Stopping powers from velocity distributions derived from Compton profiles

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In the framework of the kinetic theory of stopping it is possible to relate the stopping power of a substance to the velocity distribution of the scatterers, which can be obtained from the Compton profile. This relation is explored, and is used to determine values of the mean excitation energy for Al solid and vapor and gaseous Ar, He, N2, and CH4. The mean excitation energy is determined as the value which within the kinetic theory gives the best fit to measured or calculated stopping cross sections.

I. INTRODUCTION

The energy deposited per unit path length by a swift, massive charged projectile traversing a medium, -dE/dx, the stopping power of the medium, is generally understood in terms of Bethe's1 theory of stopping. This theory includes a material constant, the mean excitation energy I, which is frequently extracted from experimental measurements. In practice this problem is not simple.

The mean excitation energy is defined in terms of the set of excitation energies of the system ε_n and their corresponding oscillator strengths f_n as

$$\ln I = \mathbf{f} d\varepsilon \left[\frac{df}{d\varepsilon} \right] \ln \varepsilon / \mathbf{f} d\varepsilon \left[\frac{df}{d\varepsilon} \right] , \qquad (1)$$

where the integration is over all discrete and continuum states. Thus, if the experimental dipole oscillator strength distribution were known accurately, I could be determined directly. This has been done for some cases,2 but the method demands extensive spectroscopic information.

According to Bethe's formula, which is asymptotically correct at large but nonrelativistic projectile energies, E_p , the stopping power of a medium should depend on I as

$$-\frac{dE}{dx} \propto \ln \frac{4mE_p}{M_p I} , \qquad (2)$$

where M_p is the mass of the projectile and m is the mass of the electron. Thus, I can be determined^{3,4} by measuring the stopping power at large E_p (to minimize shell corrections). Unfortunately, at large incident energies the $\ln(4E_p)$ term dominates $-\ln I$, so great precision must be used in the measurements.⁴ In addition, the stopping varies only slowly with I, as ln I, so other effects such as relativisitic corrections, inner-shell corrections, and deviations from the first Born approximation (e.g., Barkas and Bloch corrections) must also be considered.

The mean excitation energy has also been obtained utilizing a different range of incident projectile energies (e.g., approximately 10-30-MeV protons) via the range function R(E), which measures the projectile penetration depth. The range as a function of projectile incident energy is an integrated stopping power, S(E),

$$R(E_p) = \int_0^{E_p} S^{-1}(E) dE \ . \tag{3}$$

The range difference t for projectiles in the appropriate energy range is thus

$$t = R(E_2) - R(E_1) = \int_{E_1}^{E_2} S^{-1}(E) dE . \tag{4}$$

One may then use I as a parameter to fit range data. The latter methods are thus both based on measuring stopping properties.

Recently the kinetic theory of scattering⁶ has provided a transformation formula for obtaining the stopping characteristics of scatterers with internal motion from that of the scatterers at rest. This formulation depends on I and on the velocity distribution of the scatterers. Another quite independent quantity, the Compton profile (CP), also depends on the velocity distribution of scatterers. This distribution can be extracted from an experimental CP and used in conjunction with the kinetic theory to produce stopping powers as a function of incident particle energy. Such a procedure requires the use of a mean excitation energy, which may be varied parametrically to obtain agreement with an experimental stopping curve and thus provide an experimentally based value of I. In contrast to most other methods of determining I, the present procedure makes use of the whole nonrelativistic energy range. This paper will outline the procedure, discuss its applicability, and report some test calculations and results based on it.

II. THEORY AND CALCULATIONS

A. Stopping power

The stopping power is conventionally related to the stopping cross section by the number density of target atoms (n)

$$-\frac{1}{n}\frac{dE}{dx} = S(v) \tag{5}$$

and then to the stopping number L(v) by

$$S(v) = \frac{4\pi e^4 Z_1^2 Z_2}{mv^2} L(v) , \qquad (6)$$

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where Z_1 is the projectile charge and, for neutral targets, Z_2 is the target atomic number and where v is the velocity of the projectile in the laboratory frame. The transformation equation provided by the kinetic theory⁶ relates the stopping number for stationary target electrons L_0 to that [L(v)] when the target electrons have an isotropic velocity distribution $\rho(v_2)$,

$$L(v) = \pi \int_0^\infty \rho(v_2) v_2 dv_2 \times \int_{|v-v_2|}^{v+v_2} L_0(v') \left[1 + \frac{v^2}{v'^2} - \frac{v_2^2}{v'^2} \right] dv'.$$
(7)

In our usual implementation^{7,8} of the transformation we assume that such an equation applies shell by shell to stationary atomic targets. Each shell is described by its electron velocity distribution $\rho_k(v)$ and its orbital mean excitation energy I_k . Appropriate choice of L_0 then leads to scattering consistent with the first Born approximation (Bethe scattering, $S(v) \propto Z_1^2$) or to higher-order deviations⁶ [Barkas, $S(v) \propto Z_1^3$, and Bloch, $S(v) \propto Z_1^4$, corrections]. Each of these terms consists of a conventional leading term and its so-called shell corrections. The total stopping number is then just the sum of orbital contributions.

At low energies, in the region of the stopping maximum, the stopping is primarily accomplished by valence electrons, and its calculation is very sensitive to a proper, shell-by-shell description of the scatterers. As one moves through the transition region to higher energies, the orbital details become less important, and the wholeatom or single-I description becomes more realistic. At yet higher energies, relativistic corrections need be made. We will confine our discussion to the projectile-energy region where relativistic corrections can be neglected.

In the present application we will consider Bethe scattering of protons. According to the derivation⁶ of Eq. (6) $L_{0,k}(v)$ must be the leading term in the Bethe stopping number for shell k when $v \gg v_2$. Here v_2 refers to the initial velocity of the target electron in the laboratory frame. It has been shown by Sigmund¹⁰ that using

$$L_{0,k}(v) = \ln \frac{2mv^2}{I_k} \Theta(v - \alpha_k)$$
, (8)

where $\Theta(v-\alpha_k)$ is the Heaviside step function and

$$\alpha_k = \sqrt{I_k/2m} \tag{9}$$

leads to the conventional expression for the shell corrections to the stopping power. We will thus here, as in the previous applications^{7,8} of the kinetic theory, use Eq. (8) for $L_{0,k}$.

B. Compton profile

If, rather than scattering swift, massive, charged particles from an electron distribution, one uses photons as the projectiles, one obtains a CP instead of a stopping power.¹¹ Such a profile measures the line shape of the shifted and broadened result of energy and momentum transfer from the photon to the electrons.

From an (in principle) anisotropic momentum density

 $\rho(\mathbf{p})$, one can obtain an isotropic distribution by angular averaging

$$\rho_0(p) = \frac{1}{4\pi} \int_{|\mathbf{p}|} \rho(\mathbf{p}) dp . \tag{10}$$

The radial, or isotropic, Compton profile is then defined

$$J_0(q) = 2\pi \int_a^{\infty} p \rho_0(p) dp$$
 (11)

In the case of atomic targets where the charge distribution is radially symmetric, $\rho_0(p) = \rho(p)/4\pi$. We define the radially symmetric charge distribution of solids as obtained from isotropic CP's through the same relation. Thus

$$J_0(q) = \frac{1}{2} \int_q^{\infty} \rho(p) dp \tag{12}$$

and

$$-2\frac{dJ_0(q)}{dq} = \rho(q)q , \qquad (13)$$

which is just the momentum (velocity) distribution needed for the integration over v_2 in Eq. (7), provided it can be obtained shellwise.

Thus, one may in principle derive a stopping-power curve directly from the experimental CP, provided the mean excitation energy is known, or conversely, determine I if both L(v) and the CP are known experimentally.

It should be noted that although the above formulation deals only with isotropic velocity distributions, the formulation certainly can be made for anisotropic cases. ¹² The precursor of Eq. (7) does contain directional dependence, and it should thus be possible to observe anisotropies in stopping-power curves which arise from anisotropic velocity distributions in samples such as molecular solids.

C. Calculation

In order to implement the scheme described above, it is necessary to have orbital Compton profiles. These are not measurable, but experimental valence CP's, and are frequently used. They are obtained by subtracting a Hartree-Fock (HF) core from an experimental profile. Such a decomposition rests on the commonly accepted belief that the atomic-core CP is well represented by HF orbitals. Consistent with this assumption, we thus represent our systems as a sum of the appropriate HF core and valence profiles. The core is itself a sum of the appropriate orbital profiles, so

$$J_0(q) = \sum_{i}^{\text{core}} J_0^i(q) + J_0^{\text{val}}(q) . \tag{14}$$

It should be noted that the valence orbitals (in the cases considered here all those with highest principle quantum number) are treated together to produce a valence CP and thus a valence momentum distribution. This is treated as a single entity when the orbital stopping numbers and cross sections are calculated.

The mean excitation energy associated 14 with the valence electrons is obtained from the total mean excitation energy (I) and the core orbital mean excitation energies (I_k) using

$$\ln(I_{\text{val}}) = \frac{1}{\omega_{\text{val}}} \left[Z_2 \ln I - \sum_{k}^{\text{core}} \omega_k \ln I_k \right]. \tag{15}$$

Here the $\{\omega_k\}$ are the orbital weight factors, which also with the orbital I_k are obtained⁷ from Inokuti *et al.*¹⁵

The effect on the stopping power of treating the valence orbitals as a common distribution is negligible. For example, our normal treatment of atomic aluminum¹⁶ uses I=123.67 eV, with orbital values of $I_{3s}=9.01$ eV and $I_{3p}=4.85$ eV. Combining the 3s and 3p orbitals according to Eq. (15) gives a valence mean excitation energy of 7.14 eV. If we compare the stopping curve for atomic Al calculated in the normal way^{7,16} to that calculated using $I_{\text{val}}=7.14$ eV, there is no difference to three decimal figures above v=3 a.u. The error rises rather rapidly to 0.2% at v=1 a.u. Thus, the common treatment of the valence orbitals introduces no significant error into the calculation.

In each of the cases reported below, an experimental valence CP was fit to a set of functions by a linear least-squares procedure using Gaussian elimination. Several forms of trial function were used, and Lorentzians $[f_i(q)=(k_i^2+q^2)^{-1}]$ were ultimately chosen. These functions have the desirable property of representing the proper¹⁷ limiting behavior of $J_0(q)$ at large,

$$J_0(q) \sim \frac{8Z^2}{3} \rho_0 q^{-6} + O(q^{-8})$$
, (16)

and at small,

$$J_0(q) \sim J_0(0) - 2q^2 \rho_s + O(q^4)$$
, (17)

values of q for the proper values of the fitting coefficients. Here ρ_s is a constant related to the s orbitals of the target.¹⁷ A more detailed study of the fitting of Compton profiles with a hydrogenic Lorentzian basis has been made by Thakker et al. 18 and shown to be quite satisfactory for producing the lower moments of the momentum. Other workers have also used Gaussian¹⁹ and polynomial²⁰ bases. As a test case a theoretical CP of atomic Al, obtained in conjunction with previous stopping-power calculations,²¹ was fit. A satisfactory fit was found to a set of six Lorentzian functions with $k_i = 0.1$, 0.3, 0.6, 1.0, 2.0, 3.0, 5.0, and this sequence was used in all further fits. Using twenty points distributed over the profile, a fit was obtained with a root-mean-square error of 8.57×10^{-3} . As expected, the percentage errors were much larger in the wings of the profile than at the peak. It is expected that use of better fitting schemes 18 will not alter the values of I

that we infer from this method. The fit obtained for the theoretical CP is better than those typically obtained to experimental CP's (see Table I), as a theoretical CP provides more fitting points with higher numerical precision, a finer grid, and no scatter.

The derivative of the fitted valence function was generated analytically on an exponential grid, and the stopping power calculated directly from Eqs. (6) and (7) using methods described elsewhere.^{7,21} The total stopping is then the shellwise sum of core (HF) and valence contributions.

III. RESULTS AND DISCUSSION

The scheme considered above relates the Compton profile, through the scatterer velocity distribution, to the stopping power and thus to the mean excitation energy. Thus the interrelation of the three quantities $J_0(q)$, S(v), and I can be explored. We restrict our discussion to proton stopping.

A. Phase effects

A problem of current interest is the origin of sample phase effects in stopping powers.²²⁻²⁴ Within the framework of the kinetic theory these differences must be due to either changes in the velocity distribution of the scatterers or in the mean excitation energy of the target. Since the CP depends on $\rho(v)$ but not on I, phase differences in $J_0(q)$ indicate that there are differences in the velocity distribution of scatterers. By using the CP for the solid and gaseous phase, we can thus separate out the phase differences in S(v) due to differences in the velocity distributions (but do not determine their importance in determining the stopping power). The CP for solid Al has been determined²⁵ and can be compared with a theoretical CP generated from atomic wave functions,²¹ which should approximate the vapor well. The profiles are indeed quite different, with the vapor being approximately 25% higher at the peak. The profile derivatives, shown in Fig. 1, are also disparate, and reflect the difference between bandlike and orbital- (atomic-) like valence electrons.

Table II reports the stopping cross section calculated at several projectile velocities based on the theoretical (vapor) and experimental (solid) CP's and for several values of I. It is clear that use of the rather different distributions has only a minor effect in the stopping, and it is differences in mean excitation energy that are responsible for the changes in S(v).

TABLE I. Characteristics of the Compton-profile fit

System	Al (atom)	Al (solid)	He	Ar	N_2	CH ₄
Experimental CP from Ref.	21	25	35	35	35	46
Number of experimental points fitted	20	20	18	23	23	22
rms error in fit $(\times 10^2)$	0.857	3.802	0.229	1.185	1.690	2.105

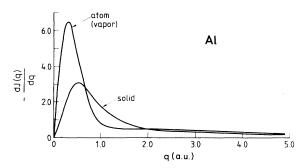


FIG. 1. Compton-profile derivatives as a function of momentum for Al. Curves for solid (Ref. 25), and theoretical ("gas") samples (Ref. 21) are given.

In this regard, there is a question as to the origin of the unexpected significant phase differences in low-energy stopping powers of the van der Waals solids N_2 (Ref. 26) and CO. We speculate that the phase differences arise from changes in the valence mean excitation energy on condensation, and not primarily from changes in the velocity distribution of the targets.

B. Determination of I

Another possibility is to extract a target mean excitation energy by comparison of experimental stopping curves to those obtained from experimental Compton profiles as described in Sec. II C. In this method we treat I as a parameter in the calculation of S(v) from $J_0(q)$, and look for the I that gives the best agreement with the measured S(v) curves. We report here several cases: aluminium in its solid and vapor state and gaseous helium, argon, molecular nitrogen, and methane.

Although the experimental stopping power of aluminium vapor has not been reported, theoretical atomic calculations should serve quite well. In Fig. 2 we present generalized-oscillator-strength (GOS) calculations of the stopping power of Al,²⁷ and we compare this to results derived from theoretical atomic CP's (Ref. 21) and to the results obtained from the kinetic theory, both with I=123.6 eV. The agreement between the GOS stopping points and the curve for the generally accepted²⁸ atomic value of I=123.6 eV is quite good. This is not unexpected, as although the GOS stopping power and atomic CP calculations are not directly related, they are both computed for an isolated atom. The fact that the CP-derived points fall on the directly calculated S(v) curve also shows that there are no serious errors introduced by the fitting procedure.

A more stringent test is with solid Al. In Fig. 3 we present experimental stopping curves for solid Al (Ref. 29) and compare them to curves derived from experimental CP's, 25 using various values of I. Before experimental stopping curves can be compared to calculated results, the Barkas correction needs to be subtracted out. This is the major deviation from the first Born approximation at the energies under consideration, and removal of the Barkas term reduces the experimental curve to (nearly) Bethe stopping. The experimental points in Fig. 3 have thus had an estimate of the Barkas correction, calculated according to Ritchie and Brandt³⁰ with b=1.4, removed. The experimental points clearly agree best with the CP-derived curve with I=163 eV.

In Table III we present various previously reported values of the mean excitation energy of aluminium. Although there are no experiments on aluminium vapor, it is generally agreed that the calculated values for single atoms should represent the vapor state in lieu of experimental measurements, and that the appropriate mean excitation energy should be approximately 124 eV. This is in excellent agreement with the results found here. For the solid, we are very close to the generally accepted mean excitation energy of 166 eV. It should be noted that attempts to fine tune this procedure are probably not worthwhile, due to the inherent uncertainty of the experimental data (1-4%), the correctness of the Barkas term, and the imprecision of the comparison of experimental points with the theoretical curves.

The CP-derived³⁵ stopping curves for argon at several

TABLE II. Proton stopping cross sections for aluminium, S(v), derived from theoretical (Ref. 11) and experimental (Ref. 25) Compton profiles.

Mean excitation energy (eV)		S(v) (10 ⁻¹⁵ eV cm ² /atom)		
	Projectile velocity (a.u.)	From theoretical $J(q)$ vapor	From experimental $J(q)$ solid	
123.6	5	9.873	9.996	
	10	4.224	4.726	
	15	2.397	2.552	
	20	1.565	1.585	
143.0	5	9.173	9.281	
	10	4.061	4.508	
	15	2.322	2.463	
	20	1.520	1.540	
163.0	5	8.542	8.638	
	10	3.914	4.311	
	15	2.253	2.383	
	20	1.480	1.499	

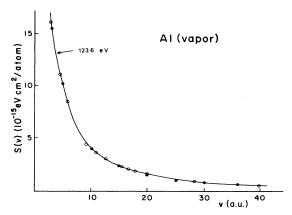


FIG. 2. Stopping cross sections for Al vapor. Values from the GOS (Ref. 27) calculation (\bigcirc) are compared to values obtained from theoretical atomic Compton profiles (Ref. 21) (\blacksquare) and from the kinetic theory (Ref. 7) (solid curve). I=123.6 eV.

values of I are presented in Fig. 4 along with some Barkas-corrected³⁰ experimental points.^{36–39} There is some spread in the experimental data. It appears that the Brolley and Ribe data³⁷ is most consistent with I=154 eV, while the Andersen and Ziegler data³⁸ agrees better with I=175 eV. This is on the lower edge of the generally accepted range for I of 174 to 194 eV (Refs. 2,32,39–41) but is still in reasonable agreement. A similar situation is presented for helium in Fig. 5. Here CP-derived³⁵ stopping curves for several Is are compared to Barkas-corrected³⁰ experimental points.^{37,39,42,43} The scatter of the data here is greater than for Ar, but again the data suggest a mean excitation energy in the range 42-62 eV, in reasonable agreement with accepted values^{2,32,39,42} (\sim 42 eV). There are some problems at lower energies (v < 7 a.u. or $E_p < 1.2$ MeV) where the experimental points seem to deviate upwards from the calculated curves.

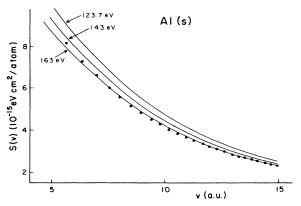


FIG. 3. Measured stopping cross sections for solid Al (Ref. 29) with Barkas corrections subtracted (\bullet) and calculated from experimental isotropic Compton profiles (Ref. 25) using various values of I.

TABLE III. Values of the mean excitation energy, I, for aluminium.

I (eV)	Ref.	
121.0	31	calculation
122.8, 118.3	27	calculation
123.7	28	calculation
124	32	recommended gas value
132.0	31	calculation
142.2	27	calculated value
		at $E_p = 10 \text{ MeV}$
145-150	33	calculated value
		for solid
163	34, 14	fit to solid data
166	32	recommended value
		for solid Al
167	4	experimental value
		for solid Al

Similar studies were carried on the molecular gases N_2 and CH_4 , using experimental isotropic Compton-profile data. In Fig. 6 we present the CP-derived³⁵ curves for N_2 along with several Barkas-corrected³⁰ experimental stopping measurements. The shapes of the curves are in good agreement with experimental measurements and the data agree very well with the I=65-eV curve. This is, however, about 20 eV lower than the commonly accepted value^{2,32,38,39,45} of about 82 eV for N_2 .

The analogous data for CH₄ is presented in Fig. 7. The experimental isotropic CP (Ref. 46) is again used to produce calculated curves at several values of I, which are compared to experimental measurements.^{37,42,44} As in the case of N₂, the shape of the calculated curves is good, and the I=31-eV curve agrees almost perfectly with the experimental data. Again, however, we find an I which is too low compared to the commonly accepted value for CH₄ of about 41 eV.^{32,47}

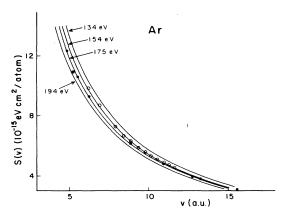


FIG. 4. Experimental stopping cross sections for Ar from Swint *et al.* (\bigcirc) ,³⁶ Brolley and Ribe (\triangle) ,³⁷ Andersen and Ziegler (\bullet) ,³⁸ and Baumgart *et al.* (\blacksquare) ,³⁹ with Barkas corrections subtracted, and calculated from the experimental³⁵ Compton profile using various values of I.

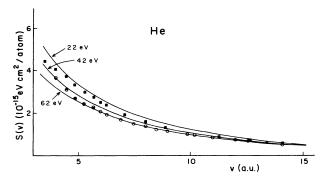


FIG. 5. Experimental stopping cross sections for He from Brolley and Ribe (\triangle) , Northcliffe and Schilling (\square) , and Baumgart *et al.* (\bigcirc) , and calculated values from Bichsel and Porter (\bigcirc) , and from the experimental Compton profile using various values of I.

The reason for the differences between the mean excitation energies determined here and those determined directly from stopping-power measurements is not clear. There are, however, several possibilities. An important step^{2,48} in an experimental determination of mean excitation energies is the determination of the shell correction (C/Z_2) . These are automatically included in our formulation, ^{7,8}

$$S(v) = \frac{4\pi e^4 Z_1^2 Z_2}{mv^2} \left[\ln \frac{2mv^2}{I} - \frac{C}{Z_2} \right]$$
 (18)

but must be explicitly considered when extracting Γ s from experimental stopping data. The commonly used shell corrections of Bonderup⁴⁹ are numerically smaller than ours^{7,8} and we would thus expect I determined using the Bonderup shell corrections to be larger than ours. This is in fact what is observed, and is probably the major source of difference in the atomic results. Another contributing factor is the uncertainty in the Barkas correction L_1 , which is important at lower energies. We have used

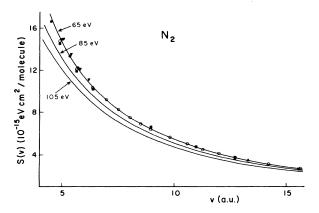


FIG. 6. Experimental stopping cross sections for N_2 from Baumgart *et al.* (\blacksquare),³⁹ Brolley and Ribe (\triangle),³⁷ Anderson and Ziegler (\bullet),³⁸ and Whillock and Edwards (\blacktriangledown),⁴⁴ and calculated values from Bichsel and Porter (\bigcirc),⁴² and from the experimental isotropic Compton profile³⁵ using various values of *I*.

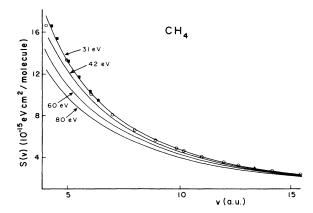


FIG. 7. Experimental stopping cross sections for CH₄ from Brolley and Ribe (\triangle) ,³⁷ and Whillock and Edwards (\square) ,⁴⁴ and calculated values from Bichsel and Porter (\bigcirc) ,⁴² and from the experimental isotropic Compton profile⁴⁶ using various values of I

the parameter b=1.4 in the Ritchie and Brandt³⁰ formulation, as recommended by Bichsel and Porter. ⁴² Use of a smaller value of b would give a larger correction to the experimental values and thus lead to a larger value of I, again in closer agreement with recommended values. The Bloch term L_2 is nearly an order of magnitude smaller than L_1 , in this energy region, and has the opposite sign. We have neglected it, but its inclusion would have the opposite effect on the results as does L_1 . The sum of these factors are felt to be responsible for the differences in the recommended and calculated mean excitation energies for the atomic cases.

The molecular results agree less well with the recommended I values. Although the preceding comments also appertain it is expected that their effects will be reasonably small, as they are in the atoms. A more important problem is that isotropic Compton profiles are used, producing isotropic momentum densities, while the targets are certainly not spherical. Methane is, however, expected to be closer to a sphere than is molecular nitrogen, and thus one would expect the magnitude of the error in CH_4 to be less than that in N_2 , as is observed.

Finally, it is expected that some error will be introduced by the numerical fitting and derivative generation procedures, but as discussed above, this error should not be inordinately large.

IV. CONCLUSIONS

It is possible to compute the stopping cross section as a function of velocity from the Compton profile of a material using the kinetic theory of stopping, provided the mean excitation energy of the target is known. Equivalently, given the Compton profile and the stopping cross section, the two may be matched to yield an experimentally based value of I. The procedure as implemented here considers only Bethe stopping of protons in the energy range $0.5 \le E_p < 6$ MeV $(4 \le v \le 15$ a.u.). Shell corrections, whose choice can greatly influence the determina-

tion of an experimental I, naturally arise in the kinetic theory²¹ and need not be explicitly considered, but it is important to take account of the Barkas correction. This is particularly important at lower energies, and for heavier nuclei.

When the kinetic theory is used in conjunction with experimental measurements, it can be used to help explain the origin of certain sample phase changes in the stopping power. It is clear from our results that changes in the scatterer velocity distribution cannot be responsible for large changes in S(v); only changes in I can affect them significantly.

Although the relationship between $J_0(q)$ and S(v) can be exploited to determine a value for I, the scheme does not lend itself to fine tuning (adjustment of I on the order of eVs) due to the scatter of experimental data and prob-

lems in comparison of calculated curves to experimental data. The calculations do show, however, that values of I may be obtained from measurable Compton profiles with accuracy of 10% and that this can be done utilizing the convenient 0.5-6-MeV proton energy range rather than higher energies with their attendant accuracy problems.

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- ¹H. Bethe, Ann. Phys. (Leipzig) **5**, 325 (1930); Z. Phys. **76**, 293 (1932).
- ²Cf., e.g., G. D. Zeiss, W. J. Meath, J. C. F. MacDonald, and D. J. Dawson, Radiat. Res. 70, 284 (1977); Can. J. Phys. 55, 2080 (1977); Mol. Phys. 39, 1055 (1980). See also J. Geertsen, J. Oddershede, and J. R. Sabin, Phys. Rev. A 85, 1104 (1986) for further references.
- ³F. Besenbacher, H. H. Andersen, P. Hvelplund, and H. Knudsen, K. Dan. Vidensk. Selsk., Mat.-Fys. Medd. 40, No. 3 (1979).
- ⁴H. H. Andersen, A. F. Garfinkel, C. C. Hanke, and H. Jørgensen, K. Dan. Vidensk. Selsk., Mat.-Fys. Medd. 35, No. 4 (1966); H. H. Andersen, Danish AEC, Risø Report No. 93, 1965 (unpublished).
- ⁵C. Tschalär and H. Bischsel, Phys. Rev. 175, 476 (1968).
- ⁶P. Sigmund, Phys. Rev. A 26, 2497 (1982).
- ⁷J. R. Sabin and Jens Oddershede, Phys. Rev. A 26, 3209 (1982).
- ⁸J. Oddershede and J. R. Sabin, Phys. Rev. A 29, 1757 (1984).
- ${}^{9}E_{p}(\text{MeV}) = 0.024\,98\,v^{2}$ (a.u.).
- ¹⁰See Sec. V A of Ref. 6 for details.
- ¹¹For a review of the subject see P. Kaijser and V. H. Smith, Jr., Adv. Quantum Chem. 10, 37 (1977); Compton Scattering: The Investigation of Electron Momentum Distributions, edited by B. Williams (McGraw-Hill, New York, 1977).
- ¹²The anisotropic form of the transformation equation is Eq. (19) of Ref. 6. The anisotropic, or directional, Compton profile is discussed in Ref. 11.
- ¹³Cf., e.g., F. Bell and H. Böckl, Nucl. Instrum. Methods B 2, 311 (1984).
- ¹⁴This is done in the spirit of E. Shiles, T. Sasaki, M. Inokuti, and D. Y. Smith, Phys. Rev. B 22, 1612 (1980).
- 15J. L. Dehmer, M. Inokuti, and R. P. Saxon, Phys. Rev. A 12, 102 (1975); M. Inokuti, T. Baer, and J. L. Dehmer, *ibid.* 17, 1229 (1978); M. Inokuti, J. L. Dehmer, T. Baer, and J. D. Hanson, *ibid.* 23, 95 (1981). The details of the procedure are given in Ref. 7.
- 16J. Oddershede and J. R. Sabin, At. Data Nucl. Data Tables 31, 275 (1984).
- ¹⁷R. Benesch and V. H. Smith, Jr., in Wave Mechanics, the First Fifty Years, edited by W. C. Price, S. C. Chissick, and T. Ravensdale (Butterworth, London, 1973), p. 357.

- ¹⁸A. J. Thakkar, A. M. Simas, and V. H. Smith, Jr., Mol. Phys. 41, 1153 (1980).
- ¹⁹G. A. Gadre and P. T. Narasimham, Mol. Phys. 31, 1613 (1976)
- ²⁰R. W. Klapthor and J. S. Lee, Chem. Phys. Lett. 45, 513 (1977).
- ²¹J. Oddershede and J. R. Sabin, Chem. Phys. 71, 161 (1982).
- ²²J. Oddershede, J. R. Sabin, and P. Sigmund, Phys. Rev. Lett. 51, 1332 (1983).
- ²³J. R. Sabin, J. Oddershede, and P. Sigmund, Nucl. Instrum. Methods B 12, 80 (1985).
- ²⁴For a summary see D. I. Thwaites, Radiat. Res. 95, 495 (1983).
- ²⁵S. Manninen, T. Paakkari, and K. Kajantie, Philos. Mag. 29, 167 (1974).
- ²⁶N₂: P. Børgesen, Chen. H.-M. and H. Sørensen, Nucl. Instrum. Methods 194, 71 (1982); 212, 517 (1983); CO: J. Schou, H. Sørensen, H. H. Anderson, M. Nielsen, and J. Rune, Nucl. Instrum. Methods B 2, 159 (1984).
- ²⁷E. J. McGuire, J. M. Peek, and L. C. Pitchford, Phys. Rev. A 26, 1318 (1982).
- ²⁸J. L. Dehmer, M. Inokuti, and R. P. Saxon, Phys. Rev. A 12, 102 (1975).
- ²⁹H. H. Andersen, J. F. Bak, H. Knudsen, and B. R. Nielsen, Phys. Rev. A 16, 1929 (1977).
- ³⁰R. H. Ritchie and W. Brandt, Phys. Rev. A 17, 2102 (1978).
- ³¹E. J. McGuire, Phys. Rev. A 28, 49 (1983).
- ³²M. J. Berger and S. M. Seltzer, Stopping Powers and Ranges of Electrons and Positrons, 2nd ed., U.S. Dept. of Commerce Publ. No. NBSIR 82-2550-A (U.S. GPO, Washington, D.C., 1983), Table 5.7.
- ³³E. J. McGuire, Phys. Rev. A 28, 53 (1983).
- ³⁴L. E. Porter and S. R. Bryan, Nucl. Instrum. Methods 178, 227 (1980); H. Bichsel, M. Inokuti, and D. Y. Smith, Phys. Rev. A 33, 3567 (1986).
- ³⁵P. Eisenberger and W. A. Reed, Phys. Rev. A 5, 2085 (1972).
- ³⁶J. B. Swint, R. M. Prior, and J. J. Ramirez, Nucl. Instrum. Methods 80, 134 (1970).
- ³⁷J. E. Brolley, Jr. and F. L. Ribe, Phys. Rev. 98, 1112 (1955).
- ³⁸H. H. Andersen and J. F. Ziegler, Hydrogen Stopping Powers and Ranges in all Elements (Pergamon, New York, 1977).

- ³⁹H. Baumgart, W. Arnold, H. Berg, H. Huttel, and G. Clausnitzer, Nucl. Instrum. Methods 204, 597 (1983).
- ⁴⁰E. J. McGuire, Phys. Rev. A 28, 2096 (1983).
- ⁴¹L. Porter and R. G. Jeppesen, Nucl. Instrum. Methods 204, 605 (1983).
- ⁴²H. Bichsel and L. E. Porter, Phys. Rev. A 25, 2499 (1982).
- ⁴³L. C. Northcliffe and R. F. Schilling, Nucl. Data Tables A 7, 233 (1970).
- ⁴⁴M. J. Whillock and A. A. Edwards, Phys. Med. Biol. 24, 518

(1979).

- ⁴⁵S. P. Ahlen, Rev. Mod. Phys. **52**, 121 (1980).
- ⁴⁶A. L. Bennani, H. F. Wellenstein, A. Duguet, B. Nguyen, and A. D. Barkas, Chem. Phys. Lett. 41, 470 (1976).
- ⁴⁷G. F. Thomas and W. J. Meath, Mol. Phys. 34, 113 (1977).
- ⁴⁸Cf., e.g., H. H. Andersen, J. F. Bak, H. Knudsen, and B. R. Nielsen, Phys. Rev. A 16, 1929 (1977).
- ⁴⁹E. Bonderup, K. Dan. Vidensk. Selsk., Mat.-Fys. Medd. 35, No. 17 (1967).