Stopping-power calculations for semiconductors

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(Received 23 June 1982)

The method developed by Brandt and Reinheimer which explicitly includes the effect of the semiconductor gap has been used to calculate the proton and α-particle stopping powers of the valence-electron gas of C (diamond), ZnTe, and U. These values, as well as those existing for Si and Ge, have been combined with the stopping contribution of the electronic core obtained from the statistical atomic model of Bonderup. Stopping powers have also been calculated using the statistical model alone. The calculated curves, which are valid for all incident projectile energies, reproduce the overall features of the semiempirical slowing-down curves, but not always the absolute values.

INTRODUCTION

A recent theoretical formalism by Brandt and Reinheimer[1] (BR) based on a model of an electron gas with energy gap permits calculation of several fundamental quantities, including stopping powers for energetic charged particles, in a manner independent of the usual Bethe approach. Their theory, which takes into account close single collisions and collective excitations, is a generalization of that of Lindhard and Winther.[2] With this extension it is possible to include the effect of the gap in stopping powers, and this without limitation on incident energy or necessarily resorting to adjustable parameters. The only existing calculations are the implicit ones given by Reinheimer[3] for Si and Ge.

The BR formalism was derived for the valence-electron gas of semiconductors, which, per electron, dominate the slowing-down process. To obtain a total atomic stopping power, provision should be made for the other electrons also. In the present case, the stopping of these other electrons, which we call the "core," was obtained from the statistical model of the atom much in the way described by Bonderup[4] by considering that the electron cloud is composed of "inner" and "outer" electrons depending on whether the velocity of an atomic electron is, respectively, greater or less than the velocity of the incident projectile. The core, as we use it, can then contain part of Bonderup's outer electrons. The stopping due to the total number of electrons is thus obtained. These values can be compared to the stopping derived from the Bonderup statistical model alone, integrated over the total number of atomic electrons.

SUCCINCT SUMMARY OF THE THEORIES

Brandt-Reinheimer formalism

Before going through some of the details of the formalism developed by Brandt and Reinheimer, we first define (with the same notation as in Ref. 1) the different elements given in this theory. The Fermi momentum k_F is related to the electron density n by $k_F=(3\pi^2 n)^{1/3}$, the Fermi velocity $v_F=k_F$ (a.u.), and the Fermi energy $E_F=\frac{1}{2}k_F^2$. The reduced wave vector and frequency variables are, respectively,

$$z=q/2k_F\ , \tag{1}$$

$$u=\omega/qv_F\ . \tag{2}$$

In the usual notation

$$r_s=(3/4\pi n)^{1/3}\ , \qquad \chi^2=r_s/6.02\ . \tag{3}$$

The quantity $\gamma=\frac{1}{4}\epsilon_g=\frac{1}{4}E_g/E_F$, which is small compared to unity, occurs naturally as an expansion parameter. E_g is the energy gap. Another quantity of smallness is $E_g/\omega_p=\sqrt{3}(\gamma/\chi)$ where

$\omega_p=(4\pi n)^{1/2}$ is the plasma frequency. In this case the dielectric function $\kappa(z,u,E_g)$ can be written as

$$\kappa(z,u,E_g)=1+g(z,E_g)\times[f_1(z,u,E_g)+if_2(z,u,E_g)]\ , \tag{4}$$

where

$$g(z,E_g)=\frac{\chi^2}{3\gamma^2+z^2}\ . \tag{5}$$

In Eq. (4) the functions f_1 and f_2 are algebraically complicated; they are given in detail in Ref. 3.

The electronic stopping power of a dispersive medium for a particle of charge Z_1e and velocity v_1 is given by[1,3]

$$-\frac{dE}{dX}=\frac{Z_1^2e^2\omega_p^2}{v_1^2}L\ , \tag{6}$$

where L is the stopping number per target electron,

$$L=\frac{6}{\pi\chi^2}\int_0^{v_1/v_F}u\,du\times\int_0^{\infty}z\,dz\,\mathrm{Im}[\kappa^{-1}(z,u,E_g)-1]\ . \tag{7}$$

For the quantity L, one can distinguish two contributions,

$$L=L_s+L_r\ , \tag{8}$$

where L_s comes from single collisions and corresponds to the part $\mathrm{Im}\kappa\neq 0$. The part L_r represents the collective excitations. In practice, considering a reduced variable y proportional to the incident particle energy,

$$y=\frac{2v_1^2}{(\omega_p^2+E_g^2)^{1/2}}\ , \tag{9}$$

the integral L_r can be obtained once L_s is determined. At y large enough, the following two relations are satisfied[1]:

$$L_r+L_s=\ln y\ , \tag{10}$$

$$L_s=L_r+C\ . \tag{11}$$

From Eqs. (10) and (11) the constant C can be determined:

$$C=[2L_s-\ln y]\ \text{ for large } y\ . \tag{12}$$

The total integral L of Eq. (8) can then be calculated using Eqs. (11) and (12) as follows:

$$L=2L_s-[2L_s-\ln y]\ \text{ for large } y\ . \tag{13}$$

From Eqs. (6) and (13) the stopping power dE/dX can be calculated as a function of the incident particle energy.

The energy gap used in the theory is not an experimental gap but a value obtained by adjusting E_g so that $\kappa(0,0,E_g)$ is equal to the static dielectric constant of the material. E_g also depends on n. To calculate the integral L of Eq. (7) one needs to know the two functions f_1 and f_2 of Eq. (4), which have been evaluated to high accuracy using a computer program in double precision.[5]

Statistical-model formalism

The stopping number per target electron L of Eq. (6) has been proposed by Lindhard and Scharff[6] to be

$$L=\frac{1}{Z_2}\int_{r_{\min}}^{\infty}4\pi r^2\rho(r)\ln\frac{2mv_1^2}{\sqrt{2}\hbar\omega_0(r)}dr\ . \tag{14}$$

In Eq. (14), m is the electron mass, $\rho(r)$ is the electron density of an atom of the target material, $\omega_0(r)$ the corresponding local plasma frequency $[4\pi e^2\rho(r)/m]^{1/2}$, and Z_2 the target atomic number. Equation (14) is expected to give a fair approximation even down to rather small values of v_1 the projectile velocity. For the determination of $\rho(r)$, the Thomas-Fermi statistical model is usually used. Lindhard and Scharff made a distinction between outer electrons,

$$2mv_1^2[\sqrt{2}\hbar\omega_0(r)]>1\ ,$$

whose stopping contribution was calculated as if they were at rest, and inner electrons,

$$2mv_1^2[\sqrt{2}\hbar\omega_0(r)]<1\ ,$$

that were considered to give no stopping at all. With a cutoff of this kind and the use of the Thomas-Fermi expression for $\rho(r)$, L remains a function of x only:

$$x=\frac{v_1^2}{v_0^2Z_2}\left[v_0=\frac{e^2}{\hbar}\right]\ . \tag{15}$$

For a gas with plasma frequency ω_0 and average kinetic energy $\langle T\rangle$ the first correction term[2] $(\Delta L)_1$ to the asymptotic formula

$$L=\ln\frac{2mv_1^2}{\hbar\omega_0} \tag{16}$$

is given by

$$(\Delta L)_1 = -\frac{\langle T\rangle}{mv_1^2/2} . \tag{17}$$

In the treatment of a free electron gas Lindhard and Winther[2] pointed out that for the outer electrons the expression for L can be given by

$$L(r,v_1) = \ln\left[\frac{2mv_1^2}{\sqrt{2}\hbar\omega_0(r)}\right] - \frac{\langle T\rangle(r)}{mv_1^2/2} . \tag{18}$$

The average kinetic energy $\langle T\rangle(r)$ of a unit volume at a distance r from the nucleus, as in the statistical description of the atom, can be obtained from $\rho(r)$ by

$$\langle T\rangle(r) = \frac{3}{5}\frac{\hbar^2}{2m}[3\pi^2\rho(r)]^{2/3} . \tag{19}$$

The contributions to L due to the outer and inner electrons can be given by Eqs. (20) and (21), respectively,

$$L(r,v) = \begin{cases} \ln\left[\dfrac{2mv_1^2}{\sqrt{2}\hbar\omega_0(r)}\right] - \dfrac{\langle T\rangle(r)}{mv_1^2/2} & \text{if } \geq 0 \qquad (20) \\ \left[\dfrac{\chi^2(r)}{3}\right]^{3/4}\dfrac{1}{2}\left[\ln\left[\dfrac{1}{\chi^2(r)}\right]-1\right]\left[\dfrac{2mv_1^2}{\hbar\omega_0(r)}\right]^{3/2} & \text{otherwise} . \qquad (21) \end{cases}$$

An analytical expression has been used for $\rho(r)$ by Lenz-Jensen[7] as follows:

$$\rho(r) = \frac{Z_2^2}{a_0^3}3.675\frac{e^{-\eta}}{\eta^3}(1+0.265\eta)^3 , \tag{22}$$

$$\eta = 3.303\left[\frac{r}{a_0 Z_2^{-1/3}}\right]^{1/2} , \tag{23}$$

where $a_0 = 0.528$ Å is the Bohr radius. The distance R is determined such that the expression of

TABLE I. Some calculated stopping powers for α particles and protons in carbon (diamond). The atomic stopping power of graphite has been found experimentally to be 1.0604±0.0090 times that of diamond for 1.1-MeV protons (Ref. 12).

	dE/dX (keV cm^2/μg)		
	Brandt-Reinheimer[a]	Core (2 e)	Statistical model (all e)
E_α (keV)			
100	0.7087	0.4375	2.8084
500	2.5535	0.2614	2.1612
1000	2.2856	0.3314	1.6854
2000	1.2722	0.4157	1.2258
5000	0.6526	0.3137	0.7257
10000	0.3798	0.2328	0.4557
20000	0.2162	0.1422	0.2732
40000	0.1212	0.0856	0.1583
E_p (keV)			
100	0.5384	0.0587	0.5766
500	0.3180	0.1039	0.3065
1000	0.1930	0.0912	0.2082
2000	0.1133	0.0667	0.1331
5000	0.0540	0.0356	0.0683
10000	0.0303	0.0214	0.0396

[a] $n = 7.047\times10^{23} e/\text{cm}^3$ (4e/atom); $E_g = 13.49$ eV (from static dielectric constant $\epsilon_s = 5.7$); $\chi^2 = 0.2163$.

TABLE II. Some calculated stopping-power values for α particles and protons in ZnTe.

	dE/dx (keV cm^2/μg)		
	Brandt-Reinheimer[a]	Core[b]	Statistical model (all e)
E_α (keV)			
100	0.1185	0.1320	0.3212
500	0.3738	0.1345	0.3579
1000	0.2214	0.1508	0.3221
2000	0.1273	0.1667	0.2754
5000	0.0596	0.1576	0.2083
E_p (keV)			
100	0.1096	0.0329	0.0912
500	0.0318	0.0417	0.0688
1000	0.0180	0.0405	0.0562

[a] $n=7.024\times10^{22}$ e/cm^3 (4e/molecule); $E_g=3.050$ eV (from static dielectric constant $\epsilon_s=10.1$); $\chi^2=0.4665$.
[b] Zn core of 28 e; Te core of 50 e.

$L(r,v)$ in Eq. (20) is ≥ 0. For $r \leq R$ we have L_2 corresponding to the inner electrons while the contribution L_1 of the outer electrons corresponds to the range of $r \geq R$. The total value of L is L_1+L_2, which was obtained with a statistical-model computer code.[8]

RESULTS

To apply the statistical-model theory to the electronic core of a semiconductor atom of atomic number Z, the stopping-power expressions were integrated out to a radius corresponding to all except the valence electrons, i.e., to a radius corresponding to $Z-4$ electrons for C, Si, Ge, to $Z-6$ in the case of U (Rn core), and to $Z-2$ for Zn and Te. The stopping of the valence electrons is given by BR. For ZnTe, additivity of core-stopping powers was assumed, as it was also in obtaining the semiempirical values.

For comparison, stopping powers were computed using only Bonderup's statistical model over the entire atomic electron distribution. Again Bragg's

TABLE III. Some calculated stopping-power values for α particles and protons in uranium.

	dE/dX (keV cm^2/μg)		
	Brandt-Reinheimer[a]	Core (86 e)	Statistical model (all e)
E_α (keV)			
100	0.1702	0.0639	0.1182
500	0.2808	0.0638	0.1507
1000	0.1843	0.0508	0.1419
2000	0.1129	0.0452	0.1268
5000	0.0558	0.0522	0.1029
10000	0.0319	0.0547	0.0838
20000	0.0179	0.0489	0.0650
E_p (keV)			
100	0.0774	0.0186	0.0378
500	0.0282	0.0113	0.0317
1000	0.0166	0.0131	0.0273
2000	0.0096	0.0138	0.0225
5000	0.0045	0.0122	0.0162

[a] $n=2.839\times10^{23}$ e/cm^3 (6e/atom); $E_g=0$; $\chi^2=0.2929$.

TABLE IV. Some calculated stopping-power values for α particles and protons in Si.

	dE/dX (keV cm^2/μg)		
	Brandt-Reinheimer[a]	Core (10 e)	Statistical model (all e)
E_α (keV)			
100	1.240	0.3073	0.9387
500	1.680	0.1550	0.9451
1000	1.095	0.1311	0.8455
2000	0.680	0.1760	0.6995
5000	0.333	0.1946	0.4807
10 000	0.184	0.1644	0.3307
E_p (keV)			
100	0.470	0.0450	0.2861
500	0.165	0.0440	0.1829
1000	0.096	0.0461	0.1361
2000	0.055	0.0416	0.0947
5000	0.025	0.0296	0.0533
10 000	0.015	0.0185	0.0325

[a]Values obtained by graphical interpolation of results in Ref. 3.

rule was assumed for ZnTe.

Nuclear stopping corrections have not been added to the calculated values. They are given as a function of projectile energy in Refs. 9 and 10. For protons on the stoppers and energies considered here, the corrections are completely negligible. For α particles, in all cases the nuclear stopping is negligible at 100-keV incident energy and 3% or less at 50 keV, and thus does not affect the comparisons.

Tables I—V contain a few of the values calculated for C (diamond), ZnTe, U, Si, and Ge. The second columns correspond to the formula prescribed by BR, i.e., the valence electrons as participating electrons, and to E_g for κ set equal to the static dielectric constant. The third columns are values calculated for the electron core using Bonderup's version of the statistical model with the Thomas-Fermi charge distribution (to be added to BR); the fourth columns are the stopping powers calculated using only Bonderup's statistical model

TABLE V. Some calculated stopping-power values for α particles and protons in Ge.

	dE/dX (keV cm^2/μg)		
	Brandt-Reinheimer[a]	Core (28 e)	Statistical model (all e)
E_α (keV)			
100	0.550	0.1655	0.2942
500	0.650	0.1209	0.3500
1000	0.425	0.1030	0.3427
2000	0.260	0.1226	0.3134
5000	0.129	0.1379	0.2481
10 000	0.072	0.1269	0.1896
E_p (keV)			
100	0.184	0.0334	0.1202
500	0.064	0.0307	0.0880
1000	0.037	0.0360	0.0707
2000	0.022	0.0335	0.0536
5000	0.010	0.0241	0.0338
10 000	0.006	0.0167	0.0221

[a]Values obtained by graphical interpolation of results in Ref. 3.

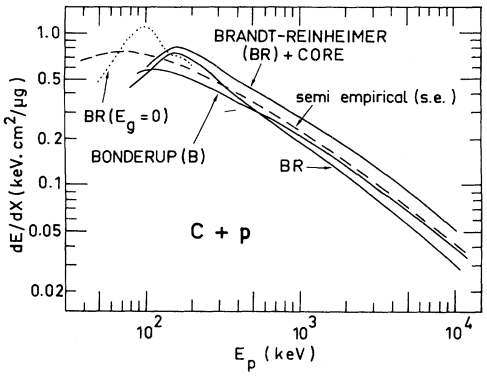

FIG. 1. Calculated and semiempirical stopping powers for protons in carbon (diamond). The semiempirical values are for graphite.

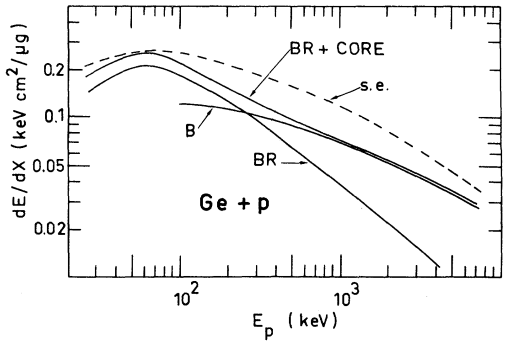

FIG. 3. Calculated and semiempirical stopping powers for protons in Ge. The BR values were obtained from the implicit ones of Ref. 3.

with a Thomas-Fermi charge distribution. The corresponding plots are given in Figs. 1—10. Semiempirical values are taken from Refs. 9 and 10.

DISCUSSION

Inspection of the figures shows the overall agreement of the calculated curves with experiment. It is interesting to compare the two calculations that consider all of the electrons in the slowing down, namely BR plus core and the statistical model of Bonderup. One notices the following:

(1) Statistical-model calculations tend to reproduce the semiempirical values at the higher projectile energies; with decreasing energy these curves do not rise as fast as the semiempirical ones.

(2) In all cases the BR plus core curves show more pronounced peaking (due to the BR contribution) than semiempirical; the curves show a systematic shift with Z in the positions of the maxima relative to semiempirical.

(3) In the BR plus core curves, the values of the stopping at the maxima vary systematically with target Z compared with semiempirical.

(4) In all cases, inclusion of the core contribution renders the BR curves parallel to the semiempirical curves at energies above the maxima. In general, BR plus core agrees better with semiempirical than the statistical model.

(5) In the statistical model, for proton projectiles, the energies of the maxima agree with experiment; the computed stopping-power values at the maxima are systematically lower than semiempirical with increasing target Z.

(6) In the statistical model for α particles, the calculated maxima are a few hundred keV lower than

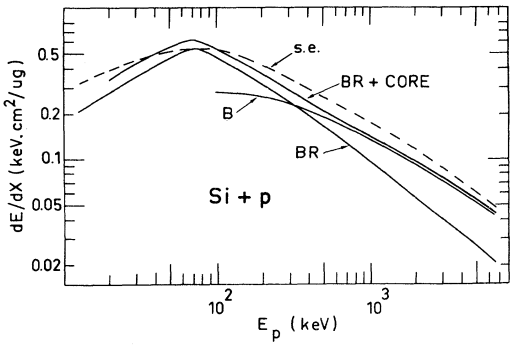

FIG. 2. Calculated and semiempirical stopping power for protons in Si. The BR values were obtained from the implicit ones of Ref. 3.

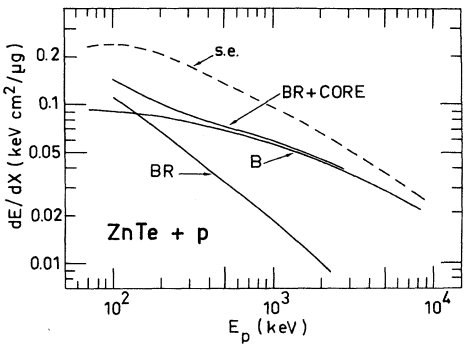

FIG. 4. Calculated and semiempirical stopping powers for protons in ZnTe.

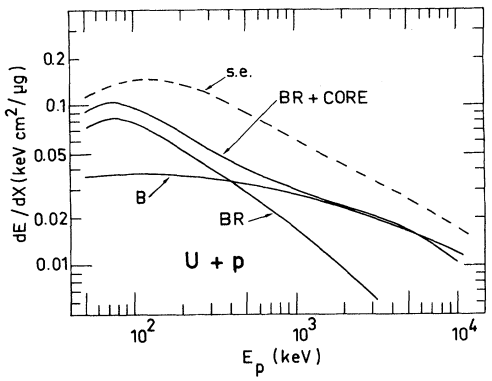

FIG. 5. Calculated and semiempirical stopping powers for protons in U.

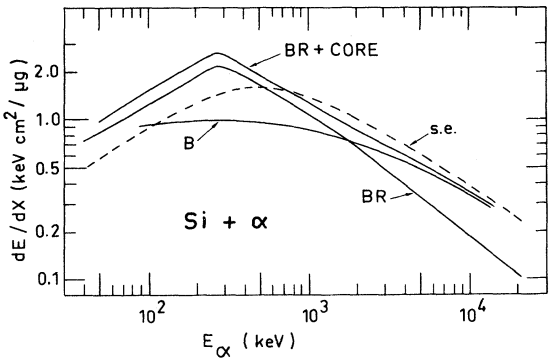

FIG. 7. Calculated and semiempirical stopping powers for α particles in Si. The BR values were obtained from Ref. 3.

semiempirical; there is again a systematic deviation with target Z of calculated values from semiempirical when values at the maxima are considered.

At projectile energies below the maxima, the behavior of the calculated curves relative to the semiempirical ones appears much more erratic. This is probably due on the one hand to the drawing of the curves between the plotted points, and on the other hand, to large experimental uncertainties upon which the semiempirical curves are based in this energy region. Note the rather impressive agreement of the BR plus core curve for Si+p with experiment (and still good agreement for the Si+α curves).

Comparison of the BR plus core curves with those of the statistical model shows that the stopping of the outer electrons is greater in the BR theory. The calculated stopping is model dependent, especially towards lower projectile energies. In the case of the BR plus core stopping, there was little flexibility in choosing the number of electrons to be considered in the valence gas or with the core, or of changing the respective stopping of either. This is because starting with BR, which was formulated for the valence electrons, the core to be described by the statistical model was defined. There remains the possibility of using other atomic charge distributions.

We have used semiempirical stopping-power curves to serve as the basis of comparison. Most existing experimental data for protons and α particles are compiled in Refs. 9 and 10, which likewise give semiempirical curves that represent the most ambitious effort yet to describe all elemental stoppers consistently. Relatively abundant data exist for the stopping of protons in C and Ge, little data in Si, Zn, and ZnTe (Ref. 11), and no data in Te and U. For α particles, there are many measurements in C, Si, and Ge; few in Zn, Te, ZnTe,[11] and U. From the spread of points in cases where mea-

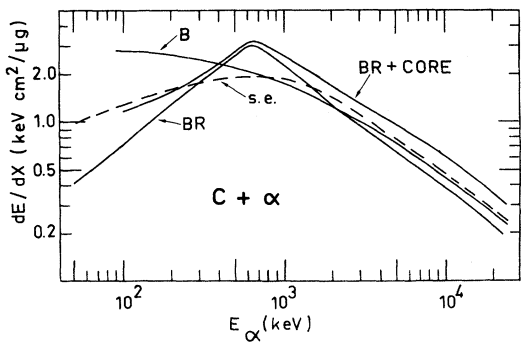

FIG. 6. Calculated and semiempirical stopping powers for α particles in carbon (diamond). The semiempirical values are for graphite.

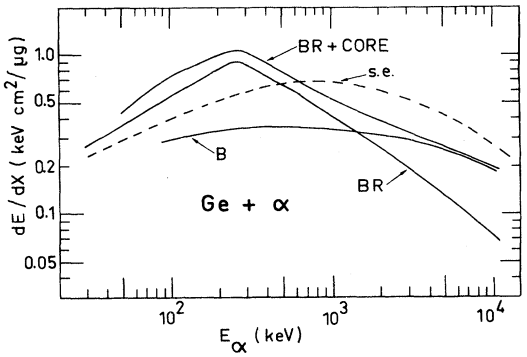

FIG. 8. Calculated and semiempirical stopping powers for α particles in Ge. The BR values were obtained from Ref. 3.

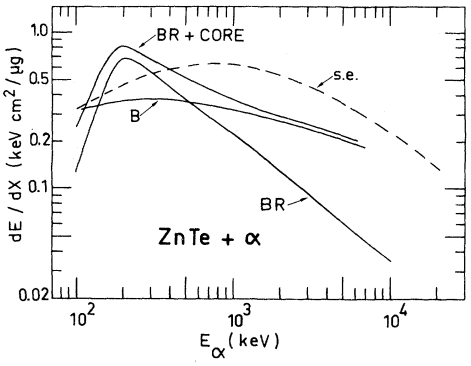

FIG. 9. Calculated and semiempirical stopping powers for α particles in ZnTe.

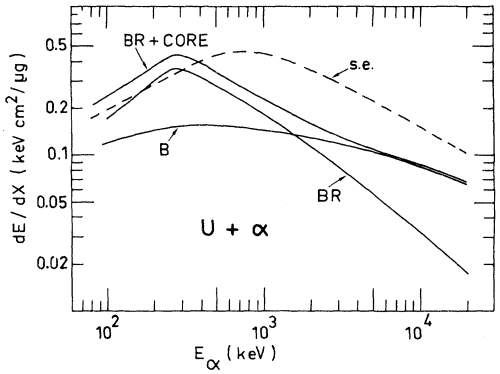

FIG. 10. Calculated and semiempirical stopping powers for α particles in U.

surements have been repeated, one might estimate an uncertainty on the semiempirical curves of the order of 10% over most of the projectile energy range, including the region of the maxima where there are no well-defined theoretical guidelines. Possibly a smaller uncertainty can be attributed to the much studied targets C (p and α) and Si (α). For projectile energies below 100 keV, experiments have been notoriously fraught with difficulties, and errors can become larger. There may be non-negligible deviations from simple additivity of stopping powers at lower projectile energies in the case of ZnTe.

The value of the stopping of graphite has been measured to be 1.0604 ± 0.0090 times that of diamond for 1.1-MeV protons.[12] It would be very interesting to have similarly accurate measurements as a function of proton energy to study experimentally the effect of the allotropic forms and the energy gap. For such measurements the C (diamond) system is the most accessible. The dotted curve in Fig. 1 was calculated as for the analogous BR curve except setting $E_g = 0$. If this is an indication of experimental results, the main differences will be seen in the C (diamond) system at $E_p < 150$ keV.

ACKNOWLEDGMENTS

The authors would like to thank J. Reinheimer for furnishing a listing of his computer code and for useful correspondence. We are likewise indebted to E. Bonderup for his program and for the enlightening discussion on the subject of the statistical model. We acknowledge the encouragement of G. Monsonego, Director of the Computer Center of Strasbourg-Cronenbourg, and the personnel for their considerable help.

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