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P. Boccaccio and G. Viesti: HEAVY-ION STOPPING-POWER CALCULATIONS.

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ABSTRACT

A computer program (ELOSS) for heavy- ion stopping-power calculations is presented.

The basic Bethe-Bloch theory is employed, incorporating corrections for the projectile low-velocity effect and charge state.

Results are compared with several experimental data sets and with Northcliffe and Schilling's evaluations.

1. - INTRODUCTION

Energy losses of particles and heavy ions in matter are of general interest in experimental physics. Frequently, very accurate stopping powers are required, for several projectile-target combinations, and in wide ranges of incident ion energies, for which experimental data are not always available.

The analytical approach to the calculations of particle-and heavy-ion stopping powers by the Bethe-Bloch theory(1), is known to give estimates which are generally in good agreement with experimental data. However, some quantities, as the mean excitation energy and the shell corrections, which are included in the formalism, in general cannot be realiably calculated, and are usually evaluated through fits to experimental data. Furthermore, in the low-velocity region corrections to the Bethe-Bloch theory are important(2).

Since the formalism rests on the applicability of the first-order Born approximation, it follows that the predicted stopping powers depend on the square of the projectile charge Ze. Experimental data from Barkas and coworkers(3), however, showed that oppositely-charged projectiles of the same mass and velocity did not lose energy at equal rates in traversing matter. It was suggested(4) that higher-order approximations would be necessary to account for this effect in the Bethe-Bloch theory.

Successive analysis(5) showed that the introduction of the projectile - Z^3 correction represents a significant contribution to stopping powers, especially in the case of heavy projectiles.

Another correction to the B.-B. theory, for low incident velocities, arises from the projectile charge state, which depends on its velocity(1) and charge Ze.

Each of these corrections requires the preliminary evaluation of some characteristic parameters, which are usually estimated through fits to experimental data.

The computer program ELOSS was written for the calculation of heavy-ion stopping powers; the basic B.-B. theory was employed, incorporating the corrections for the low-velocity projectile - Z^3 effect and the ion effective-charge state.

In the present paper, the basic theory and some features of the program are described (Sects. 2-3); some calculations are reported and compared both with experimental data and with existing compilations (Sect. 4); discussions of the results and conclusions are presented (Sect. 5).

2. - THEORY

2.1. The stopping power S_o of a target composed of atoms with atomic number Z_2, mass A_2, for a projectile with atomic number Z_1, mass A_1, and energy E_1 in the laboratory frame, is written, in the first-order Born approximation[6], as:

$$(1) \qquad S_o(Z_1,A_1,E_1) = \frac{\gamma^2 Z_1^2}{\gamma_p^2} \cdot Sp\,(E_1/A_1),$$

where Sp is the stopping power for a proton having the same velocity as the incident ion, γ is the correction for the ion effective charge and γ_p is the same quantity for the proton.

In the usual B.-B. formalism[1], the proton stopping power, S_p is calculated as:

$$(2) \qquad S_p(\beta^2) = \frac{K}{\beta^2} \cdot \frac{Z_2}{A_2} \cdot (f(\beta) - \ln I - \sum_i C_i/Z_2 - \tfrac{1}{2}\,\delta)$$

where β is the ratio of the projectile velocity, in the laboratory frame, to the velocity of light in vacuum, I the mean excitation energy of the target atoms, C_i the shell correction for the i-th atomic shell, δ the high-velocity density correction, K a numerical constant, and:

$$(3) \qquad f(\beta) = \ln\left(\frac{2\,m\,c^2\ \beta^2}{1-\beta^2}\right) - \beta^2$$

where mc^2 is the electron rest mass.

Recently[6,7], this theory was extended to include the Z_1^3-dependent correction. The contribution of this effect was calculated by Ashley and coworkers[6] in a classical treatment which is equivalent to a second-order Born approximation. Introducing the reduced parameter $x=v_1^2/(v_0^2 \cdot Z_2)$, in which v_1, v_0 stand respectively for the projectile and the Bohr velocity, the stopping power, S(x), is written as[6]:

$$(4) \qquad S(x)=S_0(x) \cdot \left(1+ \frac{Z_1^*}{Z_2^{\frac{1}{2}}} \cdot \frac{K(b,x)}{x}\right)$$

Here, $S_0(x)$ is the stopping power in first-order Born approximation (formula (1)), $Z_1^* = \gamma Z_1$ is the projectile effective charge, and K(b,x) is a calculated function[6,7], which depends on the parameter b, as well as on x. The best trial value for b, from comparison with some available experimental data, was $b=1.8 \pm 0.2$. Combining formulas (1), (4), the following expression results:

$$(5) \qquad S(x)= \frac{\gamma^2 Z_1^2}{\gamma_p^2} \cdot S_p(x) \cdot \left(1+ \frac{Z_1^*}{Z_2^{\frac{1}{2}}} \cdot \frac{K(b,x)}{x}\right)$$

which is employed in program ELOSS calculations.

In the following, details of some terms in (5) will be discussed.

2.2. - Effective-Charge Correction. The effective-charge theory for heavy-ion stopping powers is reported in several papers[(8-10)].

Pierce and Blann[(11)] proposed the following expression for the effective-charge factor γ:

(6) $$\gamma = 1 - \exp(-\lambda \cdot v_r),$$

in which v_r is the ratio of the incident ion velocity, v_1, to the Thomas-Fermi electron velocity $(e^2/\hbar) \cdot z_1^{2/3}$; λ is a free parameter (the effective-charge parameter), its value being stated as $\lambda = 0.95$ (for $v_r > 2$) from fits to experimental data.

The term γ_p in (5) accounts for the proton charge state in the low-velocity region, and is important only in the range $E/A \lesssim 0.3$ MeV/a.m.u., where it is significantly < 1.

However Porter's analysis[(2)] showed that, from fits to several heavy-ion stopping-power experimental data, in which the projectile-Z_1^3 effect was accounted for, different values for λ are obtained, according to the particular projectile-target combination. In his procedure, the "best" value was found for λ such that the quantity[(12)]:

(7) $$\sigma = \left(\frac{1}{N} \sum_{i=1}^{N} (S^i_{exp} - S^i_{calc})^2 / (\Delta S^i_{exp})^2\right)^{\frac{1}{2}},$$

called the "minimum error function", was minimized.

The dependence of λ on Z_2 is found very complicated, while, for fixed Z_2, the variations of λ with Z_1 exhibits fairly simple patterns.

2.3. - Proton Stopping Power. To evaluate the proton stopping power, S_p, in (2), the mean excitation energy, I, and the shell corrections, C_i(i = K, L, M, ...), have to be evaluated first (the term δ is usually neglected for non-relativistic velocities[(1)]). The shell corrections are written in the form[(13)]:

(8) $$\sum_i C_i = B_1 \cdot C_k(\beta^2) + B_2 \cdot C_L(\beta^2) + VM \cdot C_L\ (HM \cdot \beta^2) + VN \cdot C_L\ (HN \cdot \beta^2),$$

in which C_k, C_L, are the K- and L-shell corrections, respectively, as calculated by Walske[(14,15)]; B_1, B_2, are the corresponding strenght parameters. For the M- and N-shell, the same corrections are used as for the L-shell with scaling parameters HM, HN[(1)].

The six quantities mentioned above, as well as the mean excitation energy, are usually evaluated through analysis of experimental data and are generally found in literature.

2.4. - The Low-Velocity-Projectile Z^3 Effect. In formula (4), the Z_1^3 contribution to the stopping power is calculated for the statistical model of the target atom, in the Lenz-Jensen approximation[(6,7)].

In ref. (6), the function K(b,x) is tabulated, for b=1.6, 1.8, 2.0; it shows a very slow variation with the argument x.

3. - PROGRAM ELOSS

3.1. The computer program ELOSS, written in Fortran IV language, uses the basic Bethe-Bloch formula with the corrections included in (5), for the calculation of heavy-ion stopping powers. For simplicity, the shell corrections C_i and the function K(b,x) in (5), are approximated by polinominal expansions from the tabulations in refs. (6), (16).

For stopping-power calculations, the following input data are required:

a) projectile: charge (Z_1), mass (A_1), effective-charge parameter (λ);
b) target: charge (Z_2), mass (A_2), mean excitation energy (I), shell correction parameters (B_1, B_2, VM, HM, VN, HN).

The program is completely interactive and the following calculations are performed:

- stopping powers;
- energy loss vs. target thickness, and conversely target thickness vs. projectile energy loss;
- fits to experimental data for the evaluation of theory parameters.

3.1. - Energy Loss Calculations. The energy lost by ions in target materials, ΔE, is calculated by numerical integration of the stopping power, solving for ΔE:

$$\Delta x = \int_{E_0-\Delta E}^{E_0} S^{-1}(E)\, dE, \qquad (9)$$

in which Δx is the target thickness. To check convergence of the integral (9), repeated evaluation is performed, reducing the integration step, until percent difference between two successive evaluations falls under a fixed amount.

3.2. - Parameter Evaluation. By minimization of the function σ (formula (7)), each of the eight parameters of the formalism may be fitted to experimental data by program ELOSS.

However, a careful choice of the parameters and the data under analysis is necessary, according to physical considerations. A simultaneous search for all the parameters, in principle, is possible, but in this case more than one set of parameters may result from least-squares fitting procedures. This lack of unicity is related to the presence of several minima for chi-square statistics in multi-dimensional space, especially when measurements are affected by large errors(13). The best one can do is to evaluate separately those parameters only, which are influent in the energy range covered by the experimental data under analysis. The shell correction parameters in (8) and the mean excitation energy, I, have been determined for many atomic elements from the analysis of a number of experimental data(1), relative to proton and light-ion stopping-powers. Thus employing the values found in literature for these parameters, one can focus the attention on the study of the effective-charge parameter, λ , which is of crucial importance in heavy-ion stopping-power calculations. In next section, some calculations will be reported, employing best-fit values for λ , in comparison with the same calculations employing values found in literature; as will be evident, a fairly better agreement with experimental data was achieved.

4 - RESULTS

Using the values found in literature for shell correction parameters and mean excitation energies, as displayed in Table I, and effective-charge parameters(2), stopping-powers were calculated for various projectile-target combinations.

In those calculations, only energies above 0.5 MeV/a.m.u. were considered.

TABLE I Mean excitation energies and shell correction parameters employed for stopping-power calculations.

Stopping Material	I (eV)	B_1	B_2	VM	HM	VN	HN	Ref.
Al	169.0	1.0	1.0	0.7	1.4	0.0	0.0	(13)
Si	173.0	1.0	1.0	0.7	1.4	0.0	0.0	(2)
Ti	230.0	1.0	1.0	1.0	4.6	0.0	0.0	(2)
Fe	284.0	1.0	1.0	1.0	5.5	0.0	0.0	(2)
Ni	337.0	1.0	1.0	1.0	5.5	0.0	0.0	(13)
Cu	320.0	1.0	1.0	1.0	5.0	0.0	0.0	(2)
Ag	571.0	1.0	1.0	0.4	3.0	1.0	2.5	(13)
Au	950.0	1.0	1.0	1.6	2.3	2.7	9.8	(13)

4.1. - As a preliminary check of the program, light-ion stopping-power calculations were performed and compared with recent experimental data[17,18]. In this case, an evident advantage is the large availability of high-accuracy experimental data for proton and alpha-particle stopping-powers.

Furthermore, for incident velocities greater than $\sim$ 0.5 MeV/a.m.u., those projectiles get almost completely stripped of electrons, then no correction for the charge state is required. The results of these calculations are displayed in Table II, in which average absolute deviations of calculated to experimental data are reported.

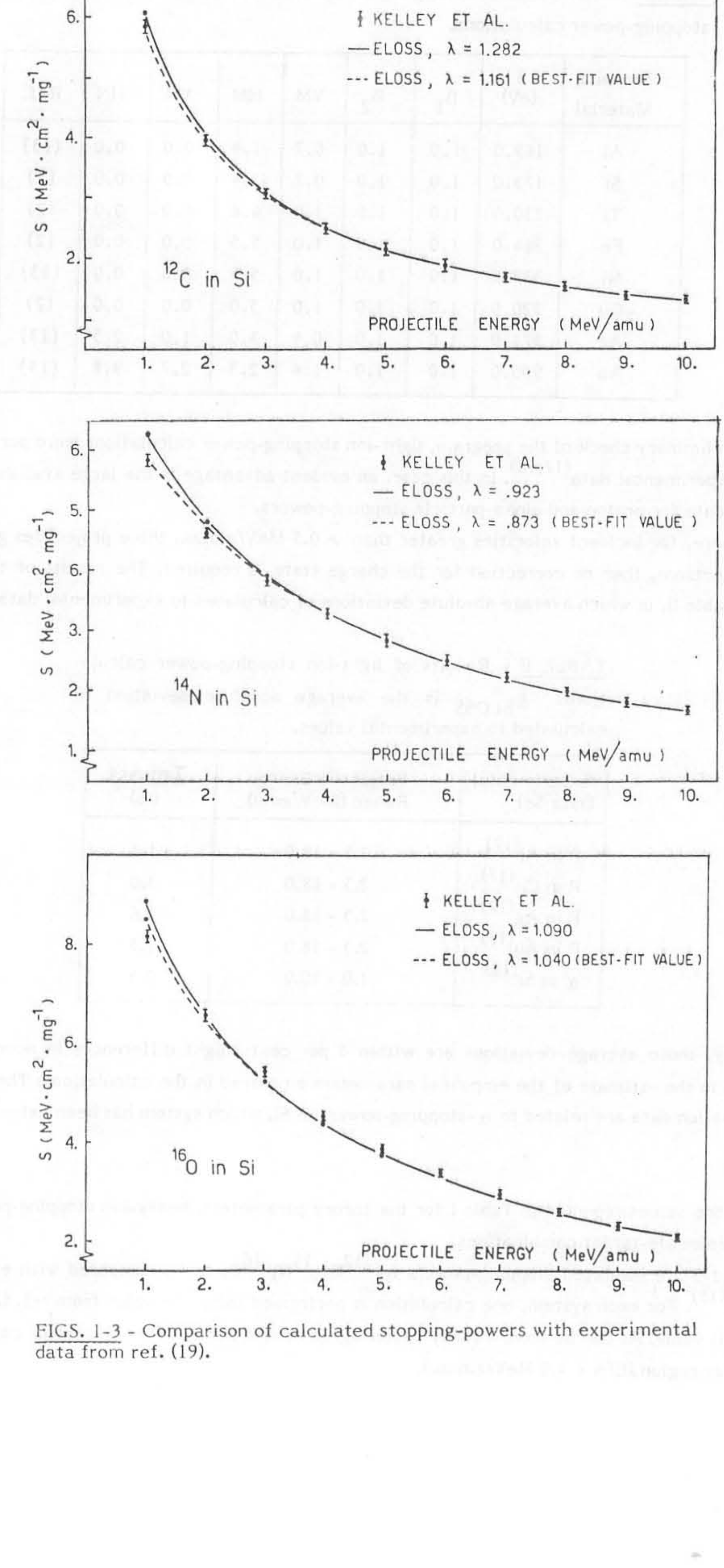
TABLE II - Results of light-ion stopping-power calculations. $\bar{\Delta}_{ELOSS}$ is the average absolute deviation of calculated to experimental values.

Experimental Data Set	Projectile Energy Range (MeV/amu)	$\bar{\Delta}$ ELOSS (%)
P in Al[17]	2.5 - 18.0	1.1
P in Cu[17]	2.5 - 18.0	3.0
P in Ag[17]	2.5 - 18.0	1.6
P in Au[17]	2.5 - 18.0	2.5
α in Si[18]	1.0 - 10.0	0.3

Generally, those average deviations are within 3 per cent; slight differences in accuracy probably reflect uncertainties in the estimate of the empirical parameters employed in the calculations. The best results achieved in fitting light-ion data are related to α-stopping-powers in Si, which system has been extensively studied.

4.2. - Using the values reported in Table I for the theory parameters, heavy-ion stopping-powers were calculated for several projectile-target combinations.

In Figs. 1-3 are displayed stopping-powers for ^{12}C, ^{14}N, ^{16}O, in Si, compared with experimental data from Kelley et al.[19]. For each system, one calculation is performed using the value from ref. (2) for λ ; the other one uses a best-fit value. As can be seen, a fairly better agreement is achieved for the latter calculation, especially in the low-energy region (E/A < 4.0 MeV/a.m.u.).



FIGS. 1-3 - Comparison of calculated stopping-powers with experimental data from ref. (19).

In figs. 4-5 are reported stopping-powers for ^{16}O and ^{35}Cl in Ag, compared with experimental data from ref. (20), and with Northcliffe and Schilling's tabulations[21].

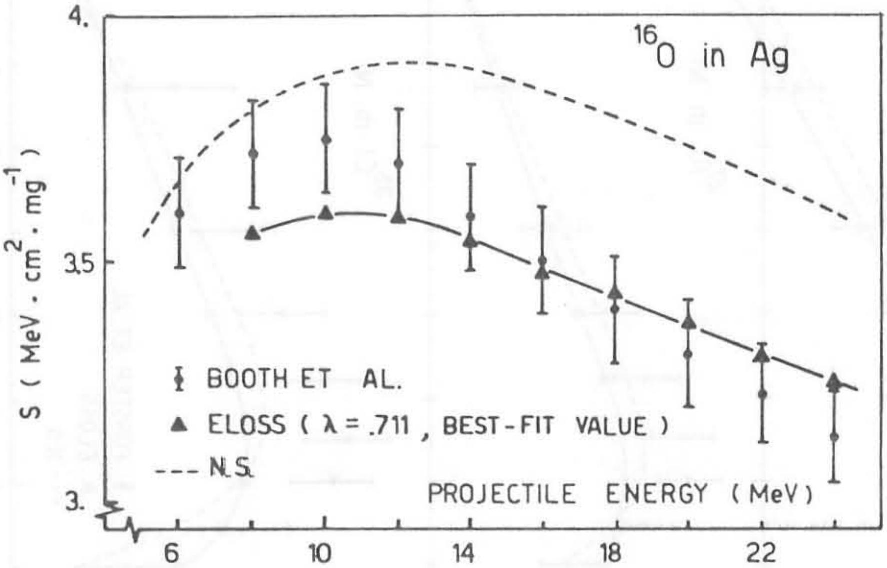


FIG. 4 - Comparison of calculated stopping-powers with experimental data from ref. (20), and with Northcliffe and Schilling's evaluations.

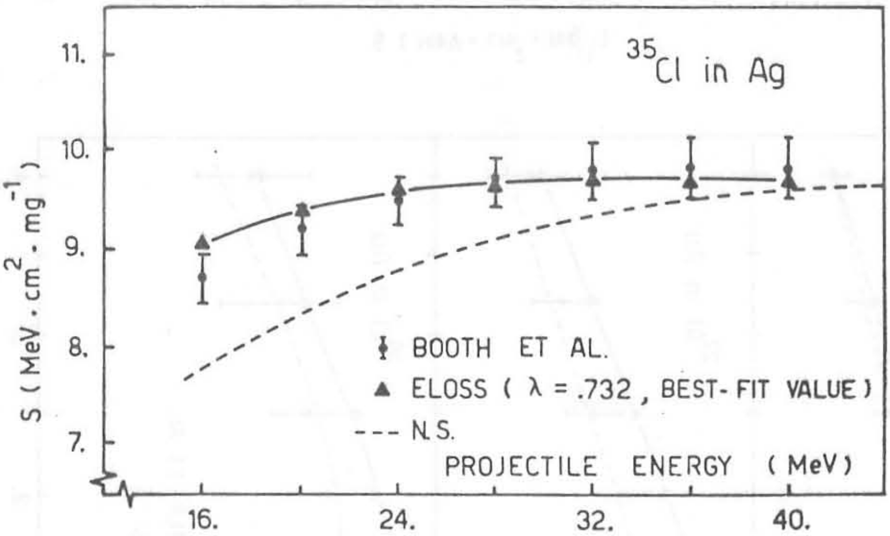


FIG. 5 - Comparison of calculated stopping-powers with experimental data from ref. (20), and with Northcliffe and Schilling's evaluations.

In both calculations, best-fit values for λ were employed.

Figs. 6-10 display calculated stopping-powers for ^{19}F, ^{27}Al, ^{35}Cl, in Au, Ni, Cu, Fe, Ti, compared with experimental data from Forster et al.[22], and when possible, with N.-S. tabulations[21]. In Table III the results of these calculations are summarized. As can be seen, the calculations agree with the corresponding experimental data within ∽ 2.0 to ∽ 7.0 per cent in the average, depending on the particular system analyzed.

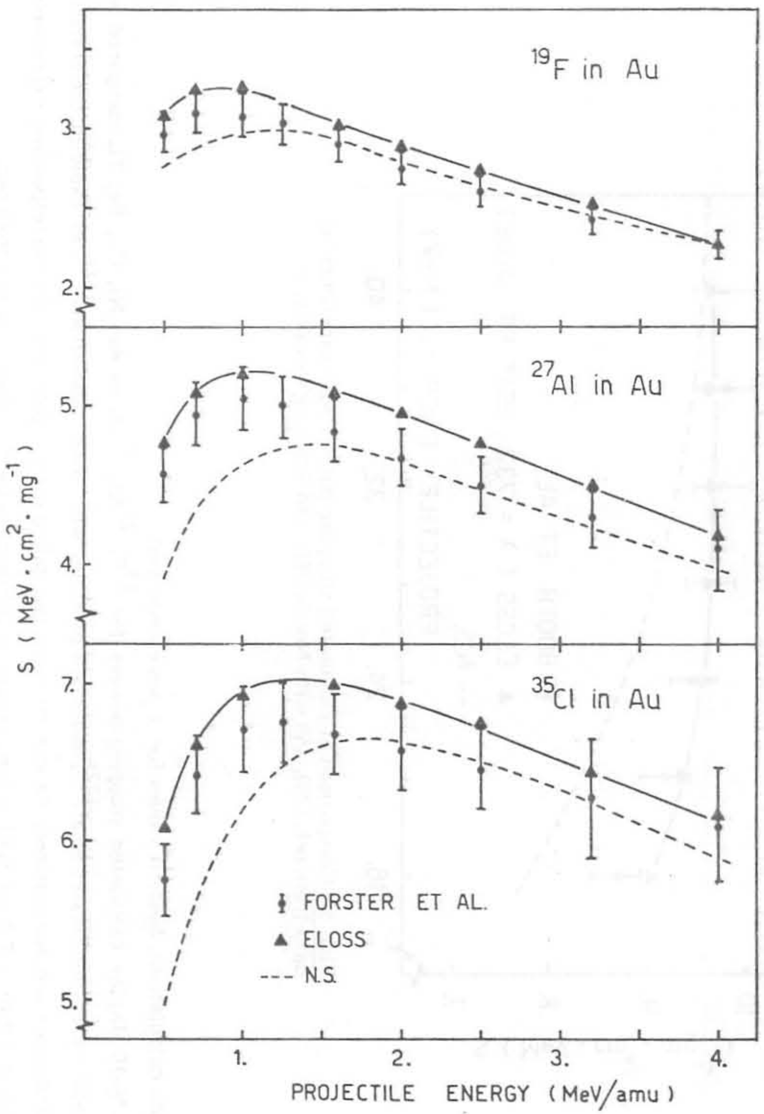


FIG. 6 - Comparison of calculated stopping-powers with experimental data from ref. (22), with Northcliffe and Schilling's evaluations.

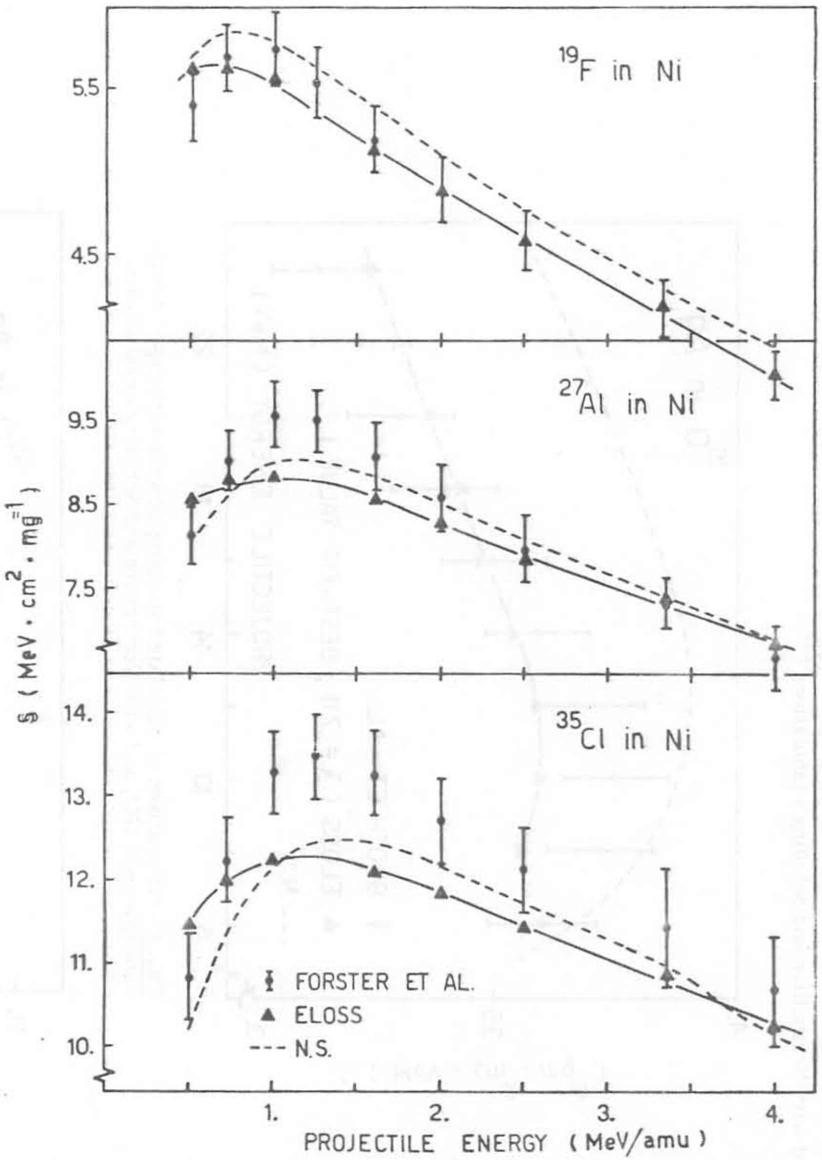


FIG. 7 - Comparison of calculated stopping-powers with experimental data from ref. (22), and with Northcliffe and Schilling's evaluations.

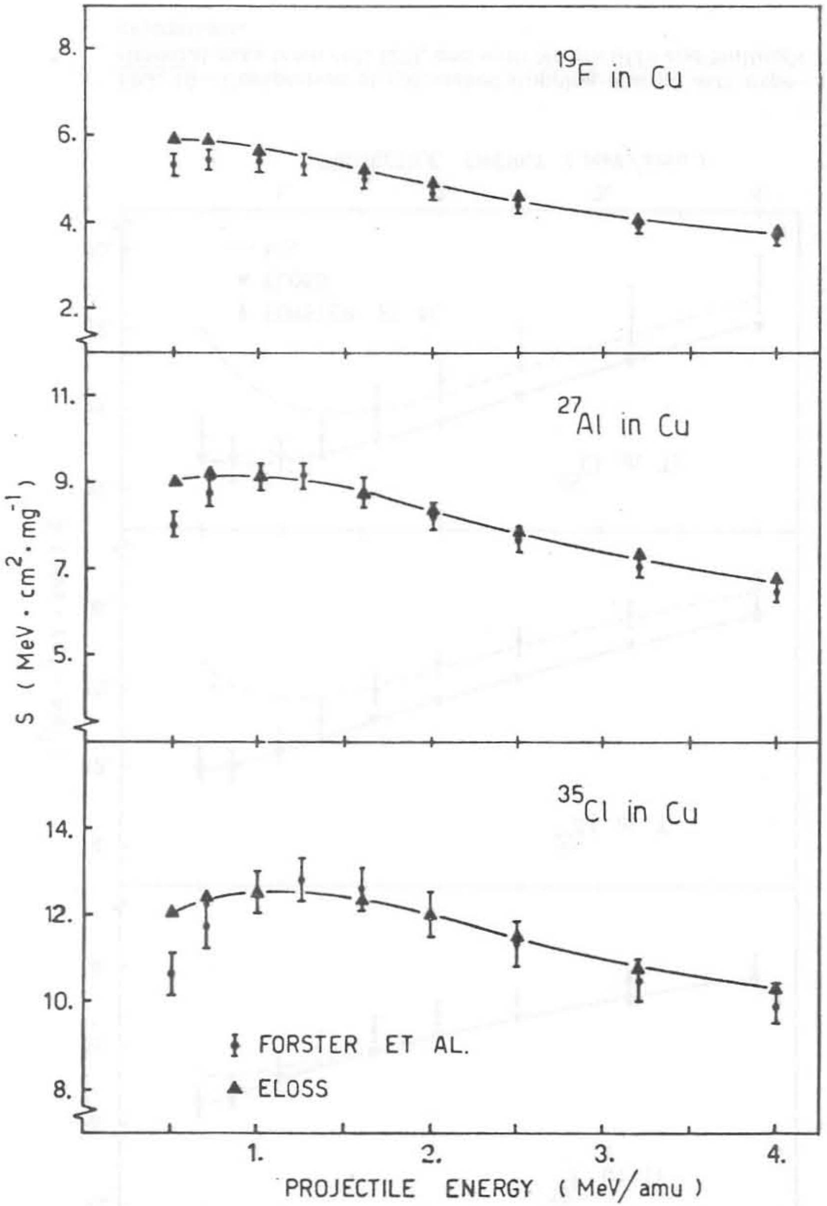


FIG. 8 - Comparison of calculated stopping-powers with experimental data from ref. (22).

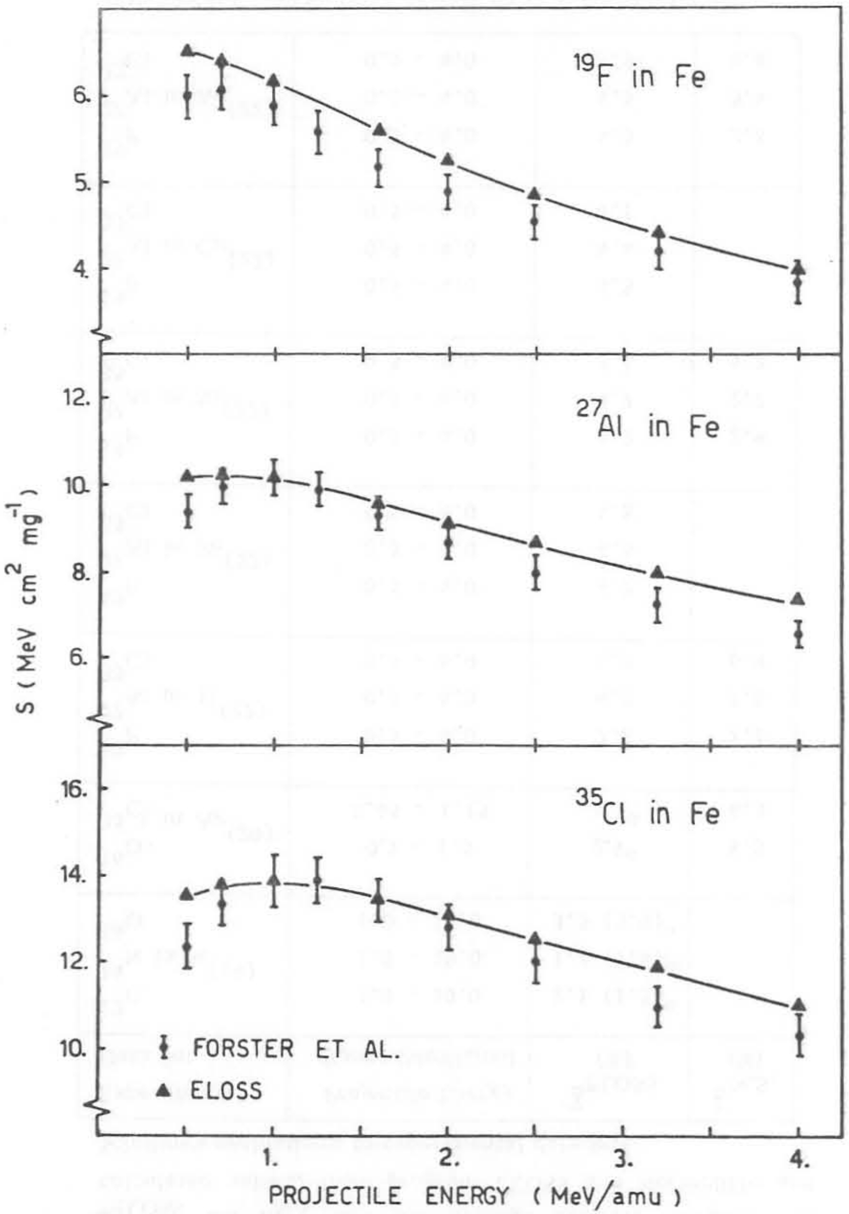


FIG. 9 - Comparison of calculated stopping-powers with experimental data from ref. (22).

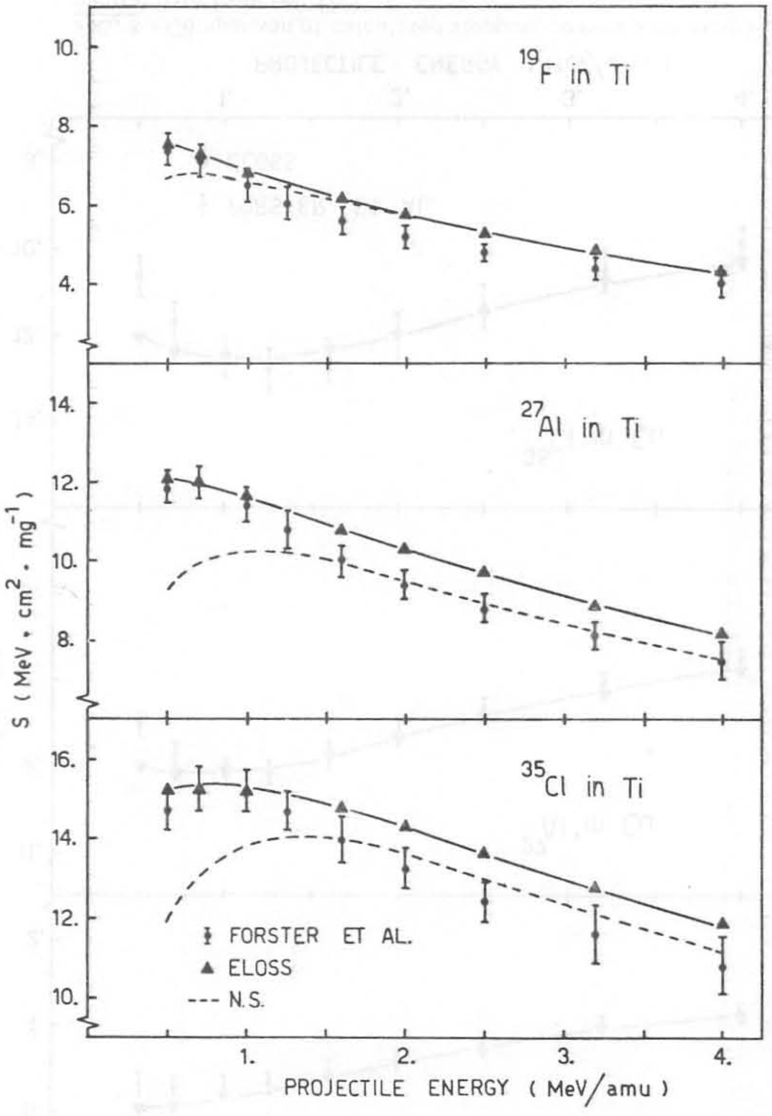


FIG. 10 - Comparison of calculated stopping-powers with experimental data from ref. (22), and with Northcliffe and Shilling's evaluations.

TABLE III - Results of heavy-ion stopping-power calculations. $\bar{\Delta}_{ELOSS}$ and $\bar{\Delta}_{N.S.}$ are the average absolute deviations of calculated values, from program ELOSS and Northcliffe and Schilling's evaluations, to experimental data sets.

Experimental Data Set	Projectile Energy Range (MeV/amu)	$\bar{\Delta}_{ELOSS}$ (%)	$\bar{\Delta}_{N.S.}$ (%)
^{12}C	1.0 - 10.0	2.1 (1.5)[a]	
^{14}N in Si (19)	1.0 - 10.0	1.7 (1.4)[a]	
^{16}O	1.0 - 10.0	3.5 (3.0)[a]	
^{16}O in Ag (20)	0.5 - 1.5	2.4[a]	8.8
^{35}Cl	0.45 - 1.15	1.5[a]	6.3
^{19}F	0.5 - 4.0	7.6	7.1
^{27}Al in Ti (22)	0.5 - 4.0	6.5	7.6
^{35}Cl	0.5 - 4.0	6.3	6.9
^{19}F	0.5 - 4.0	6.7	
^{27}Al in Fe (22)	0.5 - 4.0	6.5	
^{35}Cl	0.5 - 4.0	4.8	
^{19}F	0.5 - 4.0	1.2	2.9
^{27}Al in Ni (22)	0.5 - 4.0	3.7	2.7
^{35}Cl	0.5 - 4.0	5.6	5.7
^{19}F	0.5 - 4.0	5.3	
^{27}Al in Cu (22)	0.5 - 4.0	4.4	
^{35}Cl	0.5 - 4.0	4.1	
^{19}F	0.5 - 4.0	4.5	2.8
^{27}Al in Au (22)	0.5 - 4.0	4.5	5.4
^{35}Cl	0.5 - 4.0	3.9	4.8

a) Values obtained by least-squares fit to experimental data.

5 - CONCLUSIONS

The evolution of heavy-ion physics, in connection with the operation of several heavy-ion facilities, has brought in last years an increasing interest for massive-particle stopping-powers, in data analysis as well as in laboratory practice.

In many cases, the lack of experimental information can be compensated by the use of suitable calculations. In this frame, the Bethe-Bloch theory, widely used in the past for light-ion stopping-power calculations, with a suitable set of built-in corrections, represents a fairly good approach to stopping-power estimates.

Program ELOSS, written to satisfy these requirements, can also be employed to extend the analysis of the Bethe-Bloch corrected theory to new experimental data sets, for the evaluations of theory parameters. A further interesting use of the program may be in the analysis of experimental data for particle identification, in E- ΔE telescope measurements.

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