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Cross Sections for Electron and Photon Processes Required by Electron-Transport Calculations

MASTER

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CROSS SECTIONS FOR ELECTRON AND PHOTON PROCESSES
REQUIRED BY ELECTRON-TRANSPORT CALCULATIONS*

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ABSTRACT

Electron-transport calculations rely on a large collection of electron-atom and photon-atom cross-section data to represent the response characteristics of the target medium. These basic atomic-physics quantities, and certain quantities derived from them that are now commonly in use, are critically reviewed. Publications appearing after 1978 are not given consideration. Processes involving electron or photon energies less than 1 keV are ignored, while an attempt is made to exhaustively cover the remaining independent parameters and target possibilities. Cases for which data improvements can be made from existing information are identified. Ranges of parameters for which state-of-the-art data are not available are sought out, and recommendations for explicit measurements and/or calculations with presently available tools are presented. An attempt is made to identify the maturity of the atomic-physics data and to predict the possibilities for rapid changes in the quality of the data. Finally, weaknesses in the state-of-the-art atomic-physics data and in the conceptual usage of these data in the context of electron-transport theory are discussed. Brief attempts are made to weight the various aspects of these questions and to suggest possible remedies.

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CROSS SECTIONS FOR ELECTRON AND PHOTON PROCESSES REQUIRED BY ELECTRON-TRANSPORT CALCULATIONS

I. INTRODUCTION

The following material constitutes a critical review of the atomic-physics information required in the numerical treatment of electron transport. The scope of this review is limited in several respects; however, it reflects the types of problems most often encountered at Sandia Laboratories. Processes involving particles or photons with energies less than 1 keV and the "high-energy" model of target structure that assumes an appropriate superposition of properties derived either from pure substance or from free-atom properties will receive only incidental comment. The most representative discussion of the transport code for which these following comments apply is given in Ref. C1. This reference also defines the actual atomic-physics data now in use; it will often be cited.

The range of topics that must be covered is staggering; no single document or author could present a detailed critical review of each quantity in use and recommend the best value available at this time. The compromise approach for this presentation consists of documenting existent reviews that achieve this ideal for at least some parts of the subjects under consideration. Attention will be directed to any changes in the existing data base that would represent an improvement in accuracy. No recent critical review exists for most of the subjects under consideration. In these cases, an admittedly incomplete survey of the literature, terminating at the end of 1978, is attempted. The object is not to present a scholarly review but to identify potentially weak areas in the data base. Once identified, the ability to improve the weakness in terms of existing data or additional work is evaluated. The fact that the data base must encompass the entire periodic table and a large range of

base must encompass the entire periodic table and a large range of kinematic variables means that a great deal of careful work on some small segment will not necessarily be cited. I hope the authors of these publications will accept in advance my apologies and understand the reasons for this approach. Much of this discussion is theoretical in nature; this is not always a reflection of the author's bias, but indicates that theoretical work often provides the only available data and serves as a convenient interpolation/extrapolation device when incomplete experimental data are available. The observation that a carefully designed experimental measurement could remove some question is always implied, if not explicitly stated.

The criteria for evaluating the atomic-physics data is based on the present state-of-the-art of that particular quantity and not on the potential importance to some particular transport problem. It is impossible to avoid all speculation on the latter point, and these statements should not be weighed too heavily when they are encountered.

An obvious difference in quality of data was found; Section VI serves as a dividing line. The cross sections for electron-target collisions and the quantities derived from them are much less well understood than are the quantities based on photon-target interactions and relaxation phenomena. This difference in maturity is reflected by a rather more detailed discussion of electron-target processes which is presented in Sections II through V.

Each section starts with a very abbreviated description of the atomic-physics data under consideration. Referral to the cited references is necessary if one wishes to see how these data are used in the context of electron-transport calculations. Appendix A provides a table of definitions for various symbols used throughout the text. In the event one symbol is used for different quantities, the text definition takes precedence over Appendix A. Appendix B presents a very terse tabulation of many of the questions raised in the text and identifies the section that presents the details concerning this problem.

II. COLLISIONAL ELECTRON ENERGY-LOSS DISTRIBUTION FUNCTION

The energy-loss, or straggling, distribution function $f(x, \Delta E)$ for an electron that has lost an energy ΔE by collision, as contrasted to radiative energy loss after transversing a distance x in some material, is required in the transport calculation.^{C1} An appropriate transport equation^{B3} determines $f(x, \Delta E)$ from a theoretical point of view, and is an experimentally observable quantity under properly controlled conditions. The form used in the transport calculation^{C1} is based on the original work of Landau,^{L1} f_L , as modified by Blunck et al,^{B1,B2} f_B . The straggling is corrected for the density effect^{C1} in a manner outlined below.

The quantity, f_L , is based on the sum of the relativistic Rutherford cross section for large transfer of the initial collision energy E_0 , and the Bethe approximation to the first Born cross section^{B20,M5} for small transfers. (This device for constructing a cross section, the Q+BEM method, is discussed at some length in Section IV. This method is potentially as reliable as any commonly available technique, although additional approximations often severely and unnecessarily restrict its applicability.) The f_L result is obtained by truncating an infinite series in the energy moments of the inelastic cross section to the first term and by ignoring energy conservation requirements when computing the first moment. The resulting f_L distribution is a universal curve if an appropriately scaled independent variable is used to represent ΔE . The f_B distribution is obtained by retaining the second energy moment of the cross section. The shape of f_B is not found to be a universal curve, and it depends on a parameter representing the binding energy of the target's electrons. This is sometimes referred to as the resonance broadening effect. The Vavilov distribution, f_V , which is mentioned below, differs from f_L in that a cruder approximation to the cross section is used, but

the first energy moment of the cross section does maintain energy conservation requirements.

Ideally, the straggling and stopping power used in a transport calculation (see Section III) should be based on the same set of cross sections for the inelastic collision events.⁵⁶ This should guarantee that this average energy loss predicted by the straggling function is equal to that predicted by the stopping power as used in the continuous-slowing-down approximation. This criterion would be satisfied if the Møller binary-encounter cross section replaced the Rutherford cross section in constructing f_B . The one available test of this point is based on recalculating f_L with the Møller cross section.^{R4} The effects appear to be small near the maximum of f_L for high energy ($E_0 \sim 1$ MeV) electrons. The changes in the tails of the distribution can be quite large, but the width at half-height is decreased only by a few percent or less.^{R4} One could conclude that use of the Møller cross section will not make a great deal of difference for large E_0 ($E_0 \gg 1$ MeV), although the evidence is rather limited. For example, no consideration has been given to the extreme relativistic range, $\beta \sim 1$ or $E_0 \gg 1$ MeV.

The situation is clear for $E_0 < 10$ keV. It is shown in Section III that due to defects in energy conservation in the version of the Q+BEM cross section being used,^{R4} the stopping power has serious errors in this energy range. Since this stopping power is proportional to the first moment being used in the calculation of f_B , any straggling prediction must be questioned.

Experimental data for $f(x, \Delta E)$ are relatively sparse. Tests with $E_0 > 1$ MeV on a wide variety of materials show that the most probable energy loss is accurately predicted by f_L , provided the density effect is properly included in the calculation.^{H1,H2,G1,K1,Z1} A measurement of the straggling of high-energy electrons in a gas and its solid polymer^{G2} verifies the density effect on the most probable energy loss, and also indicates that the shape of $f(x, \Delta E)$ is independent of the density effect. (Note that the additivity of the constituent-atom effects^{B23} is

an implicit assumption underlying this test. Experimental studies indicate that this hypothesis is in only a few percent error except for small-Z materials.^{T3}) This supports the use made in the transport code^{C1} of the density-effect correction. (See the discussion in Section III for possible reservations about the density effect.)

Recent measurements^{N1} of the most probable energy loss ΔE_p in thin gas samples are systematically lower than predicted by f_L or f_B theory. This discrepancy decreases for increasingly thicker targets, and an explanation^{G6} of the thin-target results is apparently acceptable.^{N1} Another recent study^{P1} of ΔE_p in solids shows the relative success of f_B over f_L . Reference P1 does not give results for the usual f_B most probable energy loss, $\Delta E_p(B)$, but includes higher order correction terms in their predictions of the most probable energy loss, labeled $\Delta E_p(C)$. For conditions typical of their measurements, the theoretical ordering $\Delta E_p(C) < E_p(L) < E_p(B)$ is satisfied. In addition, their experimental values are lower than $\Delta E_p(L)$, and $\Delta E_p(C)$ lies within their experimental error bars. They make no comment about density effect corrections.^{P1}

The experimental shapes of $f(x, \Delta E)$ for relativistic electrons in solids have been observed^{K1, H2, Z1} to be considerably broader than the f_L curve at 1/2 height, while reasonable agreement with the f_B theory has been claimed.^{K2} The situation is similar for gas targets if the target is not too thin, although a tendency for f_B to be too wide at 1/2 height is noteworthy.^{N1} In addition, the study of thin Al targets^{P1} observes the same tendency and adds the observation that comparison with experimental results is improved when higher-order corrections are added to the f_B theory.

This is an interesting situation, when one notes that f_L and f_B average energy losses are systematically lower than the values predicted by the Bethe stopping-power formula used in conjunction with the continuous-slowing-down approximation.^{V1} The full meaning of this

disagreement is not yet clear, but Ref. V1 proposes that Monte-Carlo sampling methods be biased to better reflect the continuous-slowing-down results. This is motivated by the detailed experimental verification of stopping-power theory based on the best available Q+BEM cross sections.^{R4} The simplest resolution of this discrepancy depends upon the success of the Vavilov approximation based on Q+BEM cross sections used in the stopping-power calculation, a study not yet completed.

The few experimental data for $E_0 > 1$ MeV seem to support the conclusion reached for the high-energy data with respect to ΔE_p . The shapes of the observed $f(x, \Delta E)$ are not in good agreement with theory. It has been suggested in a review of these data^{R4} that the origin of the disagreement in shape can, in many instances, be ascribed to factors in the experimental measurements.

Some purely theoretical evidence pertaining to $f(x, \Delta E)$ is available. A study^{R3} of proton straggling in aluminum for 20-MeV protons indicates that the accuracy of f_B is a strong function of x . In brief, a modification of the Vavilov distribution, f_V , in the spirit of the modification of f_L to obtain f_B , worked well for "large" and "intermediate" x while f_B and f_L were accurate only for intermediate x . The f_B , modified f_V , and f_L predictions were all inaccurate for small x . No data were presented for the usual f_V theory. Variants of the theoretical methods described here have been developed and applied to straggling by heavy particles.^{R5, P11, T4} They will not be discussed here because of their specialized use, but the useful transfer of these techniques to the electron problem may be possible.

The analogy between cross sections for protons at 20 MeV and electrons at about 10 keV is strong; hence, there may be a similarity in the straggling for these two cases. There are no data, however, to justify this inference.

A series of theoretical studies is available that predicts straggling-like quantities for electrons in the energy range $0 \leq E_0 \leq 10$ keV. This work utilizes cross sections more realistic than the Q+BEM cross sections would be in this energy range. Unfortunately, these authors do not present a comparative study that could yield information of use to this discussion.

There are no data for the straggling of electrons in partially ionized media.^{B8} Since the BEM part of the Q+BEM cross section assumes a binary scattering of one electron at rest (representing a bound electron) and the incident electron, one might expect the treatments being discussed here to automatically be representative of the ionized media case. Free electrons can be better stopping materials than bound electrons under certain conditions (see Section III). This should be reflected in an adequate straggling theory by displaying dependence on such parameters as the degree of ionization, the Debye radius, etc. Such a theory is not yet available.

Summary

The information cited above indicates that the transport code use^{C1} of f_B is fairly well documented and accurate for relativistic electrons. As long as straggling due to radiation is correctly included, the ultra-relativistic region should also be well treated. Both gaseous and condensed media are included in this evaluation; the density-effect corrections become more important as E_0 increases and some reservation concerning this quantity may exist for extremely relativistic electrons (see Sections III and IV). There appears to be little documentation of straggling for $E_0 < 1$ MeV. The paucity of experimental data for $E_0 < 1$ MeV indicates that comparative theoretical studies^{B3} could fill this gap in information. Such a study could be done with the cross sections discussed in Section IV, at least down to $E_0 \sim 1.0$ keV, where solid-state effects may become important. The electron case may be more sensitive to q , energy conservation effects than is the proton case,^{H3} as expressed by the

differences between f_V and f_L , so too close an analogy between the proton and electron straggling cases is not advised. There are no data for the straggling of electrons in partially ionized media.

III. STOPPING POWER

The collisional stopping power is a basic quantity used in the transport code^{C1} and is based entirely on theoretical methods, except for a parameter determined from experimental measurements for protons. This stopping power is defined as

$$-p^{-1} \langle dE/dx \rangle = (N/A) \left\{ \sum_i \Delta E_i \sigma_i + \int_0^{\infty} d\xi (\xi + 1) (d\sigma/d\xi) \right\}, \quad (\text{III.1})$$

where ΔE_i is the energy threshold for the i th inelastic event, the summation is over all possible inelastic events for all degrees of freedom, and the integral over the kinetic energy of the ionized electron represents contributions from collisional ionization. The usual treatment^{D1} replaces the cross sections with their first-Born-approximation form and considers only the electronic degrees of freedom.

Bethe^{B12} derived an extremely simple stopping formula for large E_0 by modeling separately the small- and large-momentum-transfer contributions.^{P3} (This is an application of the Q+BEM cross section technique discussed in more detail in Section IV.) Sum rules over electronic degrees of freedom play an important role in this development. In addition, Bethe's methods are quite similar to those developed earlier by Møller^{M7} in treating the scattering and stopping by relativistic electrons. The results due to Bethe^{B12} are the more comprehensive and slightly supersede Møller's work.^{M7} Bloch derived nonrelativistic results quite similar^{A5} to Bethe's by starting with an impact parameter treatment. The main advantages gained by the impact parameter approach become more apparent when treating incident particles with internal degrees of freedom.^{S5} Hence, Bloch's result will be dismissed with the comment that

the usual non-relativistic stopping-power formula (see the form displayed by Eq. III.8) is often called the Bethe-Bloch formula.

The collisional stopping power now being used in the transport code^{C1} has the form

$$-\rho^{-1}(dE/dx) = 2\pi e^4 ZN (mc^2 \beta^2 A)^{-1} \times \left\{ \ln \left[\frac{\tau \beta^2}{2(1-\beta^2)(I/mc^2)^2} \right] + F(\tau) - \delta \left(\frac{\beta^2}{1-\beta^2} \right) \right\}, \quad (\text{III.2})$$

where $\tau = (1-\beta^2)^{-1/2}$ is the kinetic energy of the electron in units of mc^2 and β is its speed in units of the speed of light (c). The quantity $F(\tau)$ is a function defined in Ref. C1 and its analytic behavior for real and positive τ is the only property required for this discussion. The quantities δ and I are defined in the following discussion.

Equation III.2 was derived^{R4} by using Bethe's result for small-momentum transfers and the Møller binary-encounter collision theory for large-momentum transfers. The use of the Møller cross section is believed to be somewhat better than Bethe's original binary-encounter model. The difference involves only a very small term in $F(\tau)$. (These theories do not depend upon any cut-off parameter representing the partitioning of the momentum transfer.) This result has a very attractive feature when restricted to relatively large collision energies, $\tau = E_0/mc^2 \gg I/mc^2$, but $\beta \ll 1$ (so that $\delta = 0$ is an accurate approximation). Its derivation is based on sum rules for electronic degrees of freedom and depends only upon the actual quantum nature of the stopping material through the parameter I . Hence, the use of inappropriate theoretical models (such as isolated atoms) to represent a solid or molecule is immaterial as long as the number of electrons is known, a reliable I is available, and other degrees of freedom are not important. Other degrees of freedom include rotation-vibration. Free electrons as encountered in a plasma or electron within a conduction band are usually treated by different methods.^{B8} This

situation is reflected by the common practice of forcing agreement between Eqs. III.1 and III.2 at large E_0 by altering the list of σ_i 's used to evaluate Eq. III.1.^{D3,G12}

The parameter I appearing in Eq. III.2 arises from the Q contribution to the $Q+BEM$ collisional stopping and is defined by

$$\ln I = \left\{ \sum_i + \int \right\} f_i \ln \Delta E_i / \left\{ \sum_i + \int \right\} f_i, \quad (III.3)$$

where f_i is the optical oscillator strength and the $\{...\}$ symbol implies the appropriate sum over discrete states and integration over the continuum. However, there are few theoretical data available^{D1} for I (see Table III.I and Refs D2 and D3). However, a general formula is available from the work of Bloch,^{B7}

$$I = CZ, \quad (III.4)$$

where various estimates of the constant C are available.^{B21,C4} The value $C \approx 13.5$ eV is often used.^{B8}

Equation III.4 is considered relatively crude; the usual method for determining I is based on empirical fits of proton-stopping-power measurements to the appropriate analogue^{A4} of Eq. III.2. The use of such I values seems appropriate, since this fitting is done at large proton speed where first-Born-theory inelastic cross sections are independent of the incident-particle mass. There are some problems with using experimental data to determine I ; these have been discussed in Ref B8. The values currently in use,

$$I = 9.76Z + 58.8Z^{-0.19} \text{ eV} \quad (III.5)$$

for $Z \geq 13$ and from tabulated values for $Z < 13$, are from the work of Sternheimer.^{B5} Other more recent interpolation schemes, similar to Eq. III.5, exist.^{D9} Newer determinations of I also exist and are summarized in Ref. A4, which presents I data for all atoms with $Z \leq 92$, based on a combination of the most recent experimental information and certain theoretical calculations.^{C4}

Comparisons for selected Z between the code values, the available values based on Eq. III.3, and those data given in Ref. A4 are presented in Table III.I. The general agreement is good for all small Z except $Z = 1$. For $Z > 13$ the values from Eq. III.5 are systematically larger by nearly 10% than the values from Ref. A4, and in the worst cases this difference approaches 20%. Error estimates for the code values or those given in Ref. A4 for I are not available, so one set cannot clearly be recommended over the other. The only difference between these data is the availability of additional experimental information and more recent theoretical work for constructing I values given in Ref. A4.

The effect of possible change in I will not be too large for $\tau \gg 1$ ($E_0 \gg I$) but becomes increasingly important for smaller τ . For example, the maximum in the stopping power as a function of E_0 depends exponentially upon I . It is important to remember that the density-effect term, δ , in Eq. III.2 is dependent upon the choice of I .^{B5} Since τ is large for $\beta \sim 1$, any changes made in I should be reflected by corresponding changes in δ if one is considering $E_0 \geq 1$ MeV.^{B5}

The Density Effect

The first term in Eq. III.2 approaches infinity as $\beta \rightarrow 1$. The density-effect correction term, δ , serves to correct for this unreasonable behavior. The first and second terms in Eq. III.2 were derived for an isolated atom, so δ characterizes the non-zero density of the stopping medium. The contribution of δ to Eq. III.2 is observed to be significant^{B8} for most materials when $E_0 \geq 10$ MeV. This property is

estimated theoretically from the dielectric behavior of the stopping medium. The results of Sternheimer^{B5} are used in the transport code,^{C1} as they were the only generally applicable data available at the time the code was written. These determinations of δ have been reconsidered, and simplified numerical procedures for this evaluation are described.^{S2} Comparisons of these data with relative experimental measurements in the GeV energy range for electrons indicate a satisfactory energy dependence,^{C2} and Ref. S2 claims quite small absolute errors.

With respect to the use of δ in the transport code,^{C1} two points must be made. First, the method for constructing this term for composite materials is not clearly identified with the procedures recommended in Ref. S2. It does seem likely, however, that the method used in the transport code is "correctly" based on the Bragg-Kleeman additivity rule.^{B23} It should be pointed out that there are no examples of exceptions to this rule for electron stopping. On the other hand, proton and α -particle data do show $\sim 10\%$ changes due to density effects that are not contained in the additivity rule. (See Ref. M6 for a summary of these problems in stopping by H_2O and Section II for a discussion in the context of straggling.) Second, the transport code implicitly assumes that the stopping medium is at normal temperature and density. Techniques are available to treat the variation of δ with these parameters,^{B5} and they should prove satisfactory, except for conditions under which the stopping medium may be partially ionized. The argument of the log term in Eq. III.2 changes for ionized media (see the implications of Eqs. III.6 and III.8), and it seems probable that the derivation of δ must reflect this change. In any event, there are no experimental tests of δ for partially ionized media. Such tests, and further theoretical studies of the decrease in stopping due to δ , may be of some importance, since there are practical needs^{W3} for tailoring the stopping of very high-energy electrons by a plasma. The usual approach to this problem concentrates on other parameters,^{C5, W3} but the behavior of stopping by ionized plasmas (see the following topic), coupled with the behavior of δ for plasmas and $E_0 \geq 10$ keV, is not a well-documented subject.

Section IV will discuss some experimental ionization measurements in solids for $E_0 \sim 1$ GeV, and some comparable theoretical calculations that both include and ignore the density effect.^{D10} The methods used to obtain the density effect corrections were essentially the same as Sternheimer's techniques. The fact that the experimental data strongly favor the theoretical data without the density-effect corrections is noteworthy. Further evidence of this type may provide an excellent alternative test of the density-effect correction term. No conclusion seems obvious at this point, but future developments in this area certainly could have an influence on the status of our understanding of δ .

Partially Ionized Stopping Media

The stopping of electrons by partially ionized or plasma media has long been a topic of interest; see Ref B8 for a review of the earlier literature. The reason for this can easily be seen by following a suggestion by Salpeter.^{B22} If one calculates the plasma electron stopping by assuming two-body Coulomb collisions are the only important processes, one can easily obtain for relatively large but non-relativistic E_0

$$-dE/dx = 2\pi e^4 Z N(E_0 A)^{-1} \times \left\{ \ln \left[\frac{b_m E_0}{\epsilon} \right]^2 + \ln \left[\frac{\bar{b}_m}{b_m} \right] + \text{constants} \right\} \quad (\text{III.6})$$

where $b_m < \bar{b}_m$ are two impact parameters that must be specified. The choices $b_m = l_d$, the Debye length, and $\bar{b}_m = l_d (v/v_p)$, where v_p is the plasma (thermal) speed, cause the first term to take the often-used binary-collision form, and the second term becomes (excluding some 'screening constant') the Kramers or Pines and Bohm result for the collective effect of free electrons.^{B8} The combination of the two log terms in Eq. III.6 produces an energy dependence different from that observed for media with completely localized electrons. This, plus the existence of discrete energy losses due to the excitation of plasma oscillations has been, with some qualifications, verified experimentally.^{B8}

Depending on the choice for $\bar{b}_m$ or $\tilde{b}_m$, stopping by plasma electrons can be made much more efficient than by an equivalent number of bound electrons; see Eq. III.8 below. Unfortunately, the choice of these parameters or alternate derivations is not obvious. The choice of $b_m = I_d$ seems appropriate for stopping by the plasma's positive ions, but b_m equal to the inter-electron distance seems more appropriate for the electrons,^{D8} and the above choice of $\tilde{b}_m$ is motivated only by the early results for plasma effect.^{B22} There have been a series of studies of weakly ionized plasmas with $E_0 \leq 200$ eV (less than 1% single ionization) based on a result^{S4} similar in form to Eq. III.6 (see Ref. F2 and the citations therein). They observe that about 35% of E_0 , for $E_0 < 200$ eV is lost to the thermal electrons, with this percentage decreasing as E_0 increases. Other parameters also reflect a dependence on the ionization fraction and can qualitatively be related to the frequent collisions between free electrons that exchange small amounts of energy.

Another group^{N2,G10} is studying energy deposition of $E_0 \sim 400$ keV electrons in relatively high-temperature ($kT \approx 1$ keV) plasmas. Their approach uses a relativistic version of the first term and unmodified second term appearing in Eq. IV.6. They calculate deposition profiles that show enhanced range shortening with decreasing target density and increasing target temperature. These plasmas show a large degree of ionization, but still the target material is not completely stripped of electrons. The contributions from the bound electrons are found by using Eq. III.2, together with an adaptation of standard methods, to estimate an I value appropriate for their plasma. This is probably accurate for their conditions of $E_0/kT \sim 400$, but there is some question as to the applicability of Eq. III.2 to the treatment of electron-ion scattering with $E_0/kT \leq 10$. This is seen by investigating Fig. III.1, where the collision strength Ω (proportional to $E_0\sigma$) is shown as a function of $x = E_0/\Delta E$ for the $(2s)^2S - (2p)^2P$ transition in Ne VIII. The curve labeled BU is the Born cross section on which Eq. III.2 is based. The DWU curve is based on distorted-wave theory, which is believed to be very

accurate.^{P5} The important features are the finite value for the cross section at threshold, $x = 1$, for DWU theory, while Born theory predicts a zero value at $x = 1$ and the lowering of DWU below Born values for $x > 5$. Both features are due to the Coulomb interaction between the ionic target and the incident electron.^{P5} It is expected that these changes will be less noticeable but still present for ionization.^{B16} A quantitative study of these Coulomb effects is not available, but some differences can be expected, especially for $E_0/kT < 10$.

The low-energy region, $E_0 \leq 10I_i$ where I_i is the ionization energy of the i th ion, probably cannot be treated by methods outlined above if the ionization fraction is reasonably large. Each ionization stage, together with its expected distribution in excited states, will have to be treated as a separate constituent, and then the Bragg-Kleeman additivity approximation must be used to describe the macroscopic plasma properties.

A very few experimental data are available to test the above theoretical arguments. Little has been accomplished in testing stopping by the collective effects of electrons in plasmas.^{B8} Alternative procedures have been developed for room-temperature solids (see below), but these also remain untested. The qualitative predictions of other quantities, such as certain line emissions, have had some experimental verification^{F2} but, again, detailed comparisons of experimental data and theory are rare.

$E_0 < 10 \text{ keV}$ Considerations

One difficulty with using Eq. III.2 at small E_0 is the failure of the first Born approximation to accurately represent the σ_1 . Using Eq. III.1 and better cross sections than Born is not yet a viable alternative, since adequate data are not generally available. (See Refs. D3, G12, and G3 for examples of the approximate σ_1 data necessarily used in treating a specific substance by this approach.) This situation is probably more serious for more massive incident particles than electrons (see Ref. D1

for an example for protons), and is compounded by rearrangement-collision events not included in the sum indicated in Eq. III.1.

The remaining difficulty with Eq. III.2 for small E_0 is its failure to adequately represent sums over first Born cross sections due to the neglect of energy conservation. So-called shell corrections have been constructed^{B9} for this problem and are much in use for heavy particle stopping power predictions. These shell corrections are currently available for the K and L shells for protons or more massive particles.^{B9, W1, B11} The range of Z in this work is unfortunately not optimal. Some additional data have been created from the study of experimental measurements,^{B10} but they seem to have little use in the setting of electron stopping.^{B8}

The statement has been made^{B10} that shell corrections are small for large E_0 and can be made for electrons by using the heavy-particle results.^{W1} The first part is true, but the interesting range of E_0 for electron stopping includes regions for which these corrections are large. The second part, that the heavy-particle corrections can be used for electrons, is not correct, because the basic form of Eq. III.2 is different from that for heavy particles,^{D1} and available theoretical shell corrections make a simplifying approximation not appropriate for electrons.^{W1} However, a method capable of extracting shell correction data will be described in the following paragraphs. The ranges of E_0 and Z for which these corrections are important will be illustrated by numerical examples.

The value of the closure-relationship results, discussed above, makes the use of Eq. III.2 to as low an energy as possible very attractive. (The data shown below indicate the use of Eq. III.2 for $E_0 \leq 5$ -10 times I is open to serious question.) Appropriate shell corrections will serve to better define and extend to smaller E_0 the range for which Eq. III.2 can be used. Correction terms for the i th collection of target electrons to

be added to Eq. III.2 are defined in the non-relativistic limit as

$$C_i = -\rho^{-1} (dE/dx)_i + \overline{\rho^{-1} (dE/dx)_i}, \quad (\text{III.7})$$

where

$$-\rho^{-1} (dE/dx) = 2\pi e^4 Z_i N(E_0 A)^{-1} \ln \left[\frac{E}{2} \frac{E_0}{I_i} \right] \quad (\text{III.8})$$

This definition of C_i differs somewhat from the usual definition.^{B8} The quantity $-\rho^{-1} (dE/dx)_i$ is to be calculated from the best available cross-section data by using the analogue to Eq. III.1 appropriate for the i th set of electrons. Equation III.8 is presumed to be the stopping from the i th electrons, which constitutes their contribution to Eq. III.2. Equation III.8 is written in its non-relativistic form, since shell correction terms are expected to be unimportant for relativistic E_0 .

If one is fortunate enough to have good data for $-\rho^{-1} (dE/dx)_i$, the Z_i and I_i parameters appearing in Eq. III.8 can easily be assigned by fitting Eq. III.8 to these data. This fit should be done for large E_0 and care that these data fit the appropriate functional form should be exercised. An alternative determination of Z_i and I_i for K and L shells can be obtained from existing heavy-particle data.^{W1}

Some typical data for C_i are shown for the L shell of Al in Fig. III-1. The Z_i and I_i used in this calculation were extracted from the $-\rho^{-1} (dE/dx)_i$ data given in Ref. A2 by fitting Eq. III.8 to their highest-energy data, $E_0 \approx 10$ keV. These parameters are shown in Table III-II. The 2s-data appear reasonable. However, $Z_{2p} \sim 6.0$ (the number of equivalent electrons) is expected, although it is not an absolutely inflexible requirement, but I_{2p} is probably too small relative to I_{2s} .

The relative importance of the 2s, 2p shell corrections for Al can be seen by comparing the data shown in Fig. III-2 with the uncorrected prediction of Eq. III.2, which is shown as curve 1 in Figure III-3. For $E_0 > 300$ eV, it can be seen that C_{2p} and C_{2s} are no more than 10% of the uncorrected stopping power. The fact that they almost cancel for $E_0 > 300$ eV may be a result of unreliable correction data, as discussed above. Nevertheless, these corrections are relatively small for $E_0 > I_1$. On the other hand, these shell corrections become quite large for $E_0 < I_1$. The situation is qualitatively similar for heavy-particle stopping, except the shell corrections generally appear more important over a much broader energy range for $E_0 > I_1$. See, for example, Fig. 8d-2 shown in Ref. B10 or data given in Ref. A4.

The above situation suggests a method for deriving shell corrections from the existing heavy-particle shell-correction data.^{W1} Since the shell correction is relatively small in the $E_0 > 1.17 I_1$ region and

$$-d^{-1} (dE/dx)_i = 0, \quad E_0 \leq \Delta E_i \quad (\text{III.9})$$

but is otherwise unknown for the electron case, the approximation

$$\begin{aligned} C_i &= 0, \quad E_0 \geq I_1 / \sqrt{e/2} \\ C_i &= -p^{-1} (dE/dx)_i, \quad E_0 \leq I_1 \sqrt{e/2} \end{aligned} \quad (\text{III.10})$$

is suggested. Equation III.10 will be a lower bound to C_i for $E_0 < 1.17 I_1$ and smaller in magnitude for all E_0 .

The dashed curves shown in Fig. III-2 show results based on Eq. III.10 for the 2s and 2p electrons in Al. The maximum error occurs at $E_0 = 1.17 I_1$, and it decreases rather rapidly as E_0 decreases below the value. The error for larger E_0 is not too large, and the uncertainties in

Z_{2p} , I_{2p} lead one to expect that Eq. III.10 is about as good a guess as any in this E_0 range.

Figure III-3 shows typical stopping-power data for Al. Curve 1 is the usual Eq. III.2 data for Al, and curve 2 shows the effects of adding the K-shell correction data as obtained from Eq. III.10 and the parameters given in Table III-II. Curve 3 includes the L-shell correction data corresponding to the use of Eqs. III.7 and III.8. These correction data are the solid-line curves shown in Fig. III-1. The remaining theoretical curves shown in Fig. III-3 result from various model evaluations of Eq. III.1. Curve 1 certainly represents the preferred data for $E_0 \sim 1.0$ keV and curve 3 probably represents the preferred data for $E_0 > 0.1$ keV. The - - - curves in Figs. III-3 to III-6 are based on recent theoretical calculations. Although their low-energy behavior is untested, the high energy agreement with Eq. III.2 is not too satisfactory. The - - - curve in Fig. III-2 was generated by the direct evaluation of Eq. III.1, using first Born σ_i data, along with a model for the valence electrons.^{A2}

It is difficult to verify the above claims by comparison with experimental data. The measurements are apparently hard to make, and there are few data available. Fig. III-4 shows the available experimental data for Al, along with a repeat of part of the theoretical data shown in Fig. III-3. Curve 1 is the relativistic, Eq. III.2, data or the DATAPAC IV data used in various transport codes.^{H4} The agreement between the few experimental data and theory is excellent for $E_0 > 10$ keV. The data for $E_0 \sim 1$ keV are quite scattered and no conclusion is obvious.

The classical theory of stopping power derived by Gryzinski^{G7} seems to have been rather neglected and, other than the author's optimistic appraisal, little discussion is available in the electron-stopping literature. This approach does currently receive some attention in the context of heavy-particle stopping (see, for example, Ref. J2 and the references

cited therein). This approach consists of the sum-of-cross-sections method stated by Eq. III.1, where the σ_i data are based on Gryzinski's cross sections. The result is extremely simple and has form ^{G7}

$$\begin{aligned} \sigma^{-1}(dE/dx) = & \sum_i N_i \sigma_o \Delta E_i^{-1} (N/A) \left(\bar{v}_i^2 / v_o^2 \right) \left\{ v_o^2 / v_o^2 + v_i^2 \right\}^{3/2} \\ & \times \left[1 - \left(\Delta E_i / E_o \right) \right] \left\{ \bar{\epsilon}_i / \left(\bar{\epsilon}_i + \Delta E_i \right) \right\} + 1 \\ & \times \left\{ \left(\Delta E_i / \bar{\epsilon}_i \right) \ln(E_o / \Delta E_i) + (4/3) \ln \left[2.7 + \sqrt{(E_o - \Delta E_i) / \bar{\epsilon}_i} \right] \right\} \quad (\text{III.11}) \end{aligned}$$

Although Gryzinski's starting point is classical mechanics, Eq. III.11 is not a classical stopping power because of the use of semi-empirical velocity distribution for the bound electron in deriving σ_i (see the discussion in Sec. IV).

The use of Eq. III.11 is obvious once the structure of the target can be characterized in terms of N_i , $\bar{\epsilon}_i$, and ΔE_i . These data are not always readily available, however, and the problems become more acute for conducting media. A conductor has a finite occupation, N_i , of a conduction band that will allow ΔE_i to approach zero. Equation III.11 can approach infinity for this circumstance unless the target electron's speed, v_i^2 , is arbitrarily taken equal to zero, and it is, therefore, not reliable in the $\Delta E_i \rightarrow 0$ limit. However, it is obvious from Eq. III.1 that the contribution to stopping by processes for which $\Delta E_i \rightarrow 0$ is extremely small. The crude model of Al described below will illustrate the advantages that result from these circumstances. The lowest possible excitation assumed for Al is taken to be 10 eV for the $(3s)^2(3p)$ valence electrons. Every excitation greater than 10 eV is assumed to be in the continuum. The excitation energies of the L and K shells to this continuum are taken to be 100 eV and 1.56 keV, respectively. The average

kinetic energy ϵ_i of each electron is taken equal to its "ionization" energy.

The results from this model of Al and Eq. III.11 are shown in Fig. III-3 by the dotted curve. For $E_0 > 1$ keV, although not obvious from the graph, this curve shows the Gryzinski results decreasing faster than the Eq. III.2 data as E_0 increases. Again, the Eq. III.2 data are preferred in this energy range. This shape of the Gryzinski curve is probably the result of the inappropriate large- E_0 behavior of σ_i (see the discussion in Sec. IV). The Gryzinski stopping agrees rather well with the Born evaluation of Eq. III.1, the - - - curve in Fig. III-3, for $100 \leq E_0 \leq 1000$ eV. The model described above seems too crude to be of any value for $E_0 < 100$ eV.

Theoretical data are shown in Figs. III-5 and III-6 for Cu and Au. Curve 3 for these two cases was constructed from the K- and L-shell corrections based on Eq. III.10 and data shown in Table III.II. Similar shell-correction data can be constructed for essentially all relevant Z by using the methods described here and the data available in Refs. B9 or W1. It is obvious that the $Z = 79$ case shown in Fig. III-6 requires higher shell corrections for $E_0 \leq 2 - 4$ keV. Careful construction of these higher shell corrections, along the lines used in Ref. W1, can certainly be accomplished with some effort. Some methods outlined in Sec. IV could provide these data more quickly and with less reliability.

The only alternatives are the calculations represented by the dot-dash lines and Eq. III.11. The high-energy behavior of these theories is not satisfactory, so some type of empirical treatment to obtain continuity with Eq. III.2 for large E_0 is necessary before they can be used. For example, the Gryzinski model, Eq. III.11, could be used as an extrapolation formula to obtain data in the small- E_0 region. The large- E_0 defects of these data leave any such procedure open to criticism.

Summary

The collisional stopping-power information being used in the transport code, Eq. III.2, is estimated to be accurate for $E_0 \geq 10$ keV and media in a normal temperature and pressure environment. As is pointed out above, however, more recent data are available for the parameter I and the density-effect correction appearing in Eq. III.2. The interdependence of I and δ is emphasized. Some question has been raised concerning the code use C^I of δ for various temperature and pressure conditions. The use of Eq. III.2 for (partially) ionized media is questioned on grounds of principle, but no alternatives are well-documented. The Gryzinski stopping-power formula was examined and applied to one case; it is not strongly recommended as an alternative theory. The collisional stopping information based on Eq. III.2 is shown to be in error for $E_0 \leq 10$ keV and $Z > 29$ by deriving shell corrections. K- and L-shell correction data based on this derivation can be made available for all Z , but additional information for higher shells and large Z is needed.

TABLE III-I

Average Excitation Energy Comparison for Small- Z Elements

Z	I/eV		
	Code Value	Theoretical Value*	Experimental Value*
1	18.7	14.8, 15.0 (D2)	18.8 (A4)
2	42	41.7, 41.0 (D2)	41.7 (A4)
3	38	38.8 (D2)	39.0 (B6), 47.1 (A4)
4	60	66.1 (D2)	64.0 (B6), 62.7 (A4)
7	85	82 (D3), 78.8 (Z2)	86.7 (A4)
8	89	94 (D3), 93.6 (Z2)	97.7 (A4)
20	228		196 (A4)
40	420		378 (A4)
57	584		480 (A4)

*The reference citations enclosed in parentheses indicate the data source.

TABLE III-II

Bethe-Block Parameters for Use in Eq. III.8

i	Z_i	I_i	Comments
2s Electrons in Al	1.74	0.404 keV	Fit to Ref. A2 Data
2p Electrons in Al	6.33	0.208 keV	Fit to Ref. A2 Data
1s Electrons in Al	1.79	2.23 keV	Derived from Ref. W1 Data
Total Al	13.00	0.163 keV	I determined by Eq. III.5
Total Cu	29.00	0.314 keV	I determined by Eq. III.5
Cu K-Shell	1.64	10.8 keV	Derived from Ref. W1 Data
Cu L-Shell	7.91	1.53 keV	Derived from Ref. W1 Data
Total Au	79.00	0.797 keV	I determined by Eq. III.5
Au K-Shell	1.47	77.1 keV	Derived from Ref. W1 Data
Au L-Shell	6.177	11.2 keV	Derived from Ref. W1 Data

Figure III-1. The collision strengths, $\Omega \propto E_0 \sigma$, for the $(1s^2, 2s) {}^2S - (1s^2, 2p) {}^2P$ transition in Ne VIII are shown as a function of $x = E_0/\Delta E$ for various theoretical calculations. The BU curve represents first Born, the CB curve and $\blacktriangledown, \blacksquare$ points represent Coulomb-Born, and the DWU curve represents distorted wave results.²⁵

Figure III-2. Stopping-power corrections (see Eqs. III.7 and III.8) for the indicated electrons in Al are shown as a function of E_0 by the solid curves. The dashed curves are the approximate corrections discussed in the text.

Figure III-3. Stopping-power data for Al. Curve 1 is the Eq. III.2 data. Table III-II presents the parameter values used in evaluating Eq. III.2. Curves 2 and 3 include the K-shell and K- plus L-shell corrections, respectively, as discussed in the text. The -- curve is from a statistical model of Al structure, Ref. A1, and --- is from the direct use of Eq. III.1 together with first-Born cross-section data, Ref. A2. The curve is from Eq. III.11 and the model discussed in the text.

Figure III-4. Stopping-power data for Al. Curves 1, 3 and --- are theoretical data repeated from Fig. III-3. The experimental $\circ$ points are from Ref. K3, $\bullet$ are from Ref. G5, and $\cdot$ are from Ref. G4.

Figure III-5. Stopping-power data for Cu. Curves 1 and 3 are as defined for Fig. III-3. The --- curve represents theoretical data from Ref. A1.

Figure III-6. Stopping-power data for Au. Curves 1 and 3 are as defined for Fig. III-3. The - - - curve represents theoretical data from Ref. A1.

IV. COLLISIONAL IONIZATION

The ionization cross section is one of the more important quantities appearing in the treatment of electron transport or plasma phenomena, and it remains the most enigmatic. The large volume of data and the number of reviews devoted to this topic support these claims. In the context of the electron-transport problem, the ionization cross section is required directly for the generation of cascade electrons and inner-shell vacancies. The latter is fundamental to the generation of X-rays. Indirectly, this same cross section is required for the stopping power and straggling in a medium, and, ideally, the same cross-section data would appear in the treatment of each of these subjects. However, special circumstances-and/or difficulties usually result in the use of different approaches for the different problems; see Sec. III for the special methods used for treating the stopping power.

A number of recent reviews of various ionization phenomena have been published, including Refs. P2 and M1, which are mainly concerned with inner-shell processes, and Refs. K4, B15, and V2, which concentrate on the ionization of valence electrons. Inelastic cross sections for incident electrons and structureless heavy particles become identical for large and equal collision velocities, so some useful information can be gleaned from the heavy-particle literature.^{B24} Many earlier reviews are cited and summarized in these references. Because of the large amount of data available on this subject, the following discussion concentrates on the K-shell ionization process, and will illustrate the state of knowledge in its best light. Passing reference to L-shell and valence-shell ionization will be added only to outline the situation in these areas.

Despite the large number of publications, there are not many experimental data from different laboratories for the same set of independent parameters. The agreement is often poor for those few cases

where comparisons are possible.^{P2} The lack of a complete set of experimental data and the lack of unanimity for some cases cause the following discussion to be focused on theoretical methods. In addition, the electron-transport problem requires cross-section data for all atoms from threshold to extremely relativistic collision energies. Theory provides the required economic representation of such a large quantity of data and the rationale for the interpolation or extrapolation methods used to obtain missing data.

Weak-coupling theories are the most sophisticated that are routinely applied to the ionization problem. The very few distorted-wave (DW) calculations and semiclassical corrected Born (B) theory treatments [the so-called Glauber method (G)] available have been summarized in Ref. P4. Coulomb-Born (CB) calculations have been made for a limited number of targets and range of collision energy (see Ref. B16). A large number of B-approximation calculations are available (see Refs. P2, M1, B15, and V2), although these data leave parts of the desired ranges for many parameters untouched. The most plentiful data are based on some version of the binary-encounter model (BEM). Because of the well-known difficulties of the BEM as solved by classical mechanics,^{P4} the super-position of a quantum treatment of the "distant" collisions is often attempted (Q+BEM). Finally, there are any number of formulas with parameters adjusted to best represent available data. These will be designated "semi-empirical formulas" (SEF). These various approaches, and combinations thereof, are now outlined.

DW and G Methods

As indicated in the previous paragraph, there are few available data for ionization from quantum based theories more accurate than B (or CB in the case of ions) theory. These data are essentially available only for hydrogenic models of the targets.^{G13} The most interesting feature of these studies is shown by Fig. 12 in Ref. P4. There the usual tendency of standard B theory to be too large, in this case by almost a factor of two, in the neighborhood of the cross section maximum is displayed. A simple modification of B theory reduces the error by about one-half,^{B15} but various versions of DW theory are found to be in even better agreement with

experiment.^{P4} The trends of B-theory errors with increasing ionization potential, I , are not known, but DW remains superior to B theory for any circumstance.

The apparent increased reliability of DW over B (or CB) theory near the cross-section maximum is important for two reasons, if one considers the problem of K-shell ionization as a function of nuclear charge Z of the target atom. First, the value of the cross section for all collision energies, E_0 , is dominated by its "maximum" value if relativistic kinematic effects become important ^{Q1} for $E_0 \approx 5I$, where I is the ionization energy. This will occur for $Z \geq 80$. Second, and most important, as Z increases from 2, the field experienced by the scattering electron must necessarily deviate considerably from either the free or Coulomb field assumed in B and CB theories, respectively. The DW and G approaches should adequately describe this effect.

The systematic application of DW theory to the ionization problem has not been attempted. The main reason is the partial-wave decomposition required to evaluate the cross section, and the resulting large computational cost and data-organization problem. Techniques that address the computational-cost problem have shown some success (see for example, Ref. P5), and the data organization is mainly a matter of program effort not in any way limited by present-day computer technology. It appears that it is only a matter of time before thorough DW studies are performed. One alternative to the partial-wave approach for including distortion is the G method. The numerical problems encountered are not trivial, however, and great advantages of the G over the DW method have not been clearly established.^{P4}

It is unlikely that a "full" relativistic DW calculation will soon be done. Approximate treatment of parts of this problem is easily within reach, however. The relativistic effects on the target structure observed for $Z > 30$ is generally believed to be accurately treated by simple changes within the usual non-relativistic formalism.^{L4} The kinematic effects expected for large E_0 can be handled by today's computer capacity, but the effort and expense would be large. The alternative of using the available

relativistic B theory ^{B20} to extrapolate a non-relativistic calculation into the relativistic E_0 region is very attractive and will probably prevent any serious theoretical efforts in this area.

B Methods

A large number of full B calculations of the K-shell ionization cross section have been done in the non-relativistic formalism. A recent review gives a good summary of these data.^{P2} Only a few treatments systematically consider a wide range of targets, however, and Table IV-I presents a summary of some of these data. To facilitate comparison, cross sections are shown relative to the SEF Gryzinski cross section discussed below. The Gryzinski cross section is said to be reasonably accurate and these ratios should be a weak function of Z for this case.^{P2} The B data from Ref. M3 is in good agreement with Gryzinski but shows a tendency to be larger at large x. These B data, which are based on the Hartree-Fock-Slater target wave functions, are certainly preferred in the large-x range. The data from Ref. R2 relies on scaling laws for hydrogenic systems and could be considered a CB calculation appropriate only for electron-positive ion collisions. Indeed, this method has recently been extended to other configurations and is recommended for the treatment of positive-ion ionization.^{G11} The Ref. R2 data seem to agree fairly well with the other B data, but the extension of this method to other problems is severely limited because of the hydrogenic target descriptions. Neither of these theories provides data for relativistic collisions, although the information required to extend the data from Ref. R2 by techniques described below is available.

There are many B calculations of electron-atom ionization cross sections at non-relativistic E_0 for valence shells in small-Z targets. References P7 and M3 present more data than most studies. These calculations have the advantage of using Hartree-Fock^{P7} or one-electron orbitals based on Hartree-Fock wave functions^{M3} which are a considerable improvement over hydrogenic models. These data will not be considered further other than to note that Refs. P7 and M3 do provide data that perhaps could be used to describe L-shell ionization.

Several relativistic calculations of K-shell ionization, more or less complete with respect to the relativistic phenomenology, have appeared.^{A3,C3,D4,D5,P6,S13} The greatest problem with many of these calculations is the use of the scaled hydrogen model to describe the target ground state and a similarly scaled hydrogenic continuum orbital. The first of these calculations^{A3} is available in a convenient form for only a relatively restricted range of parameters, $Z < 30$ and $x \leq 20$, and has a tendency to be quite small. (See the data in Table IV-I that is given for Ref. A3.) An update of this calculation^{D5} proves to be larger and somewhat more in accord with available relativistic experimental data. (See the data presented in Table IV-I for Ref. D5.) These latter data^{D5} do not have severe restrictions on the ranges of Z and x but are not presented in a convenient form. However, abstract interpolation formulas are given that could be developed for wide-scale applications. The main differences between Refs. A3 and D5 are the retention of a few higher terms in Ref. D5 and the inclusion of a correction term in Ref. D5 that approximately accounts for the structure of the target not included in the hydrogenic model. This latter correction is by far the most important, and it is quite large as can be seen from Table IV-I. The structure correction was first used in this context by Ref. P6. References P6 and D4 present data for only a very few targets. The numerical accuracy of some of the data from Ref. P6 have been questioned.^{D4} There are a number of details unique to each of these two studies, but they will not be discussed because of their limited range of applicability. The most recent of the relativistic calculations, Ref. S13, presents many advances, although some details concerning the treatment of the relativistic interactions are not clearly stated. The target description, most important of the advances, is identical to one that has proved successful in photoionization calculations (see the discussion in Sec. VII). Simple formulas that represent the cross sections as a function of E_0 are provided. The only inconvenient aspects are the $E_0 \geq 50$ keV and $Z \geq 18$ restrictions. This reference also provides ionization cross sections for L_I , L_{II} , and L_{III} hole formation.

Figures IV-1 and IV-2 provide a comparison between theory and experiment for K-shell and 2p-subshell ionization. Cross sections for all

targets would lie on a single line in these figures if classical scaling were obeyed. Obviously, K-shell comparisons are much better than the 2p-subshell comparisons. Classical scaling is not a quantitative feature, and the disagreement between experimental data for 2p ionization of the Ar target should be noted.

A detailed comparison of these relativistic data with experiment will not be presented here. The original papers present this information along with a comparison of the various theoretical results. The following points can be made from these comparisons:

1. The agreement between experimental data from different studies is not particularly good for the few examples of overlapping measurements.
2. The data from Refs. A3 and D4 tend to agree fairly well, as they should, and be somewhat smaller than experiment.
3. The few cross sections available from Ref. P6 are in somewhat better agreement with experiment if one excludes a few selected points.
4. The Ref. D5 data seem to show the best general agreement with experiment and, as pointed out above, they are potentially available for a wider variety of targets and collision energies than are the other studies.
5. The few comparisons presented in Ref. S13 indicate these theoretical data are in reasonable agreement with experiment.

One of the earlier applications of the B approximation to this problem was made by Bethe.^{B14} He was able to express the ionization cross section for a particular nl subshell in the convenient form^{P2}

$$I_{nl} \sigma = 6.51 \cdot 10^{-14} Z_{nl} b_{nl} x^{-1} \ln \left(\frac{c_{nl} x}{1 + \sqrt{1 + c_{nl}^2 x^2}} \right)^2, \quad (IV.1)$$

where Z_{nl} is the number of equivalent electrons, and b_{nl} , c_{nl} , are constants determined by the B theory. Equation IV.1 is written explicitly for ionization and in a form that minimizes the Z dependence of b_{nl} , c_{nl} .^{P2} Reference B14 lists b_{nl} values for extensive ranges of Z and nl as calculated by a hydrogenic model. (Examples are shown in Table IV-II.)

The cross section defined in Ref. B14 is for the total excitation of the nl level, and not just its ionization. This accounts for the small- Z differences observed in Table IV-II. Bethe's definition is appropriate for the total production of K-shell vacancies. However, in keeping with standard custom, the term ionization will be used here for this cross section even though the total K-shell excitation process is more applicable to the electron-transport problem.^{C1}

The quality of the target wave functions is the single factor that determines the accuracy of the b_{nl} values. Precise b_{1s} data are not available, but the Ref. S13 determinations should be the most accurate shown in Table IV-II. However, note that the Ref. B12 data more nearly satisfy the intuitive requirement that b_{1s} approach the hydrogen value, 0.283, as Z becomes large. Many of the non-relativistic B calculations cited above contain b_{1s} information, but these data were not extracted. The only conclusion now possible is that differences in the b_{1s} values are a measure of the uncertainty in the ionization cross sections.

Unfortunately, c_{nl} values are only available for a few very simple targets^{I1} and some isolated examples based on data-fitting procedures.^{P2} The hypothesis that a reliable alternative to the missing c_{nl} values can be

constructed from the photoionization cross section, plus the appropriate use of the BEM part of the Q+BEM method described below, could be easily tested. This loosely-defined approach has not been used previously, but it is closely related to the Bethe-Born theory which has been shown to be quite useful in many studies.¹²

A complete set of b_{nl} , c_{nl} values would provide the ionization cross section for all E_0 . The relativistic equivalent to Eq. IV.1 is clearly implied in Ref. B12. Equation IV.1 is incorrect in the $x = 1$ (threshold) limit, but it is no more pathological than any of the other non-BEM theories, and any number of empirical corrections to Eq. IV.1 would not lose much information in this highly uncertain E_0 region. This construction, plus the alternative to the missing c_{nl} data described in the preceding paragraph, would provide the most complete set of non-SEF (see below) data existent for this problem. These data probably would be the most accurate of those available for essentially all target processes and all E_0 . In addition, the updating of this representation by changing the b_{nl} , c_{nl} parameters to better represent improved calculations or new experimental data would be a relatively easy process. This suggestion is similar to that made in Ref. H8, but has potential advantages due to the more general (accurate) target description and the avoidance of one approximation made in Ref. H8.

An interesting and simple method for extending the many non-relativistic B calculations into the relativistic E_0 region consists of carrying out the usual B calculation simply augmented by maintaining relativistic energy conservation. The first examples of this were the calculations by Fundamirsky, reported on page 155 of Ref. M2, for N1 K-shell ionization by $300 \text{ keV} \leq E_0 \leq 800 \text{ keV}$ electrons. An even simpler scaling based on the ratio of the relativistic to non-relativistic Coulomb velocity distribution function as used in the binary encounter method (BEM) has been proposed.^{Q1, P8} Both methods are known to fail for sufficiently large E_0 , and probably should not be used for E_0 greater than the incident electron's rest-mass energy.^{P10} The fact that such simple methods appear to work even to $E_0 \sim mc^2$ is something of a surprise, and may be illusory, since the more soundly-based theoretical studies of relativistic-

electron scattering cited above indicate there are many large terms neglected in the non-relativistic theory. The theoretical foundations for the relativistic equivalent to Eq. IV.1 (see Ref. 12) are impeccable,^{P10} however, and it provides a reliable prediction for large E_0 and all cases for which the threshold energy is not itself relativistic.

The preceding discussion is an attempt to summarize the applications of B theory to ionization by electrons. Ionization by heavy particle collisions is an active area of investigation^{B24} and can contribute information to the equivalent electron-scattering problem for large E_0 . The major thrust of these studies is directed at problems not encountered in electron scattering. Hence they seldom provide actual data transferable to the interests of this report. They do provide comparative studies of the theories being discussed here and these general observations are useful. In brief, these many studies^{K7,K8,L5} indicate K-shell ionization is relatively well described (for large E_0) by both B and BEM theories. The situation is less well-defined for L-shell ionization. The agreement between different theories and between experiment and any one theory is poorer for this case. The B theory seems to be favored over other approaches^{H7,C6} for large E_0 , but the evidence is not conclusive.

BEM and Q+BEM Methods

Binary-encounter models, based on classical mechanics as applied to ionizing collisions, have a long history.^{P4} However, they were mostly ignored until the work of Gryzinski^{G7} sparked a renewed interest in this approach. Reviews of this extensive field are given in Refs. P4 and B18. BEM methods are extremely attractive because of their relative simplicity. However, their range of applicability appears quite limited and, despite the many attempts to improve on the basic model, one essential difficulty has not been removed, that is, their failure to correctly include contributions from large-impact parameters.^{P4} The resulting cross section has an incorrect energy dependence for large E_0 and is not useful for the problems under consideration here. However, by adding the large-impact-parameter contributions ad hoc (the Q+BEM method), rather useful results can be

obtained. A different solution introduced by Gryzinski will be discussed in the paragraphs dealing with semiempirical results.

The simplest BEM results applying to the relativistic collision problem is the Møller classical cross section. This assumes the scattering electron is at rest and ignores the atomic field and binding effects experienced by the target electron. Rather more sophisticated solutions to the BEM problem are available in the non-relativistic region.^{B18} Of particular interest are the inclusion of a velocity distribution for the target electron and the derivation of a "focusing factor" that does include the effects of the atomic field on the collision event. It is of some interest that this focusing factor destroys some of the good agreement of BEM results^{B18} for small E_0 and is particularly unsuccessful for scattering by ions.^{B16} The available treatments of K-shell ionization ignore all the improved versions of BEM theory, and hence the comments presented here will be limited to the observation that a systematic study of these theories for inner shell ionization would be quite useful in the context of their use in the Q+BEM theory.

The Q+BEM model consists of adding to the BEM cross section the quality

$$Q = \left(\sqrt{3} \alpha E_0 / H \right)^{-1} \int_0^{E_0} \frac{\sigma_{PI}(\xi) g(\xi, b_c)}{\xi + 1} d\xi, \quad (IV.2)$$

where σ_{PI} is the photo-ionization cross section, g is the Kramers-Gaunt factor, and H is the Hartree unit of energy. The g -factor that appears in Eq. IV.2 depends on the choice of an impact-parameter b_c to divide the Q and BEM contributions. Obviously, the BEM contribution must also reflect the choice of b_c . There is no known best choice^{B10} for b_c , and this is of some importance since, unlike the stopping power result discussed in Sec. III, the Q+BEM cross section will depend on b_c . The idea for treating high-energy collisions in this way dates back to the work of Williams^{W2} and has since been used in the Q+BEM context by a number of authors.^{B16, S3}

The so-called ECIP (exchange-classical impact parameter) theory developed by Burgess,^{B18,B25} represents the most mature and systematic study of the Q+BEM approach. A careful choice of the BEM cross section was made.^{B18} The choice of b_c and the construction of Q have also been thoroughly studied.^{B25} The many applications have been concerned almost entirely with outer-shell electrons and non-relativistic collision energies. If one makes the best choice of the remaining alternative variations available to this theory, rather good agreement with experiment is usually found,^{B16,B26}. The ECIP theory has not been adapted to relativistic E_0 or applied to inner-shell ionization, so it can contribute no data to this discussion. Its success in other problem areas does make it a likely theoretical tool.

Two examples of Q+BEM theory have been worked out in simple form for K-shell ionization and have been published by Kolbenstvedt.^{K5,K9} His first result uses a hydrogenic model for the photoelectric cross section, a non-relativistic approximation to σ_{PI} , and ignores energy conservation when evaluating Eq. IV.2. The results of this approach for non-relativistic collisions is labeled Q+BEM(K5) in Table IV-1. In his second approach, labeled Q+BEM(K9) in Table IV-1, the hydrogenic model is replaced by one which accounts for the experimental binding energy. The BEM contribution to both his results is obtained by adding the Møller cross section to his evaluation of Eq. IV.2. Some additional information for the Q+BEM(K5) cross section would be useful, since it does not reduce to the Q+BEM(K9) cross section when the original Q+BEM(K5) approximations are re-introduced. (This is probably a result of different choices of b_c in the two developments.)

The Q+BEM(K5) and Q+BEM(K9) cross sections are in reasonable agreement with experiment and the best B theoretical results for $x \geq 4$. This is easily seen by noting the relationship of these cross sections to the Gryzinski cross section given in Table IV-1 and the relationship of the Gryzinski and experimental cross sections displayed in Fig. IV-1. The Q+BEM(K5) cross section exhibits classical scaling for non-relativistic E_0 . Classical scaling implies that one universal curve, plotted in the manner of Fig. IV-1, represents the cross section for all targets. The Gryzinski

cross section also shows classical scaling, so only one result is required in Table IV-I for the Q+BEM(K5) cross section. The Q+BEM(K9) results do not show this scaling, and the extremes are shown in Table IV-I. The maximum cross section applies to the case $Z = 2$ and the minimum applies to $Z \rightarrow \infty$ or $Z = 1$ targets.

Tables IV-II and IV-III further illustrate the character of these cross sections. The values of the parameter b_{n1} appearing in Eq. IV.1 are given for a number of cross sections. The value derived from Q+BEM(K5) is very near but less than the $Z = 1$ theoretical value, as it should be, when making the indicated approximation in evaluating Eq. IV.2. (Equation IV.2 completely determines the b_{n1} that appears in Eq. IV.1, since classical or BEM cross sections do not contain terms like $O(x^{-1} \ln x)$ for x large.) The value for b_{1s} derived from Q+BEM(K9) has the hydrogenic value for $Z = 1$, increases sharply for $Z = 2$, and then appears to decrease again to the hydrogenic value as $Z \rightarrow \infty$. This is, qualitatively, the expected Z -dependence of b_{1s} , but it appears to be too extreme when compared with the available experimental and theoretical data provided in Table IV-II. (It would be very interesting to derive the values of b_{n1} from the photoelectric cross sections used in the transport code.^{C1}) It seems apparent that the "energy-correction" used in Q+BEM(K9), or in B calculations discussed above for that matter, has the correct tendencies but does not adequately correct for the errors in a hydrogenic model. Since this case is about as "hydrogenic" as one can expect, reliance on this model of an atom's structure can be anticipated to reduce any precision to one that is semiquantitative in content.

A number of comparisons of the Q+BEM(K5) and Q+BEM(K9) results with experiment have been made in the relativistic range of E_0 (see Refs. D5, M4, I3, S7, S8, and D10). In general, the most successful theories are Q+BEM(K9), B(S13), and B(D5). Features such as the Z -dependence of the cross section for fixed E_0 are reasonably well represented by these two results, while serious defects are observed in the other data.^{M4}

These relativistic studies naturally bring up the question of the density effect on K-shell ionization. A theoretical investigation^{D10} of this question, using Q+BEM(K9) theory and Sternheimer's density effect correction technique,^{S2} indicates that these corrections are large for $E_0 \approx 1$ GeV. The one experimental measurement in this range of E_0 is inconsistent with the density effect corrections. The resolution of this question is important both for the ionization cross sections and the stopping power, discussed in Sec. III.

Nonetheless, the results shown here for non-relativistic E_0 and elsewhere for relativistic E_0 argue strongly for the use of Q+BEM(K9). This single algebraic form for the cross section has as good a chance as any for being near the correct magnitude and has the added attraction of possessing some of the correct Z dependent character. A more accurate treatment of energy conservation, implied by Eq. IV.2, when deriving Q+BEM(K9) would probably be one of the more useful additions, since this should improve the cross section in the important threshold E_0 region. The extension of the K5 or K9 theory to L-shell^{I3,S7} and to M-shell^{I3} ionization has been reported. No systematic set of data or description of theoretical methods was given, so the use of these results in the transport code is not yet possible. The data that are available^{I3,S7} do agree well with isolated experimental results. Some inconsistencies were observed in one application of this theory, however, and no mention was made of this choice of the important b_c parameter.^{I3} Hence, a critical evaluation of these approaches to the higher shells is not now possible.

SEF Methods

The most often used cross section of this character is the Gryzinski result,^{G7} SEF(G7), and it is the one originally used for all collisional ionization events in the transport code.^{C1} Its simplicity and general success is often described. Its derivation consists of an approximate solution of the classical BEM problem^{B18} with a completely unphysical velocity distribution function assumed for the target electron. This velocity distribution has as its sole justification the merit of producing roughly the correct large E_0 behavior of the cross section for a hydrogenic

target. (This is demonstrated in Fig. IV-1 for the non-relativistic K-shell ionization cross section and in Table IV-III for the predicted value of b_{1s} .) The classical BEM prediction for b_{n1} is zero for any realistic choice of velocity distribution and, depending on the choice of this function, gives reasonable agreement with the measured H-atom ionization cross section only in threshold region of E_0 .^{P4} Any merits of the SEF(G7) cross section are due to its great simplicity and relative success. As can be seen in Fig. IV-1, it differs by little more than +20% from all the data shown. The main disadvantage in this case is its lack of Z-dependent structure exhibited, for example, by the Q+BEM(K9) or B(D5) cross sections.

The SEF(G7) formula as used in the transport code^{C1} is intended to be applicable to relativistic E_0 . However, one comparison made in the relativistic range of E_0 claims the SEF(G7) cross section is too small;^{D6} the reason for this claim is explained in Ref. P10. (Most of the more recent studies in this area, e.g. Refs. D5, D10, I3, M4, and S7, completely ignore the SEF(G7) formula.) The nature of the relativistic SEF(G7) derivation is such that it should not be applicable for $E_0 > mc^2 \approx 5 \times 10^5$ eV and, further, this relativistic kinematic result is appropriate only for dipole-forbidden excitation events. In other words, the relativistic form of SEF(G7) is fundamentally incorrect for ionization and does not increase for increasing E_0 at a sufficiently rapid rate.^{P10}

Further data for SEF(G7) theory are shown in Fig. IV-2 for the case of L_{23} shell ionization. The breakdown of classical scaling for experimental data is obvious for this case. Nonrelativistic B calculations also fail to show classical scaling.^{P2,M3} The SEF(G7) cross section agrees reasonably well with one set of data shown in Fig. IV-2 and the agreement has been amplified and extended to the L_1 case for this one measurement.^{L2}

The results from a number of other SEF methods are indicated in Figs. IV-1 and IV-2 and Tables IV-I and IV-II. These cross section forms are all variants of Eq. IV.1 and will not be reproduced here. They originally were constructed for non-relativistic E_0 , but recent studies suggest methods for extending these formulas into the relativistic E_0 region.^{D6,P8,Q2} This

relativistic extension is based on the incorrect SEF(G7) theory, discussed in a preceding paragraph, and will therefore tend to be too small as E_0 increases.^{P10} The Lotz formulas^{L3} are available for a wide range of targets. They have the property of tending to be too small for E_0 near threshold and more or less in line with other predictions of this class for large E_0 . (See Figs. IV-1 and IV-2, Table IV-II and Ref. P8) The Drawin fits to experimental data are also available for a wide class of processes.^{D7} As ordinarily used, they show classical scaling and agree rather well with the Gryzinski prediction except for $E_0 \gg 1$ (see Tables IV-I and IV-III).

The preceding SEF methods, as well as many others, have been carefully compared with a number of experimental data in Ref. V2. Rather than go further into these examples, it is sufficient to close with the conclusion stated in Ref. V2: "(SEF's) are simple and can be used for quick estimates of ionization cross sections. But there is no complete certainty that the result is reliable. Only quantum-mechanical computations can be fully accurate. . ."

This section is concluded with a few short remarks concerning the secondary electrons produced during an ionization event. (Cascade events are postponed to a subsequent section.) The transport code uses the Møller cross section differential in angle and energy of the secondary electron for these data.^{G1} The integral of this cross section was used to constitute part of the Q+BEM(K5) and Q+BEM(K9) cross section, so some of the accuracy claimed for these cross sections applies to this case as well. It would seem the Møller prediction may be too small, since the importance of adding the "distant" collision term, Eq. IV.2, seems well established. Because of the nature of this added term, the error will be greater for those secondary electrons emitted with relatively low energy. Hence, this may not be too serious when limiting the treatment to high-energy electron transport. However, I am not aware of any quantitative tests to substantiate this hypothesis.

A recent conference^{R3} devoted to the subject of secondary electron distributions does present data that tend to support the above statement,

and some inferences can be drawn. The BEM Mott cross section differential in secondary electron energy, which is equivalent to neglecting exchange in the Møller cross section, is too small when compared with experiment.^{01,819} Errors of 20-30% are typical. The error is larger for small secondary electron energy, but it is substantial everywhere. This difference between the experimental and Mott cross sections has been observed to resemble strongly the photoionization cross section.^{K6} Since the "missing" term in either the Møller or Mott BEM cross sections is presumed to be Eq. IV.2, this observation provides strong motivation for the Q+BEM cross section and suggests an interesting correction method. It would be relatively easy to replace the Møller cross section with one consistent with the Q+BEM treatment of total ionization. Only the photoionization cross section, together with a relatively simple computation based on Eq. IV.2, would be required to generalize this approach to other than K-shell electrons.

Summary

It is believed that only Born or more exact theories have predictive value for the collisional ionization process. Data to describe these events are, unfortunately, not uniformly available over the ranges of parameters utilized in the electron-transport code. Also, a compact representation of these data is not available although formulas do exist (see the SEF discussion) that could perhaps be adapted for this purpose. A correct extension into the relativistic E_0 region is one area where improvements to the SEF formulas are demanded. Obviously, such an SEF formula could be used to represent experimental data as well. The relativistic data from Ref. S13, limited to $E_0 \geq 50$ keV and $Z \geq 18$, for ionization of the K, L_I , L_{II} , and L_{III} subshells are as good or better than any alternative information. They certainly are an advance over the Gryzinsky data, SEF(G7), now in use. The lack of small- E_0 data from this source is a serious problem. The adaptation of one of the BEM approaches to extrapolate these data into the small- E_0 region is one technique that might provide a solution, but some development work would be required.

The so-called Q+BEM theories have demonstrated considerable empirical success, but the question of a "correct" choice of b_c still plagues this

approach. Nonetheless, the Q+BEM(K9) cross section is as good as the best available for K-shell ionization and has the added advantage of having a compact algebraic form. Its main problem occurs in the threshold region of E_0 , and some caution is advised if this happens to be a dominant region in the transport calculation. Although this cross section should replace the Gryzinski SEF(G7) cross section for K-shell ionization, it must eventually be replaced by more accurate experimental or theoretical results. The so-called ECIP version of Q+BEM theory^{B18} has met with success for a variety of problems in the threshold region, $E_0 \sim I$. Future developments with one of these Q+BEM approaches are capable of providing data to replace the SEF(G7) cross section for processes other than K-shell ionization.

The SEF cross sections are only as good as the data they represent, and the general feeling is that they are good, at best, as a semi-quantitative guide. In addition, the SEF(L3) and SEF(D7) cross sections have not as yet been correctly adapted to the relativistic E_0 region. Many articles claim quantitative agreement with the Gryzinski SEF(G7) result for a variety of ionization processes. However, it has definitely been replaced for K-shell ionization by the B(D5), B(S13), or Q+BEM(K9) cross sections. Every quantitative argument points to the fact that the SEF(G7) cross section is most reliable for K-shell ionization, so its replacement for L- and higher-shell ionization is of high priority from the point of view of reliable atomic physics data. It was also indicated that the E_0 dependence of the SEF(G7) cross section is incorrect for relativistic E_0 .

The question of density effects on the K-shell ionization cross section has been investigated in the context of the Q+BEM(K9) cross section, and these theoretical predictions are in disagreement with the one pertinent experimental observation. This problem obviously remains open. The formula used to characterize the secondary electron spectrum from collisional ionization was found to be uniformly too small, but otherwise it well represents the general behavior of the available experimental data. The simplified B theory suggested here appears to be capable of correcting the magnitude problem.

None of the discussions given above mentions the effects expected if the stopping medium is at a high temperature or partly ionized. The collisional ionization cross section for an ion is expected to behave somewhat differently from that for a neutral (see Sec. III and the discussion concerned with Fig. III-1). Little quantitative information is available, however, and there is nothing in principle to suggest the neutral cross sections are qualitatively incorrect for inner-shell ionization of ions if one excludes the little-understood threshold region. A more quantitative evaluation of this question must await further study.

TABLE IV-1

Ratios of the indicated cross sections for K-shell ionization, which are discussed in the text, are presented as a function of x . The ratio is defined as the cross section from the indicated author divided by the Gryzinski K-shell ionization cross section. If a particular target is not indicated, the ratio applies to all targets.

<u>x</u>	<u>B(HJ)</u>	<u>B or CB(R2)</u>		<u>B(A3)</u>	<u>B(D5)</u>	<u>Q+BEM(K5)</u>	<u>Q+BEM(K9)</u>		<u>SEP(L3)</u>	<u>SEP(D7)</u>	<u>SEP(Q2)</u>
	*	*	*	*	*		o	o	*		
2		1.35	1.58	1.06	1.44	1.81	1.65	0.85	0.75	0.95	1.37
4		1.06	1.13	0.80	1.35	1.17	1.11	1.08	0.81	0.92	1.01
5		1.05	1.08	0.78	1.33	1.09	1.04	1.09	0.84	0.92	0.97
10	1.02	1.03	1.04	0.69	1.28	0.98	0.95	1.12	0.89	0.96	0.93
15	1.04	1.03	1.05	0.66	1.28	0.95	0.93	1.15	0.92	1.00	0.95
20	1.06	1.03	1.07	0.63	1.31	0.94	0.92	1.17	0.93	1.03	0.97
25	1.08	1.07	1.09	0.63	1.32	0.94	0.91	1.19	0.95	1.06	0.99
30	1.10	1.09	1.11	0.62	1.34	0.94	0.91	1.21	0.97	1.08	1.00
40	1.12	1.12	1.13	0.62	1.34	0.93	0.91	1.23	0.99	1.12	1.03

*The ratio applied to the K-shell ionization cross section for carbon. The ratio should be a weak function of Z .

†This ratio is for a hypothetical hydrogenic target with $Z = 128$

°The Q+BEM(K9) ratio for $Z = 1$ and 2, respectively. The ratio for all other Z values should be bound by these ratios.

TABLE IV-II

Values of b_{1s} for K-shell ionization of targets with varying Z. The experimental data are from Ref. P2 and the Q+BEM(K9) data are discussed in the text. The parenthetical theoretical entries are interpolated values from Ref. B12 and refer to total K-shell excitation. See the discussion following Eq. IV.1.

<u>Z</u>	<u>Experiment</u>	<u>B Theory</u>	<u>Q+BEM(K9)</u>
1		0.283* (1.0)	0.276
2		0.443# (1.0)	0.606
4	0.58	(1.0)	0.653
6	0.50	(0.81)	0.581
8	0.55	(0.63)	0.556
10	0.55	(0.44)	0.534
13		(0.41)	0.493
29		0.439● (0.35)	0.404
50		0.388● (0.31)	0.351
79		0.388● (0.29)	0.297

*Ref. B12

#Ref. I1

●Interpolated values from S13.

TABLE IV-III

Values of b_{1s} for K-shell ionization from theories that give predictions independent of Z.

<u>Theory</u>	<u>b_{1s}</u>
SEF(G7)	0.336
Q+BEM(K5)	0.275
SEF(L3)	0.61
SEF(D7)	0.666

Figure IV-1. $I^2\sigma$ versus x for K-shell ionization by electrons. The shaded area represents the range of experimental data found for C, Ne, N, and O by Refs. G8, G9, and B13 and data as quoted by Ref. P2. The $\circ$ symbols represent twice the H-atom ionization data (Refs. F1 and R1); $\bullet$ symbols are for He (see summary in Ref. K4); $\blacksquare$ symbols are for Li (Ref. P3); and $\square$ symbols are for C (Ref. H6). The solid curve represents the non-relativistic Gryzinski theory, SEF(G7).

Figure IV-2. $I^2\sigma$ versus x for L_{23} -shell ionization by electrons. The various symbols represent the experimental data discussed in Ref. P2 and are shown as in Fig. 6 of Ref. P2. The symbols and the target are, respectively, (x , Ar), (o , Ar), ($\blacksquare$, P), ($\bullet$, S), and ($\blacktriangle$, Cl). The solid line is the SEF(G7) cross section and the dashed line is the SEF(L3) cross section. The dash-dot line is a scaled B calculation by McGuire (see Ref. M3) applicable to all targets with $Z > 18$.

V. CROSS SECTIONS DIFFERENTIAL IN ELECTRON SCATTERING ANGLE

The angular distribution of electrons after transversing a certain distance in the target material is determined by the Goudsmit-Saunderson solution to the multiple-scattering problem.^{C1} This calculation requires cross sections differential in scattering angle for all possible scattering events. The standard method consists of describing the elastic scattering by the Mott relativistic Coulomb cross section augmented by the introduction of a screening parameter to correct for the Coulomb divergence at small-angle scattering. Reference B27 discusses the methods used to derive values for the screening parameters. Inelastic scattering effects are introduced by assuming that the angular dependence is the same for all inelastic and elastic events. This approximation and the high-energy limit of the first Born approximation predict that the ratio of the total elastic to the total inelastic cross section is Z . Hence, in this approximation the sum of differential elastic and inelastic cross sections is obtained by replacing the multiplicative factor Z^2 appearing in the Mott cross section by $Z(Z+1)$.

Elastic Scattering

The construction described above for elastic scattering is capable of relatively high accuracy in regions where first-Born theory is adequate. The proper choice of a screening parameter can represent with reasonable accuracy the important small-angle scattering region. (See page 193 of Ref. M8 for a clear and concise treatment of multiple scattering theory.) At larger scattering angles the first-Born cross section, σ_B , and the Rutherford cross section, σ_R (the non-relativistic limit of the Mott cross section), are related by

$$\sigma_B/\sigma_R \approx 1 - 6.4 \cdot 10^{-4} \frac{(\text{cosec } 0.5\theta)^{3/2}}{\beta} Z^{1/2}, \quad \theta \text{ not small}, \quad (\text{V.1})$$

if one uses the Thomas-Fermi field to represent the atom (see page 188 of Ref. M8). Equation V.1 defines an error for σ_R relative to σ_B in terms of Z , θ , and E_0 (or β). Obviously, differences are small under any conditions for $E_0 > 10^5$ eV but for $E_0 < 10^5$ eV restrictions on θ becoming small and/or Z becoming large may be necessary.

The above arguments lead one to expect the screened Mott cross section to be a reliable representation of first Born results if one excludes certain large- Z and small- E_0 ranges. This restriction is qualitatively similar to the first-Born region of validity, so only data from a more accurate theory or experiment could be expected to provide much improvement. Unfortunately, there does not appear to be a published comparison of cross sections from the transport code's data base and other available data. Such a comparison is required to justify the expectations stated here.

Recent developments have made any questions about the use of the screened Mott cross section academic. Alternatives now exist^{R6,F5,B28} which represent state-of-the-art theoretical results.^{R7,R8} These calculations are based on the relativistic distorted-wave formalism. The only known difficulties with this theory are its failure to include non-weak-coupling effects, such as target polarization and loss of flux due to other open scattering channels. The elastic scattering in the important small-angle region exceeds the weak-coupling prediction in part due to target-polarization effects. There is no known acceptable correction for this problem within weak-coupling formalisms, but it is not too important for relatively large E_0 .^{R9} For example, first-Born is reasonable for $E_0 > 500$ eV elastic scattering by He (see pages 185-187 of Ref. M8 and Ref. R9) while it is questionable for $E_0 < 500$ eV. Full distorted-wave results are, in any event, better than first-Born, although they are nearly equal for He and $E_0 > 500$ eV. In the cases of Xe and Hg, significant errors occur in the distorted-wave results for scattering angles less than 10 degrees at $E_0 = 500$ eV.^{R7,R9} For example, experimental and distorted-wave data differ

by nearly a factor of two for Hg at $E_0 = 500$ eV and a scattering angle of 3 degrees. Reference R7 estimates the energy dependence of the reliable range of scattering angles for the heavy elements is bounded for small θ by the relationship

$$\sin 0.5 \theta \geq 0.5[E_0 / (13.6 \text{ eV})]^{-1/2} \quad (V.2)$$

for non-relativistic E_0 . As an illustration, experiment and theory for Xe are in good agreement for all θ and $E_0 \geq 37$ keV.^{R9} This agrees with the Eq. V.2 prediction that this theory is reliable for $\theta \geq 1$ degree. Any improvements in these small-angle and small- E_0 data will probably first become available from fitting experimental data with weak-coupling calculations that include polarization by the addition of an empirical correction term (see Ref. K10 for a typical example). Interpolation procedures might be developed to augment the limited information of this type.

The assumption that molecular targets can be treated by the appropriate superposition of cross sections for the constituent atoms has been tested and found to be acceptably accurate for certain diatomic molecules.^{R9} The troublesome cases of molecules containing hydrogen or the properties of molecules more complex than diatomics have not been considered in this context.

With the one reservation concerning loss of flux to other channels, it seems probable that there will be very little change in the distorted-wave predictions for the entire periodic table and for $E_0 \geq 1.0$ keV. This exception may become a factor in the range of large E_0 and Z where bremsstrahlung can be important. No data are available to quantify this point, but the loss of flux to this channel may provide a significant change in the weak-coupling predictions. Similar considerations occur for $E_0 < 1.0$ keV and for the larger- Z targets. Here the inelastic-excitation

channels will modify the weak-coupling prediction. A priori theoretical solutions to this problem will not soon be available for large ranges of Z and E_0 , and any improvement must come from experiment.

The data from Ref. R6 are the most useful. Data are presented for the entire periodic table in a convenient form for use in the transport problem. The energy range, $1 \text{ keV} \leq E_0 \leq 256 \text{ keV}$, when supplemented with the screened Mott cross section for larger E_0 , is adequate for most purposes. The methods used in Ref. R6 to solve the weak-coupling scattering problem, including the theory for treating exchange effects^{R8} and the wave functions required to describe the target, are consistent with the best techniques available.

Inelastic Differential Cross Sections

Very little analysis of the formula used to represent the contributions from inelastic events is available in the literature. However, qualitative theoretical results can lead to some conclusions. Inelastic collisions for E_0 greater than the threshold energy tend to be dominated by small angle scattering. This is reflected by the Born-theory result that the ratio of inelastic to elastic differential cross sections for hydrogen is θ^{-1} if $\theta > 1/E_0$ (see page 239 of Ref. M8). For general targets, Z times the ratio of inelastic-Born to screened-Rutherford cross sections can be calculated.^{P12} For large non-relativistic E_0 and $\theta > 1/E_0$ the result takes the simple form

$$Z \left\{ \sum_i + \int \right\} \left[\frac{d\sigma_i/d\theta}{d\sigma_{\text{elastic}}/d\theta} \right] \\ = \frac{S(1 - \cos \theta + 2\eta)^2}{(1 - \cos \theta)^2} \approx \frac{16S\eta^2}{\theta^4}, \text{ small } \theta > 1/E_0 \quad (\text{V.3})$$

where $S \sim 1$ for large E_0 and θ not too small (see page 240 of Ref. M8) and η is the elastic scattering screening parameter.

The right-hand side of Eq. V.3 should be equal to unity for all θ if the construction described at the beginning of this section is to be valid. This restriction is not satisfied for small angle scattering, i.e., $2\sqrt{\eta} > \theta > 1/E_0$, and as η is proportional to $Z^{2/3}$ for large E_0 ,^{B27} the situation becomes worse with increasing Z . Equation V.3 therefore indicates that the number of scatterings through small angles is seriously underestimated by the $Z(Z+1)$ scaling, while this scaling is reasonably accurate for the larger angles. It is important to note that Eq. V.3, although not directly comparable, disagrees with the more rigorous Born ratio found for the H atom.^{M8}

All deflections due to inelastic events were assumed to be the result of target excitation in the derivation of Eq. V.3. It has been pointed out that bremsstrahlung should also be included in this calculation of inelastic events.^{M11} This means that the ratio defined by Eq. V.3 is a lower bound to the desired result. Furthermore, bremsstrahlung becomes more important with increasing Z , so the error anticipated by Eq. V.3 undoubtedly underestimates the trend with increasing Z .

The above information seems to cast a severe doubt on the procedure used in the transport code to construct the inelastic contributions to the small-angle differential cross section. Reference F4 also discusses this point. In addition, there are transport data that show the improvement resulting from switching to the weak-coupling data of Ref. R6 for elastic scattering, although even larger changes are required to bring these experiments and predictions into good agreement.^{L6} It is tempting to speculate that the solution to this remaining problem is the inelastic scattering contribution. There is some information on the sum of elastic and inelastic total cross sections,^{H9} but no data were found that bore directly on the problem at hand.

The techniques described in Sec. IV for obtaining the ionization (total inelastic) cross section could be adapted to the study of this

problem and be useful in the region of E_0 for which first-Born theory is applicable.^{P12} A rather crude analysis of this problem would undoubtedly represent an improvement in our understanding, and further development of Eq. V.3 could provide compact and, perhaps, improved results.^{P12}

Miscellany

There are electron-transport applications that involve regions of parameters for which little or no information appears to be available. These areas and a brief definition of the missing information are discussed below.

The use of σ_M to extend the weak-coupling data for $E_0 > 256$ keV may be reliable, but little pertinent information is available. Also, the question of density effects in the ultra-relativistic region of E_0 has not been explored. As pointed out in the preceding discussion, density effects have been identified for the stopping power but not for individual cross sections. The use of free-atom cross sections to describe other media such as solids or plasmas are also areas that have not been explored. Experimental data for condensed media necessarily involve the use of the multi-scattering formalism, so direct tests of single-scattering cross sections are impossible.

Summary

The elastic scattering cross sections differential in scattering angle now available are of high quality, and little improvement is anticipated. Some reservations about the small-angle scattering for large Z and small E_0 are expressed, but the information now available does not indicate these questions are very important. Open questions about the application of these data to condensed media or plasmas are briefly discussed. The treatment of the inelastic cross sections differential in scattering angle was shown to be of questionable validity. This is an important area that deserves attention.

VI. BREMSSTRAHLUNG

Bremsstrahlung cross sections, both total and differential in photon energy, are required in the treatment of high-energy electron transport.^{C1} The data currently in use^{C1} are based on an adaptation^{B5} of recommendations made in 1959.^{K11} These semi-empirical data well represent the sum of experimental and theoretical knowledge available at that time. Subsequent developments have been primarily based on theory, and the following discussion will reflect this fact. In addition, the transport code must assign a direction to the bremsstrahlung photon. The bremsstrahlung cross section differential in both photon energy and direction, normalized to unity when integrated over all photon directions, is required for this purpose.^{C1} The cross section currently in use^{C1} is described below in more detail. A short analysis of the data now available for these cross sections follows a brief review of the theory.

Weak-coupling scattering theory presents the bremsstrahlung cross section in terms of a matrix element of the appropriate operator between two functions describing the elastic scattering of electrons by the target. The energies and normalizations of these elastic-scattering functions are chosen to represent the initial and final conditions. This matrix element provides the bremsstrahlung cross section differential in photon energy, photon polarization, and various angles representing the photon and electron directions in space. (The polarization effects are of no interest for the purposes of this discussion and no further mention of them will be made.) After making certain approximations, this photon-production matrix element can be related to elastic scattering in the limit of zero-energy photons (see Ref. B28 and the citations therein), and to the photoionization cross section in limit of large-energy photons.^{J3} Hence, one can

expect a strong correlation between the strengths and weaknesses found for theoretical treatments of these three processes.

There are many choices that one can make for the elastic-scattering wave functions. Many of the more approximate choices are reviewed in Ref. K11. If one is considering bremsstrahlung from an atomic target, one of the more appropriate weak-coupling choices would be that for scattering from a static potential, determined by the electronic structure of the target, that includes exchange. This is just the approach used to generate the recommended elastic-scattering cross sections discussed in Sec. V. Such an approach has occasionally been termed "exact"^{T5} but more precise elastic-scattering functions could be used and an even better theoretical model, including the bremsstrahlung as a channel in a close-coupling scattering calculation, is available.^{B29}

There is little chance that much data will soon be available from the full close-coupling approach, but fragmentary data do exist for weak-coupling theories that utilize rather sophisticated elastic-scattering functions. These elastic-scattering functions most often are the result of an independent electron-atom close-coupling calculation. Photon-production data of this type usually pertain to the $E_0 < 100$ eV range and may be presented for the inverse process of free-free absorption. The available theoretical data for several neutral targets are summarized in Ref. G14, where a maximum uncertainty of $\pm 30\%$ was placed on effects due to the choice of wave function. An experimental study is not completely in agreement with this theoretical estimate.^{R10} Part of the observed discrepancy is identified with known errors in the elastic-scattering functions, part is related to experimental difficulties, and part remains to be explained.^{R10} The situation for atomic nitrogen targets is summarized in Ref. J4. In this case there is little agreement between theoretical results based on different close-coupling elastic-scattering functions, or with any of these calculations and the few available experimental data. Because of the low incident energies used in these calculations, very little can be concluded

in the context of electron transport, but future developments in this area should not be ignored.

One other theoretical study of improved elastic-scattering functions, more directly related to the range of E_0 appropriate for electron transport calculations, is available.^{A6} This work shows the effects on the bremsstrahlung cross sections for Ar and K due to the polarization of the atomic target by the scattered electron. These effects were quite large under conditions associated with small-angle scattering and photon energies near the ionization threshold for the target. The neglect of polarization in calculating the elastic-scattering cross section at small angles can result in large errors (see the discussion in Sec. V), and the connection seems obvious.

In summary, the preceding two paragraphs indicate that weak-coupling calculations of bremsstrahlung based on the use of appropriately chosen static potentials to generate the elastic-scattering functions can have large errors for certain choices of parameters. However, the only problem identified for relatively large E_0 has not yet been demonstrated to be a great influence on the total cross section or the cross-section differential only in photon energy. Hence this type of weak-coupling prediction can be accepted for $E_0 > 10$ keV with only the slight reservation that full knowledge of the errors is not yet available. The $E_0 < 10$ keV range is more problematic and, because of the above observations, one can expect fairly rapid deterioration in the limits of small and large photon energies. However, these predictions may retain their validity to quite small E_0 for intermediate photon energy.

The reason for devoting so much space to the analysis of the weak coupling with static potential approach is that considerable data are available from this method.^{P13} Reference P13 presents the bremsstrahlung

cross section differential in photon energy for neutral atomic targets with $2 \leq Z \leq 92$ and $1 \text{ keV} \leq E_0 \leq 2 \text{ MeV}$. The authors claim an accuracy of 10%. Experimental data are not available to justify this claim, but these data should be of a quality similar to that achieved by the elastic-scattering cross sections discussed in Sec. V. In this respect, the only point not clearly resolved in Ref. P13 is the treatment of exchange phenomena in constructing the static potential. No explicit statement about exchange potentials is made, but a 10% or less uncertainty is attributed to the choice of different static potentials. Preliminary considerations have been given to the use of the successful exchange approximation developed for elastic scattering^{R6, R8} in bremsstrahlung calculations.^{R11} Effects as large as 20% for certain restricted ranges of the parameters treated in Ref. P13 appear possible.^{R11}

The question of how the data in Ref. P13 compare with values presently used in the electron-transport code^{C1} has been answered in a private communication from C. J. MacCallum.^{M8} Table VI-I summarizes his results. It is clear that for $E_0 \leq 2 \text{ MeV}$, significant differences can occur for both the total and differential in photon-energy cross sections. The single example shown in Table VI-I indicates that agreement between the code values and the results from Ref. P13 improves as E_0 increases. However, the errors for the case shown exceed 20% for certain photon energies, so an overlap of the data presented, within the 10% uncertainty claimed, apparently will only occur for $E_0 > 2 \text{ MeV}$. Hence, an extension of the calculation presented in Ref. P13 to larger E_0 would serve a useful purpose in the context of the electron-transport problem. Some of the formulas used in the large- E_0 region^{K11} have recently been reconsidered,^{M9} but it is doubtful that such treatments will bridge this gap. The low- E_0 cut-off of data at 1 keV in Ref. P13 was probably judicious and poses no imposition for many electron-transport problems. However, the low energy region continues to grow in importance, and a unified set of data, for $E_0 < 1 \text{ keV}$, even if known to be of qualified accuracy, would undoubtedly be used.

The normalized cross section used to assign a direction to the bremsstrahlung photon is based on the leading high-energy term in a formula given by Sommerfeld (see Ref. S9). This formula ignores all screening due to the target's electrons, assumes that $E_0 \gg mc^2$, and assumes that the angle between the incoming electron and photon propagation direction, ϕ , is small. Interestingly, this simple formula^{C1} for the probability of producing a photon at some angle, $P(\phi)$, is, independent of the photon energy and target Z,

$$dP(\phi) = 0.5 (1 - \beta^2) (1 - \beta \cos \phi)^{-2} \sin \phi \, d\phi. \quad (\text{VI.1})$$

To provide some insight into the range of validity for Eq. VI.1, $dP/d\Xi\phi$ from Eq. VI.1 and from formula 2BS of Ref. K11 are shown in Fig. VI-1. The sum of the electron's kinetic energy and rest-mass energy is designated by Ξ . Equation VI.1 is represented by the solid line, and the data from formula 2BS are spanned by the vertical bars for the indicated range of Z and E_0 . As a general rule, the full range of the bars is covered for a fixed choice of Z and E_0 as the fraction of E_0 converted to photon energy changes. A crossover occurs at $\Xi\phi = 1.5 \, mc^2$ radian. For nearly complete conversion of E_0 to photon energy, the curve lies near the top of the bars for $\Xi\phi < 1.5 \, mc^2$ radian and near the bottom for $\Xi\phi > 1.5 \, mc^2$ radian. The opposite is true for small conversions of E_0 to photon energy.

Formula 2BS from Ref. K11 is expected to be reasonably accurate for this choice of parameters and, as a consequence, Fig. VI-1 should provide a reasonable assay of the accuracy expected from Eq. VI.1. First, Eq. VI.1 has a tendency to be more accurate for high conversion of E_0 to photon energy. Second, 80% of the cross section is contained in the range $\Xi\phi \leq 2 \, mc^2$ radians, and the errors are generally less than $\pm 20\%$ in this range, although they become substantial for $\Xi\phi > mc^2$ radians.

It seems probable that many applications will be well served by Eq. VI.1, although two exceptions must be noted. The first concerns the range of E_0 for which Eq. VI.1 can be used. It is applicable only for $E_0 \gg mc^2 \sim 500 \, \text{keV}$ and, although the accuracy observed for

$E_0 = 5$ MeV is as described above, fairly rapid deterioration should be expected for E_0 decreasing below this value. The 1-500 keV angular distribution has recently been investigated theoretically and a parameterization of these data with formulas based on simple theoretical results was suggested.^{T6} It seems clear that for quantitatively accurate $dP/d\phi$ information for $E_0 \leq 500$ keV, the information from Ref. T6 must be used. The $500 \text{ keV} \leq E_0 \leq 5 \text{ MeV}$ is not well covered at the present, although it may prove possible to devise a reasonable interpolation between the Ref. T6 data and such formulas as 2BS of Ref. K11. The $E_0 > 5$ MeV $dP/d\phi$ is well represented by formula 2BS from Ref. K11, and Eq. VI.1 is a reasonable approximation in this range of E_0 .

The second problem with Eq. VI.1 is its tendency to introduce systematic errors into beam propagation problems. As discussed above and shown in Fig. VI.1, the energetic photons will have a tendency to be propagated in too narrow a beam along the electron-beam direction, while just the reverse is true for the soft photons. The errors expected from Eq. VI.1 can easily be removed for $E_0 \geq 5$ MeV, as discussed in the previous paragraph.

Plasma Effects

The data currently used^{B5} in the electron-transport code^{C1} are not intended for use on plasma targets, but the large- E_0 region is probably modified only slightly by changing the target's ionization state. (As a rough guess this large- E_0 region may occur for $E_0 > 5.0$ MeV, but it could be smaller for small- Z and larger for large- Z targets. See Ref. L7.) The use of neutral-atom bremsstrahlung cross sections for intermediate or small E_0 will seriously underestimate this phenomenon, especially in the small photon-energy region. This is due to the long-range Coulomb effects on the elastic-scattering wave functions. Data shown in Refs. L7 and Z3 for a series of ions and the $1 \text{ keV} \leq E_0 \leq 100 \text{ KeV}$ region show that underestimation by factors of 2 to 6 are common. This theory shows a logarithmic divergence for positive ions or free electrons as the photon energy goes to zero. This behavior should be modified by conditions determined by the

plasma and as a consequence some differences noted in Ref. L7 may be reduced.

There are a few studies ^{L7,Z3,M10} of bremsstrahlung by plasmas in the 1 keV to 10 keV temperature region that have been stimulated by the interest in fusion-plasma radiation losses. The principal conclusion from these studies is that bremsstrahlung may not be a dominant feature,^{M10} but it cannot be accurately treated by simple approximations unless E_0 is very large^{Z3} or unless the medium is at a temperature that guarantees that all the constituent atoms are completely stripped of electrons.^{L7} There do not appear to be any published comparisons of these data with experimental measurements. These observations on a plasma may or may not be appropriate to a particular electron transport problem, but they serve ample warning for the differences expected from a (partially) ionized medium.

Summary

Available bremsstrahlung cross-section data for both the total and differential in photon energy cross sections^{P13} are of good quality for $1 \text{ keV} \leq E_0 \leq 2 \text{ MeV}$. The authors claim 10% accuracy for these data. The semi-empirical data now in use^{C1} are probably of comparable accuracy for $E_0 \geq 50 \text{ MeV}$,^{B5,M9} while they have been shown to differ from the more reliable data by more than 20% for $E_0 = 2 \text{ MeV}$.^{M8} The $2 \text{ MeV} \leq E_0 \leq 50 \text{ MeV}$ gap should be filled in. The small- E_0 region is probably adequately covered for most present applications, but lower- E_0 data will undoubtedly continue to grow in importance. The present bremsstrahlung data appear to be inappropriate for transport in an ionized medium.

The information used for assigning a direction to the bremsstrahlung photon^{C1} is reasonably accurate for $E_0 \geq 5 \text{ MeV}$. It may provide predictions of reasonable quality for many problems at even smaller E_0 . Accurate alternatives in reasonably simple form, such as formula 2BS from Ref. K11, are available for the large- E_0 region if more accuracy is required as, for example, in the quantitative treatment of beam propagation. The situation has not been quantitatively analyzed for $E_0 \leq 5 \text{ MeV}$, although appropriate data in the 1-500 keV range of E_0 have recently become available.^{T6}

TABLE VI-I

Differences between the bremsstrahlung cross sections differential in photon energy as predicted by Ref. P13 and by Sandia's electron-transport code^{C1} for a gold target. These data were compiled by C. J. MacCallum.^{M8} A positive sign indicates that the code value exceeds the Ref. P13 value.

Photon Energy/ E_0	$E_0 = 500 \text{ keV}$	$E_0 = 2.0 \text{ MeV}$
0	+56%	+7%
0.1	+ 6%	-1%
0.2		-3%
0.3	- 6%	-6%
0.4	-11%	-8%
0.5	-16%	-11%
0.6	-22%	-14%
0.7	-27%	-19%
0.8	-34%	-24%
0.9	-40%	-20%
1.0	-47%	-7%

Figure VI-1. The probability of producing a bremsstrahlung photon at an angle ϕ is shown as a function of $\Xi \phi$, where $\Xi = E_0 + mc^2$. The solid line is an accurate representation of Eq. VI.1 for $E_0 \geq 5 \text{ MeV}$. The vertical bars represent the range of predictions of Eq. 2BS from Ref. K11 for the ranges of Z and E_0 indicated in the figure. See the discussion following Eq. VI.1.

VII. PHOTOIONIZATION CROSS SECTIONS

The total photoionization cross section is required to compute the probability of one of four events occurring when a photon interacts with a target system. (Elastic, inelastic, and pair-production scattering are the other three events.^{C1}) This same cross section in the neighborhood of an absorption edge is also used to make a statistical assignment of the atomic shell from which the photoelectron was ejected. The direction of the photoelectron is found from a normalized cross section differential in the angle between the incoming photon and outgoing electron directions. Details concerning the use of these cross sections in the electron-transport calculation are clearly outlined in Ref. C1.

The photoionization literature is extensive and there is currently considerable activity in this area. Numerous experimental measurements appear on a regular basis, and theoretical activity continues after a flurry in the late 1960's and early 1970's (see, for example, Refs. H10 and N3 and the many citations therein). The volume of this work precludes a detailed presentation that would tend to repeat and only slightly update the existing literature. An analysis of the theoretical tools available for this problem will be given and the data currently in use will be analyzed within this theoretical framework.

Theory

The basic formulation of photoionization, including relativistic effects, is well understood,^{P14} and questions about accuracy occur only when one chooses the target description before and after its interaction with the photon. As discussed in previous sections, one expects that modern data for atomic structure should be based on foundations at least

as good as Hartree-Fock (HF) theory. There are results now available that go somewhat beyond this view,^{M12} but these efforts are usually concerned with photon energies below 1 keV. This energy range is below that of direct interest; therefore, these data will not be discussed further. The existence of satellite lines in photoelectron spectroscopy is a many-electron phenomena that, generally speaking, cannot be explained by ordinary HF theory. Our view is that these details near absorption edges are not important for electron-transport calculations. Should this be incorrect in any instance, there is already a considerable amount of literature on this subject that can be consulted.^{M13}

The use of HF theory is not without its difficulties. The ground-state HF wave function for the N-electron target is generated with no ambiguity. The final target state consists of a hole left by the active electron, which now occupies an orbital in the continuum. The description of these N-1 "inactive" electrons for the final target state is the core of the problem. One model assumes that these electrons are in identical orbitals and configuration both before and after the excitation event. A second model completely ignores the existence of the active electron and then solves the (N-1)-electron HF problem again for a probable (N-1)-electron state. A more lengthy discussion of these models is presented in Ref. P14. This *second model would seem to be the more realistic*. Consider the ionization of the helium atom as an example. However, two practical problems occur with this approach. The first is that calculations for all possible configurations of the N-1 electrons must be done, an imposing task for many-electron targets. The second is that orthogonality between the initial and final N-electron wave functions is not automatic. The manner in which orthogonality is accomplished necessarily obscures much of the meaning that one initially attributes to this second model of the (N-1) electrons. The only unambiguous solution available is an exhaustive N-electron calculation that accurately includes correlation effects and all relevant configurations.

The meaning of the first model is relatively well understood.^{P15} Basically, it represents a certain weighted average over all possible final states of the (N-1)-electron core. The main approximations are that this weighting may not correspond to that found in a full N-electron treatment and that energy conservation is lost.^{P15} This model yields results for the target's ionization energy that are identical to Koopmans theorem. It is my opinion that the first model is the more useful first approximation, and only very detailed treatments will represent an improvement. This is especially true in the context of electron transport, where the statistical nature of the problem usually implies that a great deal of averaging is required to generate most quantities of interest. It is also a fact that almost all of the major sources of data for photon processes, as well as scattering, implicitly utilize some variant of this first model.

The conclusions just reached mean that the discussion of the completion of the N-electron final state for the target will be limited to the first model. Generally, some approximation to the HF potential for the active electron's initial orbital is found. This same potential is then used to compute the continuum orbital for the active electron. The information required to construct the target's N-electron final-state wave function is now complete, and there are no orthogonality problems. However, a serious problem is hidden in this model. The full HF potential contains a non-local exchange term that explicitly depends on the orbital occupied by the active electron. Hence, in principle, the initial and final active orbitals cannot satisfy the same one-electron Hamiltonian, and therefore they are not necessarily orthogonal orbitals.

There are several ways that have been used to avoid this problem. One is to completely ignore the exchange term. This is not generally done,^{H10} because the associated errors are believed to be large.^{P14} Another is to approximate the exchange term with a local operator that does not depend explicitly on the active orbital. The resulting potential is then used for

both orbitals, and orthogonality is automatic. This method has been used in most of the large-scale applications.^{H10} The resulting local exchange operator can give reasonable results near threshold but, as the energy in the continuum increases, it fails to vanish appropriately. A local exchange potential having at least the correct dependence on the continuum energy is known^{R8} and should be used. Orthogonality can be established for those cases not covered by angular momentum considerations by standard techniques. The use of a local exchange operator with the correct energy dependence has not yet been utilized in photoionization studies. Preliminary results in bremsstrahlung calculations, where orthogonalization poses no problems, indicate that 10-20% effects can occur in certain cases^{R11} (see the discussion in Sec. VI). Hence, until this point has been tested, rather large changes in the available one-electron model results for photoionization can be expected.

The exchange term in the HF potential also introduces another problem. This is most easily recognized by observing that the long-range form of the potential has a Coulomb form with a coefficient of $(Z-1)$ when the correct value is Z . This difficulty is accurately removed by simple devices.^{B30}

Total Photoionization Data

The cross sections used in computing the probability for photoionization were initially taken from the University of California Livermore Data Bank.^{C1} These data have since been replaced by a computation^{B31} that, for photon energies greater than 1 keV, is based mainly on data presented in Ref. S10.

The data from Ref. S10 for photon energies below 200 keV are basically the results found from a computer code described in Ref. B30. The frozen-core HF model described above forms the basis for this calculation. The high-energy data are based on a much cruder model of the target but comparable accuracy over the entire energy range is expected. A maximum difference of 10% between Ref. S10 data and all other data, including experimental, available at that time is claimed.^{S10}

A comprehensive review of most of the available total photoionization cross section has recently become available.^{H10,N3} Inexplicably, these reviews do not comment on the Ref. S10 data. Instead, considerable discussion of subsequent theoretical calculations is presented, and the conclusion is reached that theory and experiment are within 10% agreement for photon energies above 1 keV.^{H10}

A series of not generally available comparisons^{S11} tends to substantiate this claim for the Ref. S10 data as well, although some considerably larger differences can be noted for photon energies less than 10 keV and small-Z targets. It is nonetheless concluded that the Ref. S10 data also fall within the 10% range of uncertainty claimed in Refs. H10 and N3. The theoretical data recommended in Ref. H10 and the Ref. S10 data are both based on the frozen-core model for the target discussed above. Differences occur in that different exchange potentials were used, and Ref. S10 used experimental energies for ionization thresholds rather than the computed values used in the source for the data recommended in Ref. H10. The use of experimental data for the location of absorption edges is preferred, so preference for the Ref. S10 data is indicated for cases with large differences.

The situation described above does little to motivate an update of the data presently in use.^{B31} The large effort on experimental measurements currently in progress may change this situation, especially if the range of photon energies less than 10 keV becomes important in the transport problem. Also, the presence of the incorrect dependence on energy of the exchange term^{R11} in all available theoretical data has yet to be tested. In view of the great reliance on available theoretical data, and the many claims of agreement with experimental measurements, it seems that resolution of this question rates high priority.

The method^{C1} for estimating the shell from which the photoionization took place is based on data presented in Ref. S10. These data, as they actually appear in one transport code data-base, are listed in Ref. H13. The appropriate probabilities are computed from cross sections near the absorption edges and then are considered independent of photon energy. Reference S10 states that this energy dependence is weak and gives one example of a 10% change for a rather large change in photon energy. There is not now a clear indication that more accurate data are demanded by the electron-transport problem or that further tests of Ref. S10's conclusions should be made. Theoretical shell-by-shell photoionization data from one large-scale tabulation are available.^{S14} Should improvements be required, extrapolation estimates based on these theoretical results probably offer the quickest, if perhaps an uncertain, solution.

Angular Distributions

A normalized angular distribution is used to compute the direction assigned to the photoelectron. A simple result applicable to K-shell photoionization is used for all shells.^{C1} This formula has long been known to be relatively accurate for subshells consisting of s orbitals, K, L_I, etc., but qualitatively inaccurate for subshells with lower symmetry, L_{II}, L_{III}, M_{II}, etc.^{B30}

Several tests of simple formulas for these angular distributions have been performed,^{B30,T7} and it appears that much of the known information for photon energies greater than 1 keV can be well represented by them.^{T7} At lower photon energies the situation becomes quite complex, and there is little hope for simple results that have a wide range of validity (see Ref. S12 for a typical example).

The quality of the data, excepting the K-shell case being used in the transport calculation,^{C1} is quite low from the atomic physics point of view. Certain tests of the approximation in use^{C1} have been performed in the context of electron transport^{M14} and, depending on the quantity tested,

errors can be large. A much-improved procedure would consist of using the formula now in use for K, L_I , . . . ionization, one of the alternate formulas^{B30,T7} for L_{II} , L_{III} , . . . ionization, and some simple representation of the available data^{B30} for subshells with higher angular momentum. This would provide some improvement, but for demanding problems such as beam propagation, the rather more careful procedures suggested by Ref. T7 should be followed.

Plasma Effects

The photoionization of an atom partially stripped of its electrons is not expected to be greatly different from that for the neutral atom except near threshold, where the long-range character of the target wave functions is important. Hence, within the accuracy outlined above, the cross sections presently in use are adequate for treating plasmas as long as the change in threshold energy is accounted for properly.^{B32} Basically, the cross section is constant for a given photon energy and changing number of bound electrons in the outer shells. The threshold energy increases as outer electrons are removed, so the edge must be "moved" to higher energy and the photoionization from the higher shells, if any, must be extrapolated to higher energies. This extrapolation process could probably be accomplished with the fitting formulas now in use.^{B31} The major task would be to obtain the threshold-energy data. All of this of course presumes the existence of intact subshells in the plasma target from which the ionization is taking place.

The recent interest in high-temperature low-density plasmas has stimulated a considerable activity in the associated atomic physics. Consequently, the effects of outer-shell electron removal on the photoionization cross section has received attention.^{H11,B32} Reasonably simple schemes have been suggested (e.g. Refs. H11 and B32) should the electron-transport calculation require improved accuracy, and their need is most marked in the low- or threshold-energy region.

Summary

The total photoionization cross sections now in use are based on fits^{B31} of the best of the available large-scale tabulations.^{S10} There appears to be little experimental evidence to suggest systematic errors greater than $\pm 20\%$ for photon energies greater than 1 keV. Indeed, claims of much higher accuracy are made.^{H10} Until further experimental evidence is accumulated and especially until the problem of using an exchange potential with the incorrect dependence on the energy of the photoelectron is removed from the theoretical work, as discussed above, the larger error estimate seems appropriate. For the same reasons, there does not appear to be a compelling reason for updating the data now used in the electron-transport codes. The data used to determine the originating subshell for the photoelectron are of similar quality. However, the energy dependence of these data should be explored in more detail.^{S10, S14} This would be a natural adjunct to a detailed study of the exchange problem discussed above.

The angular-distribution calculation is reasonable for ionization from the K and L_I subshells. Exceptions may occur in threshold regions and for photon energies below 1 keV. Alternate formulas should be used for the L_{II} and L_{III} subshells,^{B30} and even a spherically symmetric approximation probably represents an improvement over the formula now in use for the average M and N shells. More quantitative data exist for many instances, T7,^{B30} but their implementation could prove an imposing task.

Certain plasma effects were noted and rather simple procedures were outlined which would be required to update the presently available data to this problem. More accurate data for this problem exists for isolated cases.^{H11, B32} This would seem to be one of the lower-priority problems in an attempt to treat electron transport in plasmas.

VIII. ELASTIC AND INELASTIC PHOTON CROSS SECTIONS

The total elastic and inelastic cross sections for photon scattering are used in computing the probability for a photon scattering event.^{C1} The form factor (scattering factor) is required in the computation of the new photon direction resulting from elastic (coherent or Rayleigh) photon scattering. Similarly, the incoherent scattering function is used in the computation of the photon direction when inelastic (incoherent or Compton) photon scattering has occurred. The use of these data in computing quantities in the context of electron transport is discussed in Ref. C1.

All of the quantities discussed in this section require only a knowledge of the ground-state electronic wave function, so the quality and availability of theoretical data are good. Furthermore, comprehensive reviews of these data have recently been published.^{H12,G15} Due to the relative maturity of this field, rapid changes in the future and significant improvements of information dating from the late 1960's are not expected. Detailed comparisons between recommended values and experiment are presented in Ref. H12. These comparisons justify the conclusion that large-scale improvements are neither required nor expected.

One note of caution must be sounded. The use of form factors and incoherent scattering functions are in fact approximations to the quantum-electrodynamically correct formalism. Reference B36 discusses some of these theoretical questions. These effects usually become important for photons with energies much greater than $mc^2 \approx 0.5$ MeV and for relatively large-angle (momentum-transfer magnitudes approaching mc) scattering, especially by large-Z targets. These would appear to be remote ranges of

parameters for most transport problems, but the techniques now in use become qualitatively incorrect in their extremes.

The data currently in use or available for use in electron-transport codes will be identified and compared with the recommended values. Unfortunately, Ref. H12 does not present a direct comparison of all relevant data, but this evidence, plus some random checks of the remaining data, should suffice. The few data pertaining to the relativistic ranges of parameters will be cited.

Elastic Cross Sections

The total elastic cross sections now in use are from Ref. M15, and these data are based on integrals of the form factors from Ref. C8. These form factors^{C8} are also in use in the transport code, and have been represented in analytic forms convenient for use in computer format.^{B33} Hence, these elastic cross sections are based on a consistent set of data. The recommendations of Ref. H12 are based on a Hartree-Fock-Slater non-relativistic calculation of the form factors plus the use of improved results now available for $Z \geq 7$ atoms. Differences between the form factors from Refs. H12 and C8 are typically less than 5%, although larger differences exist. These differences are reflected in the total (coherent) cross section data presented in Refs. H12 and M15.

The differences between the recommendations of Ref. H12 and the one alternative large-scale source represented by Refs. M15 and C8 are small. Relativistic Hartree-Fock-Slater wave functions were used to generate the Refs. M15 and C8 data, while nonrelativistic Hartree-Fock-Slater wave functions form the basis for the Ref. H12 data. The two calculations also differ slightly in the choice of a local, or Slater-screening, approximation to the electron exchange term appearing in Hartree-Fock theory. The differences mentioned above tend to be small, and the comparisons with theory presented in Ref. H12 give no clear indication which source is the better choice.

The criteria for recommendation are reduced to choices made on theoretical grounds. The $Z \leq 7$ data represented in Ref. H12 are the best now available. The data from Refs. M15 and C8 are the data of choice because of the use of relativistic Hartree-Fock-Slater wave functions. The main defect in this recommendation is that the range of momentum-transfer magnitude $\hbar q = (\hbar 4\pi/\lambda) \sin(\theta/2)$ is limited to $q \leq 2 a_0^{-1}$. Here λ is the photon wavelength and θ is the scattering angle. High-energy photon processes, especially in large- Z targets, appear to require data from an extended range of q . Data in the large- q range are available for ⁰² certain $Z > 20$ values based on relativistic wave functions and agree well, within 1%, with the Ref. C8 data at $q = 2 a_0$. These large- q data have been recently extended and combined with the Ref. C8 data.^{H18} The coherent cross sections are also recalculated. The Ref. H18 tabulations are the most extensive available, in terms of the ranges for q , Z , and E_0 , and since these data are based on the best available information, they are the recommended source at the present time.

If an extension into the large- q range is motivated by electron-transport considerations, questions about the differences between the correctly-formulated Rayleigh scattering cross section^{B36} and the form-factor approximations should be answered. Several sources of data pertaining to this problem are available (see Refs. J5 and K12), but a systematic study of these differences has yet to be published. A recent study,^{K12} based on a rather rudimentary model of the atomic target, indicates that certain modifications^{B37} of the usual form-factor data can be effective for $\hbar q \leq mc$. Hence, existing data can be modified to accommodate these effects over a large range of q should changes in the present approach to electron transport be required. Reference K12 states that publication of an extensive set of data applicable to the large- q region is planned for the near future.

Inelastic Cross Sections

The total inelastic cross sections now in use^{C1} are also from Ref. M15 and are based on integrals of the incoherent scattering functions from Ref. C9. These incoherent scattering functions have been represented by convenient analytic forms.^{B33} The recommendations of Ref. H12 are based on the same data, Ref. C9, for $Z > 7$ atoms and on rather more detailed calculations for the $Z \leq 7$ atoms. This is reflected by almost complete agreement between Ref. H12 recommendations and the Refs. M15 and C9 sources for $Z > 7$. These data differ rather more for $Z \leq 7$, because the incoherent scattering function depends on correlation effects in the atomic wave functions. The Hartree-Fock-Slater wave functions used in Ref. C9 are not accurate with respect to this property, which is most important for small Z and small momentum transfers. Rather large differences can be found in this restricted range of parameters, and the use of the Ref. H12 recommendations is indicated.

References H12 and G15 compare the available experimental data with the suggested values and conclude that the agreement is satisfactory. One important feature of Ref. H12 is the more thorough coverage of the various independent parameters than available from Ref. C9. The usefulness of the Refs. H12 or C9 data is compromised by the fact that nonrelativistic Hartree-Fock-Slater wave functions were used. Any effects from this defect would be most important for large- Z and large- q ranges. For this reason, an extension of the Ref. C9 incoherent scattering function data to the large- q range is not strongly indicated, although the Ref. H12 data might represent some improvement. Should a relativistic Hartree-Fock calculation of the incoherent scattering function become available, an update and q -extension of the data in use would be recommended. A recalculation of the total inelastic photon cross section should be done at the same time. Developments based on the quantum electrodynamics of inelastic photon scattering should also be reevaluated when an update is attempted.

One interesting feature of the transport calculation is the treatment of secondary electron generation due to incoherent scattering. The secondary electron's direction and energy are computed by assuming the incoherent photon scattering event occurred with a free electron.^{C1} Since incoherent scattering is of relative importance only for high-energy photon scattering, intuitively this approximation seems reasonable. However, direct tests of this point were not discovered. Compton scattering is now a very active field of investigation,^{W4} and certain data from these studies could provide a basis for this test. It is conceivable that such detailed comparisons may suggest alternative methods, but there do not appear to be strong hints of such an event^{W4} at the present time.

Another feature of the transport code is the complete neglect of atomic relaxation after an incoherent scattering event. The method now used to treat inelastic photon scattering precludes any identification of the shell from which the secondary electron was ejected. These relaxation events may not contribute significantly to the transport problem, but tests appear to be lacking. Certainly incoherent scattering is the dominant process in photon scattering by small-Z targets for photon energies between 0.1 MeV and 10 MeV.^{H10} There appear to be sufficient data from K-shell Compton scattering^{W4} to estimate the fraction of incoherent events involving this shell. This would then make possible an estimate of the contributions from the most energetic relaxation processes.

Plasma Effects

The total cross sections are basically representative only of a neutral target, and any ionization of the target should be reflected by changes in these data. Unfortunately, no data are available from which an estimate of the size of these effects can be derived. The same can be said for the cross sections differential in scattering angle, except one of the integral components of the formulas in use^{C1} are the free point-charge formulas. That is, the Thomson cross section multiplied by the atomic form factor is used for elastic scattering, and the Klein-Nishina formula

multiplied by the incoherent scattering function is used for inelastic scattering.^{C1} The form factor and the incoherent scattering function should change as target ionization increases, until only the free-particle formulas are in use for complete ionization. Again, there does not appear to be a study of photon scattering in plasmas, although efforts along these lines appear to be in progress.^{N2}

Summary

All data now in use for elastic and inelastic photon scattering are of high quality. The elastic cross-section data could be improved somewhat by changing to the recommendations of Ref. H12 for $Z \leq 7$ targets and an extension of the form factor data to larger- q values for $Z > 7$ targets by using the information presented in Ref. H18. Quantum-electrodynamic refinements exist and should be used in the large- q range. The inelastic data now in use could be improved by following the recommendations of Ref. H12. Changes in the remaining inelastic data would be strongly recommended if relativistic Hartree-Fock calculation of the incoherent scattering function were available. Lacking such information, the only advantage to be gained would be to make use of the more extensive coverage of the range of q presented in Ref. H12.

Questions about the methods used to compute the energy and direction for the secondary electrons produced by incoherent photon scattering are raised. The neglect of any possibility for inner-shell relaxation processes after incoherent scattering is also noted. No estimates of the importance of these questions to electron transport problems were found and no priority for changes in these procedures is assigned.

The direct application of the methods now in use for transport in ionized media is questioned.

IX. PAIR-PRODUCTION AND PHOTONUCLEAR EVENTS

The electron-positron pair-creation event from a photon in the field of a nucleus or an electron is usually included in electron-transport calculations.^{C1} The threshold for pair production in a nuclear field is $2(mc^2) \sim 1$ MeV and in the electron field is $4(mc^2) \sim 2$ MeV. The latter event is often referred to as triplet production since three tracks, or a "fork," are produced in a cloud chamber. The nuclear-field exceeds the electron-field cross section and, roughly, the events occur in a Z^2/Z ratio. It follows that the electron-field events are relatively important only for low-Z targets. This is of some importance since the transport calculations ignore the "third" free particle, the electron that formerly was bound, under all circumstances. This approximation could be of consequence for small-Z targets, since energy conservation requires the third particle to have a reasonably large kinetic energy.

The total cross section is required in the computation of the probability for a pair-production event. There remains the assignment of the energy and angle for the electron/positron pair. The process for this energy and angle assignment is discussed in some detail in Ref. C1 and in the references cited therein. It suffices to say here that the pair-production cross section differential in kinetic energy for the produced particles and the unit-normalized cross section differential in angle are required.

Photonuclear cross sections are ignored in the present electron-transport calculations.^{C1} These cross sections become important in the photon-energy range of 10-100 MeV, with some small-probability events occurring at much higher energy. A typical example is illustrated in Ref. H10 for Cu targets. The pair production and incoherent photon scattering

tends to dominate the photonuclear events by at least an order of magnitude. Hence, unless the photonuclear particles are of direct interest, this process is of minor importance.

Total Pair-Production

Two sets of total pair-production cross sections that meet the general requirement for electron-transport calculations are available.^{S10,P16} They were both generated from the same initial set of data for a limited range of targets^{H14} by interpolation and extrapolation. These data from Ref. S10 have also been represented by simple formulas convenient for numerical computation.^{B34} It is some consolation that these various interpolations and extrapolations of the same data tend to agree with each other, if one accepts a $\pm 5\%$ variation.^{S11}

A third set of total pair-production data is now available,^{G15} which appears to differ very little from the tabulations just introduced. Reference G15 also presents a detailed comparison of high-energy (10 MeV or greater) experimental data for total attenuation of photons with theoretical data which also includes photoionization, elastic, and inelastic cross sections. This comparison^{G15} tends to justify the accuracy claims made above and in the preceding two sections.

The cross-section data in use^{H14} are based on a formalism that is correct in the high-energy limit. It is essentially a Born calculation which relies on corrections for other channels and for Coulomb or screening effects (see the discussion and references cited in Refs. C1 and S10 for more details). One expects these predictions to be accurate at high energy and they are generally accepted for photon energies greater than 20 MeV. In the 1-20 MeV range of photon energies, these predictions have recently been questioned and considerable effort has been made to derive improved information from experiment (see Ref. H15). The new data presented in Ref. H15 for small-Z targets do not appear to demand any change in the existing tabulation if one accepts the $\pm 5\%$ level of uncertainty. (This observation is not based on data presented in Ref. H15, but upon direct comparisons with data presented in Refs. S10 and B34.) A number of experimental data

could be cited as supporting evidence (see Ref. A7 for example), and it appears that there is little motivation for replacing the theoretical data now in use for the total cross section. It should be pointed out that a large-scale systematic calculation of the total cross section in the field of the nucleus does exist in the threshold to 5 MeV photon-energy range.⁰³ This calculation should be an improvement but, again, the changes are small if one excepts the near-threshold region where these cross sections are small.

Differential Cross Sections

The cross section differential in the kinetic energy of one of the pair as used in the transport code is based on an uncorrected Born calculation and is therefore symmetric with respect to the electron/positron pair. Once this kinetic energy is determined, it is randomly assigned to one of the pair, and the kinetic energy of the remaining particle is determined from energy conservation.^{C1}

There does not appear to be extensive experimental data bearing on this quantity, but one calculation does exist. This work is basically a Coulomb-Born calculation for nuclear pair production in the threshold energy region, which completely neglects screening effects.⁰³ It results in an asymmetry in the particles' kinetic energies, with the positron being more energetic than the electron. This is a result of Coulomb interaction, and it is therefore difficult to estimate the effects expected in a neutral target. Since the Coulomb effects are not in any case large, there does not appear to be a great motivation to update this aspect of the transport calculation.

The angles assigned to the electron and positron are calculated from the leading-term in the high-energy limit of a Born formula. Each particle is treated independently and the directions of the pair are therefore completely uncorrelated.^{C1} The formula differential in particle direction is also completely independent of kinetic-energy considerations, so all computations of the degrees of freedom for the created pair can be done without keeping track of previous assignments. This is probably a reliable

process for high-energy photons, say greater than 20-30 MeV, but may be questionable at lower energies. More detailed formulas are available that would require a complete coupling of variables in assigning the directions and kinetic energies. There do not appear to be any attempts made to use this approach in the context of transport theory. This is undoubtedly justified for most transport problems, but caution would seem appropriate if the properties of pair production in the low-energy photon region are important.

Unfortunately, experimental data do not appear to be available to test theory for these differential processes, and appropriate measurements do not seem to be in progress. The relative simplicity of the distorted-wave theory for this process is such that these theoretical results are well within today's computational capability. A systematic test of the various high-energy approximate formulas and more quantitative estimates of the errors could be provided by data of this type.

It is important to note that all treatment of these differential processes is based on results for pair production in the field of a nucleus only. As mentioned above, the electron field provides a competitive process, at least for the smaller-Z targets, and this process is qualitatively different in these degree of freedom.

Plasma Effects

The data in use for this process are largely based on theoretical results that only incorporate atomic structure through the device of a screening correction for the total cross section.^{S10} Since these corrections tend to be relatively small, the assumption that the state of target ionization has little effect on pair production is consistent with the computational methods now in use.^{C1} Again, uncertainty remains in the relatively unexplored range of 1-30 MeV photons.

Summary

The total cross section data now in use were judged to well represent the known information, if one accepts a +5% range of uncertainty. The

cross sections differential in pair energy and direction now being used can be improved by utilizing one of the more accurate formulas available (see Ref. 13). It is impossible to present a detailed assessment because of the lack of differential experimental measurements or comprehensive theoretical treatments. One relatively sophisticated theoretical treatment is available,¹³ and it poses few questions for the procedures now in use. Intuitively, it seems that any doubts about these data are reserved for the threshold range of energy.

The most notable question concerns the treatment of pair production in the field of an electron. The recoil electron is ignored and all assignments of direction and angle for the electron/positron pair are based on nuclear-field formulas. This question is obviously most important for small- Z targets.

X. INNER-SHELL RELAXATION

Subsequent to electron- or photon-ionization events that remove an electron from an inner shell, the target will relax to its ground or lowest energy state.^{C1} The modes available for relaxation consist of fluorescence, which produces a photon, and Auger/Koster-Cronig transitions, which produce secondary electrons. The general concepts for this relaxation are simple, but the number of possibilities grows so large as the electron vacancy moves toward the outer shells that complex bookkeeping with a large number of quantities becomes necessary. The approximation that the manner in which the hole was created has no consequences in the subsequent relaxation pattern is essential in keeping this problem within tractable bounds. A particular relaxation parameter is then defined by one Z-dependent table which is independent of the kinematics or any other history of the hole formation. See, for example, the discussion in Ref. B35, and note that the transport code still requires 47 tables of data in treating this problem.^{H13}

The data now contained in Sandia's electron-transport codes are outlined in Ref. C1 and reviewed in detail by Ref. H13. Of particular interest, it should be noted that vacancies in K, L_I, L_{II}, L_{III}, average M, and average N shells receive consideration. The representation of the M and N subshells by average quantities plus leaving out higher subshells is consistent with ignoring all particles with energies less than 1 keV in the transport problem. This point would have to be reconsidered if transport at lower energies in large-Z targets is attempted. Also, the chemical composition of the target must be taken into account in the lower-energy problem, since processes involving the valence electrons then become more probable.

Reference C1 neither provides explicit lists of data that are in use nor identifies the sources for these data. The author of Ref. C1 does

indicate that his data were assembled prior to the publication of the most recent review of this field, Ref. B35, and that improvements based on this review may be possible. This exercise has not yet been attempted. The data actually being used in the transport code have recently been made available in a convenient form.^{H13}

This section will present a short outline of the theoretical problems associated with calculations of quantities used in the inner-shell relaxation problem. This seems relevant since all data now in use appear to be theoretical in origin.^{H13} This will be followed by a comparison of the Ref. H13 data with the data presented in Ref. B35.

Considering the age of Ref. B35 and the great activity currently devoted to inner-shell phenomena, it is reasonable to expect that much additional information exists. An update of Ref. B35 goes beyond the scope of this work. However, in the literature survey for this section, a number of articles that appear particularly well-adapted to the requirements of electron-transport were identified. References of interest for radiative decay and energy levels include H17, K13, L8, M17, O4, and S15. Auger and Koster-Cronig rates are considered in Refs. C10, C11, H16, W5, and Y1. This list of references is not intended to be exhaustive, but merely an indication of the data postdating Ref. B35.

Theory

The theoretical viewpoint most commonly in use starts from the "frozen-core" model described in Section VII.^{M16} The inner-shell relaxation proceeds from the initial N-electron target description, with the appropriate vacancy created by reducing one of the orbital occupation numbers by one. (The methods for determining the appropriate vacancy for photoionization are outlined in Section VII.) Relaxation occurs by transitions between various configurations of this "frozen-core" manifold of states. The wave functions used in these calculations are based on the construction of a one-electron potential from the frozen-core Hartree-Fock orbits, using the methods briefly discussed in Section VII. Matrix elements for the photon field and electron-electron interaction complete the computation.

The best theoretical model would be to treat each hole-producing collision individually, and include in the dynamics the possibility of fluorescence, multiple-electron ejection, etc. The result would be a list of cross sections for the "completely" relaxed target and the description of the modes in which the collision energy has been redistributed.

Such a calculation has not yet been attempted, and little data of this type can be expected in the near future. In addition, the incorporation of these data into an electron transport code, should they become available, would present a considerable obstacle. Occasionally, studies intermediate between this "exact" treatment and the one-electron model just described become available for limited classes of problems (e.g. Ref. H16). Meanwhile, the results from simple models, when correlated and corrected to agree with available experimental information, appear to be the standard.

The transition from the "exact" model to the frozen-core one-electron model relies on arguments concerning the time-scales for various competing events. This is not the place to present a discussion of these problems (see Ref. P14 and its citations for the identification of some of this literature), but one auxiliary point must be made. The assumption made in treating the relaxation of the target "after" a hole has been created in the context of electron-transport theory^{Q1} is that the target has unit probability for the hole being in the original location. Irrespective of the accuracy of rates for "subsequent" relaxation or the models on which they are based, this seems inconsistent with the quantum-mechanical view that there will be a distribution of hole locations. (The sudden approximation to this distribution is described in Section VII and Ref. P15.) There seems to be little information on or study of this problem, and errors due to this restrictive assumption are not known.

Relaxation Parameters

The number of parameters is too large for an individual discussion of each quantity. Instead, the majority of the quantities in use (see Ref. H13) are listed in Table X-I. The original source for some of these data

is also indicated. The main content of Table X-I is the comment section, where short summary statements are based on comparing the transport data base^{H13} with data presented in Ref. B35. Generally speaking, direct comparisons were not possible, and it was necessary to derive a quantity in one reference from a series of quantities available from the other reference. The comments will indicate how this was done.

There was no attempt made to provide a detailed definition of the quantities under consideration when Table X-I was constructed. Generally speaking, these quantities are defined in terms of fractions or probabilities for events.^{H13} Also, a number of energy-related quantities were used^{H13} that were not checked. This is because experimental knowledge of the energy levels for the various sub-shells has long been of high quality, with respect to 1-keV lower bounds on particles appearing in the transport problem, and any averaged quantity involving energy would only change if one or more of the relaxation-rate parameters were changed.

A few summary comments based on preparing Table X-I should be made. The agreement for various K-shell processes, including both experiment and theory, seems rather good. That is, a range of variation less than $\pm 10\%$ is common for K-shell relaxation parameters. The situation is otherwise for higher subshells, and often a consensus of any quality is not obvious. Of particular note, the L_1 -shell Auger-effect parameter seemed quite inaccurate when compared with data from Ref. B35. Also, the K-shell fluorescence efficiency is a rather well-studied and important parameter. It would seem that replacing these data in the electron-transport code by one of the rather accurate formulas now available^{B35} would be advisable.

Plasma Effects

There are no data pertaining to this subject, but some analogies with the comparatively well-studied problem of photoionization can be drawn. As in the photoionization case, one expects that the actual probabilities will be a weak function of removing outer electrons from the target as long as

the numbers of electrons involved in the relaxation event are not changed. However, shifts in the energy levels will change the various energy-related quantities, and associated errors would be linear in these changes. However, at least for small degrees of ionization, on the scale of a 1-keV cutoff for low-energy transport problems, these errors would probably not be too large.

Summary

Many of the relaxation parameters for inner-shell vacancies now used in electron transport codes^{C1,H13} have been compared with data given in the most recent comprehensive review of this subject.^{B35} Table X-I presents this comparison. A large discrepancy was noted for the L_I-shell Auger effect parameters, and the replacement of the K-shell fluorescence efficiency data with a formula provided by Ref. B35 was recommended. In general, the remaining data appeared to fall or nearly fall within the accuracy bounds established in Ref. B35.

The tacit assumption made in the transport-code treatment of vacancy formulation, that a vacancy is formed in any particular subshell with 100% probability rather than in a distribution over subshells, was questioned. Definitive information for assessing this question is not yet available.

TABLE X-I

Comments on the various quantities tabulated in Ref. B13 that pertain to inner-shell relaxation are provided. The source, when identified, for the data tabulated in Ref. B13 is also indicated. The abbreviations used in identifying these quantities are defined in Ref. B35, except for F and KC, which designate fluorescence and Koster-Cronig, respectively.

Quantity	Source Reference	Comments
1. M-shell F efficiency		Exp. data scattered but tend to be smaller by 20% (Ref. B35 Table V-III)
2. L_{III} -shell F efficiency	M16	Generally within range of exp. data (Ref. B35 Table IV-XII).
3. L_{III} -shell F from L_{III} -M transition		Using data from entries 2 and 3 to derive quantities given in Table V-I of Ref. B35 indicates the product of 2 times 3 is too large with factor of two differences occurring where product is small.
4. L_{III} -shell Auger Effect from L_{III} -MM transition		Data derived with entries 2, 4, and 5 are in good agreement with Table X-I information from Ref. B35.
5. L_{III} -shell Auger effect from L_{III} -MN transition		See comments for entry 4.
6. Fraction of L_{III} relaxation from L_{II} - L_{III} KC transition	M16	These data appear consistently too small when compared with quite scattered experimental information; see Table IV-XIII of Ref. B35.
7. L_{II} -shell F efficiency	M16	These data are within $\pm 10\%$ of experiment, being small for small Z and large for large Z. See Table IV-XII of Ref. B35.

TABLE X-I (cont)

Quantity	Source Reference	Comments
8. L_{II} -shell F from L_{II} -M transition		Data derived from entries 7 and 8 tend to be too large by 10% or more when compared with data from Table IV-XII of Ref. B35.
9. L_{II} -shell Auger effect from L_{II} -MM transition		Data derived from entries 7, 9 and 10 tend to be accurate for small Z and too large at large Z when compared with Table V-I data from Ref. B35.
10. L_{II} -shell Auger effect from L_{II} -MN transition		See comments for entry 9.
11. L_I -shell relaxation due to L_I - L_{III} KC transition	M16	These data are within the scatter of experimental measurements (Ref. B35 Table IV-XV).
12. L_I -shell relaxation due to L_I - L_{II} KC transition	M16	These data have a tendency to be too low in mid-Z range, but experimental data are quite scattered (Ref. B35 Table IV-XIII).
13. L_I -shell F efficiency	M16	Comment on data in use cannot be made because experimental data scatter is too large (Ref. B35 Table IV-XII).
14. L_I -shell F due to L_I -M transition		Data derived from entries 13 and 14 are quite consistent with available information (Ref. B35 Table V-I).
15. L_I -shell Auger effect from L_I -MM transition		Data derived from entries 13, 15, and 16 tend to be larger by ~ 50% than data given in Table V-I of Ref. B35.

TABLE X-I (cont)

Quantity	Source Reference	Comments
16. L_I -shell Auger effect due to L_I -MN transition		See comments on entry 15.
17. K-shell F efficiency	M16	Differences greater than + 10% are noted, especially for small Z, when compared with data from Table III-IV of Ref. B35.
18. K-shell F from K- L_{III} transition		Data derived from Table IV-IV of Ref. B35 tend to be smaller by about 10% for low Z and to agree for large Z.
19. K-shell F from K- L_{II} transition		Data derived from Table IV-IV of Ref. B35 agree for small Z and are large by 10% for large Z.
20. K-shell F from K-M transition		Experimental data are too scattered to make a comparison possible.
21. K-shell Auger effect from K-LL transition		Data derived from inform- ation in Table IV-V of Ref. B35 are consistently larger by less than 5%.
22. K-LL Auger effect from K- L_I - L_I		Data derived from entries 22, 23, 24, 25, and 26 agree well with data from Table IV-V of Ref. B35.
23. K-LL Auger effect from K- L_I - L_{II} transition		See comment for entry 22.

TABLE X-I (cont)

Quantity	Source Reference	Comments
24. K-LL Auger effect from $K-L_{I}L_{III}$ transition		See comment for entry 22.
25. K-LL Auger effect from $K-L_{III}L_{III}$ transition		See comment for entry 22.
26. K-LL Auger effect from $K-L_{II}L_{III}$ transitions		See comment for entry 22.
27. K-shell Auger effect from K-LM plus K-LN transitions		These data tend to be large by 20% at small Z and 3% for large Z when compared with data derived from Table IV-V of Ref. B35.

APPENDIX A

Definition of Symbols

A summary and the definition of many of the symbols used in the text are presented in Table A-I.

TABLE A-I

The definitions for various symbols appearing in the text are presented. On the occasions where these symbols are used for different quantities, they are explicitly defined in the local context.

Symbol	Definition
$f(x, \Delta E)$	The probability of an electron losing an energy ΔE after transversing some material a distance x
x	Length; $E_0/\Delta E$
ΔE (ΔE_i)	An energy difference (between two energy levels)
$E_0 = (1/2) m v_0^2$	Initial kinetic energy of an electron
(dE/dx)	Stopping power (energy/distance)
$f_{L,B,V}(x, \Delta E)$	Landau, ^{L1} Blunck, ^{B1} and Vavilov theories, respectively for $f(x, \Delta E)$
ρ	Density (gm/cm ³)
N	Avogadro's constant
A	Atomic weight (gm/mole)
σ	A total cross section
β	$= v/c$

TABLE A-I (cont)

Symbol	Definition
c	Speed of light
v	A particle speed
m	Electron rest mass
f_i	Optical oscillator strength for the i th inelastic event
Z	Nuclear charge
C_i	Shell corrections defined by Eq. III.5
e	Electron charge
N_i	Number of equivalent electrons in i th configuration
σ_0	$6.56 \times 10^{-14} \text{ cm}^2$
$\bar{\epsilon}_i = (1/2) m\tilde{v}_i^2$	Average kinetic energy of an electron in the i th configuration
e	Equals 2.718. . . .
α	$\cong (1/137)$ the fine structure constant
g	The (Kramers) Gaunt factor
I	Average ionization energy appearing in stopping power theory
I_i	Average ionization energy of the i th subshell appearing in stopping power theory
b_{nl}, c_{nl}	Constants appearing in the Bethe cross section, Eq. IV.1
T	Particle kinetic energy in units of mc^2

TABLE A-I (cont)

Symbol	Definition
δ	The density effect correction term appearing in stopping power theory
l_d	Deby length
$b_m, \bar{b}_m$	Impact parameter cut-off values (see Eq. III.5)
Ω	Collision strength (proportional to $E_0\sigma$)
q	The magnitude of the momentum transfer is $\hbar q$.
$\Xi = E_0 + mc^2$	The total energy of a particle with rest mass m

APPENDIX B

High Priority Problems and Additional Information

A summary of various high-priority problems identified in the text and the need for added information is presented in Table B-I.

TABLE B-I

Summary of areas where explicit changes in data are recommended and additional information would be useful.

Section	Quantity	Remarks
II	$f(x, \Delta E)$	General investigation of various theoretical approaches and correlation with any existing measurements for $E_0 \leq 1.0$ MeV.
II	$f(x, \Delta E)$	Investigate the use of cross sections consistent with the derivation of $-(dE/dx)$, especially in the Vavilov theory.
III	$-(dE/dx)$	Check of density effect corrections for partially ionized or high temperature systems and $\beta \sim 1$.
III	$-(dE/dx)$	Shell corrections for $E_0 \leq 10$ keV.
IV	Ionization	Application of distorted wave theory to ionization problem.
IV	Ionization	Application of the simplified Born theory discussed in this section to the total and secondary electron-production ionization cross sections.
IV	Ionization	Adaptation of the various semiempirical formulas correctly to the relativistic E_0 region.

TABLE B-I (cont)

Section	Quantity	Remarks
IV	Ionization	Study the use of the various BEM theories as applied to the Q+BEM theory. The SEF (G7) cross section now in use should be replaced by the Q+BEM(K9) cross section for K-shell ionization.
IV	Ionization	Study the use of better σ_{PI} , the choice of b_c , and energy conservation approximations in evaluating Eq. IV-2 for Q+BEM cross sections.
V	Total Inelastic Scattering	Further investigation of the features of formulas such as Eq. V.2.
V	Total Inelastic Scattering	Application of the Sec. IV Born approximation to the differential cross section summed over all inelastic events.
VI	Bremsstrahlung	Extend the weak-coupling static-potential calculations from $E_0 = 2$ MeV to E_0 sufficiently large for 10% agreement with semi-empirical formulas now in use. A qualitatively incorrect exchange potential used in generating currently available data should also be removed.
VII	Photoionization	The removal of the qualitatively incorrect exchange term for the calculations providing the base for these total cross section data is a high-priority item.
VII	Photoionization	The angular distribution data should be changed for L_{II} , L_{III} , and average M and N subshells.
VIII	Elastic and Inelastic Photon Scattering	The extension of the form-factor data now in use to larger-q values and the need for a relativistic Hartree-Fock calculation of the incoherent scattering function was indicated.
VIII	Incoherent Photon Scattering	The transport calculation's neglect of the decay products from the relaxation of inner-shell vacancies created by photon scattering was noted.

TABLE B-I (cont)

<u>Section</u>	<u>Quantity</u>	<u>Remarks</u>
IX	Pair- Production	The transport calculation's failure to account for the recoil particle for production in the field of an electron was noted.
X	Inner- Shell Relaxation	A replacement of the K-shell fluorescence efficiency data was recommended.
X	Inner- Shell Relaxation	A premise used in analyzing and calculating inner-shell relaxation rates was questioned. The approximation in question assumes that a vacancy is produced with 100% probability in a particular subshell and not in a distribution over different subshells.

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