIG. 1. Plot of $\sigma U I^2/R \ln U$ vs U. The data plotted are from the indicated references: $*$: Ag, Ref. 2; ◉: Ni, Ref. 4; ⊙: Cu, Ref. 5; ✹: Sn, Au, Ref. 6; ◎: Ag, Sn, Au, Ref. 8; O: Ag, Sn, Ref. 9; ✻: Al, Ref. 11; ●: Cu, Sr, Mo, In, Tm, Au, Ta, Bi, Ref. 12; ✸: Cu, Ag, Au, Ref. 13; ■: $23 \leq Z \leq 83$, Ref. 14; ⊛: C, Ref. 15; ✺: He, Ref. 30; ○: Li II, Ref. 30.

for precise data over a wide range of U for a variety of atoms, especially for U greater than 100. For U above 400 there are the data of only one experiment, and for $400 \leq U \leq 3000$ there are no data at all. Clearly, to further test the validity of the formula presented here and to see at what point, if any, additional dependence on ionization potential is needed will require data with higher precision than the data currently available. Fourth, from a theoretical viewpoint, the essential question would seem to be how to recover what appears to be a relatively simple behavior from calculations which are generally very complex.

To conclude, we have found that the data from electron-induced K-shell ionization can be described very well by the formula

$$\sigma = (828 \pm 13) \times 10^{-16}(R/UI^2) \ln U \text{ cm}^2\,\text{eV}^2 \ .$$

*Work supported by the Texas Christian University Research Foundation.

[1]D. L. Webster, W. W. Hansen, and F. B. Duveneck, Phys. Rev. 43, 839 (1933).
[2]J. C. Clark, Phys. Rev. 48, 30 (1935).
[3]A. E. Smith and P. Kirkland, Phys. Rev. 67, 153 (1945).
[4]L. T. Pockman, D. L. Webster, P. Kirkpatrich, and K. Harworth, Phys. Rev. 71, 330 (1947).
[5]M. Green, Ph.D. dissertation (University of Cambridge, 1962) (unpublished).
[6]J. W. Motz and R. C. Placious, Phys. Rev. 136, A662 (1964).
[7]H. Hansen, H. Weigmann, and A. Flammersfeld, Nucl. Phys. 58, 241 (1964).
[8]D. H. Rester and W. E. Dance, Phys. Rev. 152, 1 (1966).
[9]H. Hansen and A. Flammersfeld, Nucl. Phys. 79, 135 (1966).
[10]B. Fisher and K. W. Hoffman, Z. Phys. 204, 122 (1967).
[11]W. Hink and A. Ziegler, Z. Phys. 226, 222 (1969).
[12]L. M. Middleman, R. L. Ford, and R. Hofstader, Phys. Rev. A 2, 1429 (1970).
[13]D. V. Davis, V. D. Mistry, and C. A. Quarles, Phys. Lett. 38A, 169 (1972).
[14]S. Scholz, A. Li-Scholz, R. Colle, and I. L. Preiss, Phys. Rev. Lett. 29, 761 (1972).
[15]W. Hink and H. Paschke, Z. Phys. 244, 140 (1971).
[16]R. L. Gerlach and A. R. Ducharme, Surf. Sci. 32, 329 (1972).
[17]H. Hubner, K. Ilgen, and K. W. Hoffman, Z. Phys. 255, 269 (1972).
[18]G. Glupe and W. Melhorn, Phys. Lett. 25A, 274 (1967).
[19]H. Bethe, Ann. Phys. (Leipz.) 5, 325 (1930).
[20]E. H. S. Burhop, Proc. Camb. Philos. Soc. 36, 43 (1940); J. Phys. B 5, L24 (1972).
[21]A. M. Arthurs and B. L. Moisewitsch, Proc. R. Soc. A 242, 550 (1958).
[22]H. S. Perlman, Proc. Phys. Soc. Lond. 76, 623 (1960).
[23]M. Gryzinski, Phys. Rev. 138, A336 (1965).
[24]M. R. H. Rudge and S. B. Schwartz, Proc. Phys. Soc. Lond. 88, 563 (1966); 88, 579 (1966).
[25]H. Kolbensvedt, J. Appl. Phys. 38, 4785 (1967).
[26]M. Inokuti, Rev. Mod. Phys. 43, 297 (1971).
[27]R. Fleming, Ph.D. dissertation (Texas Christian University, 1972) (unpublished).
[28]J. N. Das, Ann. Phys.(Leipz.) 28, 6 (1972); Nuovo Cimento B 12, 197 (1972).
[29]G. R. Dangerfield, Phys. Lett. 46A, 19 (1973).
[30]W. Lotz, Z. Phys. 206, 205 (1967); Astrophys. J. Suppl. 14, 207 (1967).
[31]L. Vriens, Physica (Utr.) 31, 385 (1965).
[32]W. Hink, J. Jessenberger, and A. Ziegler, Z. Phys. 226, 463 (1969).
[33]V. M. Pessa and W. R. Newell, Phys. Scr. 3, 165 (1971).
[34]C. A. Quarles, Phys. Lett. 39A, 375 (1972).
[35]S. I. Salem and L. D. Moreland, Phys. Lett. 37A, 161 (1971).
[36]Y. K. Park, M. T. Smith, and W. Scholz, Phys. Rev. A 12, 1358 (1975).