Bethe-Bloch stopping-power parameters for Mylar, Kapton, and Havar targets derived from measurements with proton, α-particle, and carbon-ion projectiles

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Recently reported measurements of the stopping powers of Mylar, Kapton, Havar, and nickel for proton, α-particle, and carbon-ion projectiles have been analyzed with a modified Bethe-Bloch formalism in order to ascertain values of various parameters and to test the additivity rule with mean excitation energies thus obtained. Extracted values of this parameter exceeded additivity predictions by 8–17 % for Mylar and by 5–9 % for Kapton, whereas the alloy Havar yielded mean excitation energies within -4% to $+5\%$ of the additivity value.

I. INTRODUCTION

Several sets of measurements of energy loss by various projectiles in Mylar, Kapton, and Havar targets have been reported recently.[1–5] These reports held special interest for the author both because experiments with Mylar and Havar targets had been conducted about a decade earlier[6] and because studies of additivity of stopping powers of composite targets have remained a major focus of attention.[7–11] Whereas the projectiles utilized in the recent studies[1–5] encompassed protons,[1] α particles,[2] and carbon,[5] nitrogen,[3] and oxygen[4] ions, the targets employed in the latter two cases were so thick as to forbid extraction of stopping-power data. Since projectile velocities in these experiments lay in the interval of applicability of Bethe-Bloch theory, the measurements were analyzed in order to extract various parameters of the formalism and to compare results with those of previous studies as well as with additivity predictions.[6,7]

II. MODIFIED BETHE-BLOCH THEORY

Analyses of stopping-power measurements in the context of modified Bethe-Bloch theory have been described on several recent occasions.[10–15] The basic Bethe-Bloch theory can be written to express stopping power in units of MeV cm^2 g^{-1} as

$$S=\frac{0.30708z^2Z}{\beta^2 A}L \ , \tag{1}$$

where Z and A, respectively, represent target atomic number and atomic weight, z is the projectile atomic number, β is the relativistic velocity parameter for the projectile, and L is the rather complicated (dimensionless) stopping number of the target. The latter quantity consists of three terms,

$$L=L_0+\xi zL_1+L_2 \ . \tag{2}$$

The first term is the basic stopping number

$$L_0=\ln\frac{2mc^2\beta^2}{1-\beta^2}-\beta^2-\ln I-C/Z-\delta/2 \ , \tag{3}$$

where mc^2 is the rest-mass energy of the electron, I is the target mean excitation energy, C is the total of target shell corrections, and δ is the density-effect correction needed for highly relativistic projectiles. The projectile-z^3 effect (or Barkas effect) is represented by the L_1 term of L, whereas L_2 represents the Bloch term.

Shell corrections appearing in the L_0 term were calculated according to a method devised by Bichsel,[16,17] whereby the theoretical K- and L-shell corrections of Walske[18,19] are adopted, and scaling factors are then applied to the L-shell correction so as to obtain M- and N-shell corrections:

$$C=C_K(\beta^2)+V_LC_L(H_L\beta^2)+V_MC_L(H_M\beta^2) + V_NC_L(H_N\beta^2) \ , \tag{4}$$

where the C_K and C_L represent the Walske[18,19] K- and L-shell corrections, respectively, and the V_i and H_i $(i=L,M,N)$ denote the scaling factors.

The density-effect correction term of the L_0 term proved unnecessary[20] in the present study by virtue of the moderate-to-low projectile velocities utilized in the measurements.[1–5]

Of the two correction formalisms for the Barkas-effect correction which first appeared, one for low projectile velocities[21–23] and the other for both low and very high projectile velocities,[24] the former[21–23] was employed in the current analysis. In this formalism

$$L_1=F(b/x^{1/2})/Z^{1/2}x^{3/2} \ , \tag{5}$$

where F is a function tabulated in Ref. 21, $x=(18\,787)\beta^2/Z$, and b is the sole free (composite) parameter of the theory.[21–23] The presence of ξ, as an amplitude of the Barkas-effect correction, in Eq. (2) reflects a minor controversy over the proper form of this correction. A synopsis of the history of parameters b and ξ reveals that b was initially fixed at 1.8 ± 0.2 on the basis of fits to accurate stopping-power measurements,[21–23] but when the Bloch term[25] was reintroduced into the Bethe-Bloch formula a strength factor (ξ) of roughly two was proposed[26] for the Barkas-effect-correction term[24] then used[26] in order to account for contributions of close collisions to the Barkas effect. Shortly afterward, two of the designers of the low-velocity Barkas-effect formalism[21–23] suggested that ξ be held at unity, but that $b=1.4\pm0.1$, on the basis of fits to very accurate stopping-power measurements with the Bloch term[25] included.[27] Numerous studies seeking resolution of this matter have been reported by the author,[12–15] and the topic has been recently reviewed.[28]

The Bloch term,[25] L_2, appearing in Eq. (2) was evaluated in the form

$$L_2=\psi(1)-\mathrm{Re}[\psi(1+iy)]\ , \tag{6}$$

where ψ represents the digamma function[29] and $y=z\alpha/\beta$ with α the fine-structure constant.

A further modification to Bethe-Bloch theory features an attempt to account for the gain and loss of electrons by the projectile when it has slowed to a velocity comparable to those of atomic electrons of the target. A projectile effective charge of some sort is accordingly defined and inserted into the Bethe-Bloch formula. Indeed, such a quantity was required in the present study of stopping powers of various targets for carbon-ion projectiles,[5] and the form of effective charge utilized was that which has recently proved so successful in a more comprehensive study of heavy-ion stopping powers.[15] That is, the projectile charge ze was replaced by an effective charge γze, where

$$\gamma=1-\zeta\exp(-\lambda v_r)\ . \tag{7}$$

In this case v_r represents the ratio of projectile velocity in the laboratory frame (v) to the Thomas-Fermi electron velocity $(e^2/\hbar)z^{2/3}$, so that $v_r=\beta/\alpha z^{2/3}$, and ζ and λ serve as the effective-charge parameters whose values must be established for a given projectile-target combination.[15]

All of the foregoing discussion of Bethe-Bloch theory pertains to a target consisting of identical atoms isolated completely from one another, since this model serves as the basis of theoretical descriptions of energy-loss processes. Whenever atoms combine into molecules, or appear in the condensed state, or both, compensations must be made for "aggregation effects." These effects are generally categorized as chemical-bonding effects or physical-state effects, and a target manifesting aggregation effects will be called "a composite-material target" herein. In order to apply the Bethe-Bloch formula to a composite-material target, one must assume that the stopping effects of the combined atoms are a linear sum of the stopping effects of the individual atoms. This rule, formulated early in this century,[30] is called "Bragg's rule of additivity," or simply the "additivity rule." Inspection of the Bethe-Bloch formula indicates that several of the target parameters therein must be evaluated for composite-material targets by appropriate averaging. Proper procedures for calculating average parameters are described in detail elsewhere.[6,22,31] Whereas the Bloch term[25] contains no target-dependent parameters, the Barkas-effect correction term requires averaging as explained previously.[6,22] Similarly, the target parameters of L_0 such as the shell-correction parameters and the mean excitation energy must be assigned average values.[6,22] However, available knowledge of the correct values for target constituents represents an important consideration in executing such a procedure. Mean excitation energies can be calculated from first principles only for low-Z materials, and aggregation effects influence considerably the value evinced by a given target material.[6,10] Similarly, all shell-correction parameters are known accurately for only a few (elemental) target materials.[16,17] The target mean excitation energy is often selected as the parameter with which to test the additivity rule, and the calculated average value I_B is obtained[31] from

$$\ln I_B=\frac{\sum_j n_j Z_j \ln I_j}{\sum_j n_j Z_j}\ , \tag{8}$$

where Z_j, n_j, and I_j, respectively, represent the atomic number, atomic concentration, and mean excitation energy of the jth component of the composite material. In one such test, conducted with very accurate measurements of the stopping power of polystyrene for protons,[8] the value of I extracted from the data exceeded I_B by some 13%.[9]

III. ANALYSIS AND RESULTS

Stopping-power measurements can be analyzed in terms of Bethe-Bloch theory to extract various parameters of the formulation. Computer codes capable of searching one-, two-, or three-parameter space have been described in detail elsewhere.[12–15] Quality of fit is characterized with the root-mean-square relative deviation of calculated from measured stopping powers—a quantity assigned the symbol σ. The number and accuracy of stopping-power determinations in a given experiment rarely support the extraction of more than two parameters. Indeed the experiments[1,2,5] studied herein follow the general pattern. Hence, two parameters were selected for searches in data fits. In the cases of proton and α-particle projectiles, these parameters were the mean-excitation energy and one of the two parameters associated with the Barkas effect, i.e., b (the composite quantity appearing in the correction formalism[21–23]) or ξ (the strength of the correction term). In the course of data analyses the results of another investigation of α particles traversing Mylar targets[32] were also subjected to analysis. When the value of b was obtained from the fit to measurements, the prescribed value of ξ was either 1 or 2, the former value corresponding to the Ritchie-Brandt suggestion[27] and the latter corresponding to the Lindhard suggestion[26] concerning contributions of close collisions to the Barkas-effect correction. When instead the value of ξ was extracted from fits to measurements, the prescribed value of b was either 1.8 or an estimate close to 1.4, the former value corresponding to that originally selected[21–23] and the latter corresponding to the subsequently revised estimate.[27] Results of each type of two-parameter search will be described separately.

A. Mylar targets

Stopping-power measurements for protons traversing Mylar foils[1] were analyzed with b set at 1.34, the value

TABLE I. Results of searches for the best-fit parameters, mean excitation energy (I), Barkas-effect parameter (b), and Barkas-effect correction amplitude (ξ), for protons and α particles traversing Mylar targets.

		Mylar target $I_B=74.6$ eV, $1.13I_B=84.3$ eV			
Projectile	Ref.	b (fixed)	I (eV)	ξ	σ
p	1	1.34	83.36	1.28	0.247
α	2	1.34	55.36	−0.07	0.335
α	32	1.34	80.48	0.40	0.144
p	1	1.80	87.12	2.44	0.234
α	2	1.80	54.64	−0.17	0.333
α	32	1.80	81.68	0.68	0.142

		Mylar target $I_B=74.6$ eV, $1.13I_B=84.3$ eV			
Projectile	Ref.	ξ (fixed)	I (eV)	b	σ
p	1	1.0	81.68	1.20	0.252
α	2	1.0	60.72	3.43	0.397
α	32	1.0	82.64	2.16	0.141
p	1	2.0	84.56	1.72	0.238
α	2	2.0	62.80	3.78	0.408
α	32	2.0	85.20	2.80	0.139

used for C in a recent study.[15] Extracted values of I and ξ, displayed in Table I, proved eminently plausible ($1.12I_B$ and 1.28, respectively). However, the α-particle projectile data[2] yielded values of I and ξ that were much too low for credibility ($0.74I_B$ and -0.07, respectively). At this point the α-particle measurements of Ref. 32 were analyzed, with the somewhat reassuring results that $I=1.08I_B$ and $\xi=0.40$. Next, b was fixed at 1.8 for the original data set,[1] and the best-fit values of I and ξ emerged as $1.17I_B$ and 2.44, respectively. This value of ξ lies in reasonable agreement with the Lindhard suggestion.[26] Again the resulting values of I and ξ for α-particle measurements[2] were very low, with $I=0.73I_B$ and $\xi=-0.17$, but the other set of such measurements[32] yielded $I=1.09I_B$ and $\xi=0.68$. In this case the ξ value agreed poorly with the Lindhard suggestion.[26]

Similar analyses with ξ fixed at values of 1 and 2 indicated agreement of the Ref. 1 data with both Lindhard[26] and Ritchie-Brandt[27] suggestions, suspiciously high values of b for both values of ξ in the case of Ref. 32 data, and unacceptable values of both I and b for the two selected ξ values in the case of the Ref. 2 data.

B. Kapton targets

Measurements of the stopping power of Kapton for protons[1] yielded unexpectedly low values of I upon first analysis. The author noted that the cited[1] composition of Kapton was in error, and the experimenters,[1] upon notification sometime later, responded with corrected foil thicknesses which the author then used for all such reported data.[1,5] The value of b selected initially was 1.34, the value previously used[15] for C targets. The corrected proton data yielded the results shown in Table II, all of which were reasonably consistent with expectation.

TABLE II. Results of searches for the best-fit parameters, mean excitation energy (I), Barkas-effect parameter (b), and Barkas-effect correction amplitude (ξ), for protons traversing Kapton targets.

	Kapton target $I_B=76.1$ eV, $1.13I_B=86.0$ eV			
Projectile	b (fixed)	I (eV)	ξ	σ
p	1.34	80.32	1.53	0.124
p	1.80	82.96	2.70	0.138

	Kapton target $I_B=76.1$ eV, $1.13I_B=86.0$ eV			
Projectile	ξ (fixed)	I (eV)	b	σ
p	1.0	78.88	1.01	0.119
p	2.0	81.52	1.55	0.130

TABLE III. Results of searches for the best-fit parameters, mean excitation energy (I), Barkas-effect parameter (b), and Barkas-effect correction amplitude (ξ), for protons and α particles traversing Havar targets.

Projectile	b (fixed)	Havar target $I_B=295.8$ eV I (eV)	ξ	σ
p	1.36	302.64	1.256	0.061
α	1.36	303.04	0.800	0.979
p	1.80	345.44	3.856	0.098
α	1.80	309.60	1.792	0.356
Projectile	ξ (fixed)	Havar target $I_B=295.8$ eV I (eV)	b	σ
p	1.0	295.44	1.288	0.072
α	1.0	284.24	1.600	0.567
p	2.0	311.92	1.576	0.082
α	2.0	289.20	2.000	0.312

C. Havar targets

Results of analyses of stopping powers of Havar for proton[1] and α-particle[2] projectiles appear in Table III. In the case of mixtures one might at first estimate expect consistency of extracted I values with additivity predictions.[31] In this spirit one might reasonably expect that the extracted I and b values would respectively agree with I_B and a b value common to the major constitutent elements. (Such agreement did indeed occur in two previous studies of Havar stopping powers for hydrogen-isotope projectiles.[6,33]) The current study of I and ξ fits yielded excellent results except for the case of proton projectiles when b was fixed at 1.8: I exceeded I_B by nearly 17%, and ξ was 3.86 rather than the expected value of about 2. Similarly, the results of I and b fits deviated little from expectation.

D. Carbon projectiles

Analysis of stopping-power measurements with carbon projectiles[5] required careful selection of parameters to be established through the search procedure. That is, these data were collected at projectile velocities which necessitated inclusion of one or two effective-charge parameters in addition to the three already selected for proton and α-particle data. Since the two-parameter (ζ,λ) formulation had proved so successful for recent heavy-ion studies[15] (including carbon projectiles), the same form was employed herein, having selected values of the other three parameters (I,b,ξ) on the basis of the present and earlier studies.[6–9,15,17] Mean-excitation energies for nickel and Havar targets were deemed well known.[6,17,33] I values of Mylar and Kapton were selected as $1.13I_B$ in accordance with earlier results for a specific low-Z compound[9] and with an identified general trend for compounds.[17] Two sets of (b,ξ) values were utilized—one corresponding to the Lindhard suggestion[26] and one to the Ritchie-Brandt suggestion.[27] Results of these fits, appearing in Table IV, were all quite satisfactory in the sense that values of ζ and λ followed trends reasonably consistent with those displayed by carbon projectiles in a previous study,[15] although all values of ζ and λ were somewhat higher in the present study. The (simple arithmetic) average figure of merit (σ) for the fits favored neither suggestion,[26,27] but the lower magnitudes of best-fit (ζ,λ) values occurred for the (b,ξ) values following the Lindhard suggestion.[26] All values of σ lay below 0.51, indicating excellence of fits with plausible values of ζ and λ in every case.

IV. DISCUSSION AND CONCLUSIONS

Several reviews of stopping-power additivity studies have appeared recently.[7,17,34–36] Deviations from additivity are to be expected in the presence of aggregation effects, and particularly so in the case of low-Z compounds where a large fraction of the electrons are valence electrons and hence susceptible to bonding effects. Both Mylar and Kapton are low-Z compounds. (Deviations from additivity may also occur for mixtures such as alloys, but far fewer tests have been conducted for these materials.[34]) In order to test the additivity assumption when analyzing stopping-power measurements with Bethe-Bloch theory, one generally assigns to the shell-correction parameters and Barkas-effect parameters values appropriate for the average Z of the composite material. Then the additivity test is focussed on the mean-excitation energy, whose value can be compared

TABLE IV. Results of searches for the best-fit effective charge parameters (ζ and λ) for carbon projectiles traversing Mylar, Kapton, Havar, and Ni targets.

Target	I (eV) fixed	Carbon projectile b	ξ	ζ	λ	σ
Mylar	84.3	1.34	1.0	1.448	1.227	0.322
	84.3	1.80	2.0	1.198	1.029	0.371
Kapton	86.0	1.34	1.0	1.653	1.317	0.080
	86.0	1.80	2.0	1.538	1.179	0.041
Havar	296	1.36	1.0	1.304	1.106	0.508
	296	1.80	2.0	0.946	0.878	0.475
Nickel	304	1.36	1.0	1.368	1.076	0.183
	304	1.80	2.0	0.980	0.852	0.166

TABLE V. Values of selected constituent mean excitation energies for composite targets and of all assigned modified Bethe-Bloch parameters employed for composite and Ni targets.

Element	I (eV)	Ref.	Element	I (eV)	Ref.
H	20.4	37	Mn	272	17
Be	63.7	17	Fe	286	17
C	78.0	17	Co	297	17
N	82.0	17	Ni	311	17
O	95.0	17	Mo	424	17
Cr	257	17	W	727	17

					Shell correction parameters			
Target	$\bar{Z}$	$\bar{A}$	I_B (eV)	b	V_L	H_L	V_M	H_M
Mylar	4.54	8.74	74.6	1.34	0.318	1.00		
Kapton	5.03	9.80	76.1	1.34	0.379	1.00		
Havar	26.62	57.60	296.0	1.36	1.000	1.00	1.875	7.13
Nickel	28.00	58.71	304.0	1.36	1.000	1.00	2.000	6.53

with the prediction of Eq. (8).

Table V contains values assigned to various parameters of Bethe-Bloch theory, including constituent-element mean excitation energies employed for evaluation of I_B, and the source references.[17,37] It must be noted that the Havar constituent element, Ni, was given the I value of 311 eV in order to employ a consistent set of such values[17] for calculation of I_B, whereas Ni was assigned an I value of 304 eV in the carbon-projectile study (Table IV). The latter value, derived from the aforementioned study of carbon projectiles traversing Ni targets,[15] seemed more appropriate for the present analysis of measurments with the same projectile-target combination.[5] The b value common to Ni and Havar (1.36) was taken to be that employed for Ni in a recent study,[15] whereas that common to Mylar and Kapton (1.34) was taken to be the same as the value used for C in the same study,[15] when the Ritchie-Brandt suggestion[27] was followed.

Results of the fits, displayed in Tables I–IV, feature plausible values of the fitted parameters in all cases except that of the α-particle projectile data of Ref. 2 for Mylar targets. One can speculate that those particular measurements may have suffered from systematic errors. Moreover, the I and ξ values extracted from the measurements with protons traversing Havar, when b was fixed at 1.8, both strayed inexplicably to anomalously high levels. However, all of the other fits of data for light projectiles traversing Havar yielded excllent results.

In view of the remarkably good fits achieved in the present study, and of the generally plausible values of extracted Bethe-Bloch parameters, the measurements involved[1,2,5,32] can be adjudged reliable, with the one exception noted above. The low-Z compounds, Mylar and Kapton, appear to follow familiar trends for such substances in that mean-excitation energies extracted from measurements exceed Bragg (additivity) values by some 8–17 % for Mylar and some 5–9 % for Kapton—results generally consonant with the so-called "13% rule" for compounds.[17] By comparison, the alloy Havar evinces normal behavior by providing mean excitation energies within −4% to +5% of the additivity prediction. Both the Mylar and Havar results are thoroughly consistent with those of previous studies.[6,33]

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