Calculation of energy straggling for protons and helium ions*

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Energy straggling has been calculated for protons and helium ions in each of the elements, by using the Hartree-Fock-Slater charge distribution for the target atom with Bonderup and Hvelplund's formulation. The results reveal a Z_2 structure in energy straggling, and afford a ready explanation of some earlier measurements.

I. INTRODUCTION

The energy loss of charged particles passing through matter has been studied both theoretically and experimentally. The energy straggling of these particles, however, has not received broad attention, probably because it is a second-order phenomenon. It results from the statistical fluctuation of the energy-loss processes that particles are subjected to as they travel through matter.

Recently, ion backscattering has been successfully applied in investigating the elemental composition, depth distribution, and lattice location of atoms in a thin film or a bulk sample. However, the depth resolution that makes this success possible is ultimately limited by the energy straggling of the probing ions as they traverse the sample. For examining depth distribution by backscattering, therefore, it is important to know the amount of energy straggling. In this paper, we report calculations of energy straggling for protons and helium ions in matter and compare the results with earlier measurements of energy straggling.

II. THEORY

Several theories have been advanced to describe the average energy loss and energy straggling of fast-moving light ions in matter. For energy straggling Ω, Bohr has given the high-energy limiting cases Ω_B as

$$\Omega^2 = \Omega_B^2 = 4\pi Z_1^2 Z_2 e^4 N \Delta R\,, \tag{1}$$

where Z_1 is the atomic number of the projectile atoms, Z_2 is that of the target atoms, e is the charge of the electron, N is the number of target atoms per unit volume, and R is the thickness of the target. Clearly, the energy straggling described by Bohr[1] is proportional to the square root of $Z_2 N \Delta R$, the total number of electrons per unit area that the projectile has traversed. This theory was based on three assumptions: (i) that the velocity of the projectile is much greater than that of the orbital electrons of the target atoms, (ii) that the energy loss is very small by comparison to the total energy of the projectile, and (iii) that the target atoms are randomly distributed and no channeling is involved in the penetration process.

Assumptions (ii) and (iii) apply to most cases, but assumption (i) breaks down for low and medium energies. To account for this breakdown, Lindhard and Scharff[2] extended Bohr's theory by applying a correction factor for low- and medium-energy projectiles to get

$$\begin{aligned} &\Omega^2 = \Omega_B^2 L(\chi)/2 \quad \text{for } \chi \leq 3\,, \\ &\Omega^2 = \Omega_B^2 \quad \text{for } \chi \geq 3\,, \end{aligned} \tag{2}$$

where χ is a reduced energy variable

$$\chi = v^2/(v_0^2 Z_2)\,. \tag{3}$$

Here v is the velocity of the projectile, and v_0 is the orbital velocity in a Bohr hydrogen atom, defined as

$$v_0 = e^2/\hbar\,.$$

Finally, $L(\chi)$ in Eq. (2) is the stopping number, which appears in the energy-loss formula

$$\frac{dE}{dx} = \frac{4\pi Z_1^2 e^4}{mv^2} N Z_2 L(\chi)\,, \tag{4}$$

where m is the electron mass.

Equation (2) indicates that energy straggling approaches Bohr's value at high energy and is energy dependent at low energy. Bonderup and Hvelplund[3] have refined Lindhard and Scharff's expression by using a more realistic formula for the atomic charge distribution $\rho(r)$ together with a more accurate expression for $\Omega^2(r, v)$, the contribution from the various parts of the electron cloud to the straggling. Their formula[3] for the energy straggling is normalized to Bohr's energy straggling value Ω_B by

$$\frac{\Omega^2}{\Omega_B^2} = \frac{1}{Z_2} \int 4\pi r^2 \rho(r) \frac{\Omega^2(r, v)}{\Omega_B^2} dr\,, \tag{5}$$

where the localized contribution $\Omega^2(r, v)/\Omega_B^2$, de-

rived in Ref. 3, is a function of the velocity of the projectile and a function of the charge distribution $\rho(r)$, which is normalized such that

$$Z_2 = \int_0^\infty 4\pi r^2 \rho(r) dr . \tag{6}$$

Bonderup and Hvelplund[3,4] have measured the stopping power and the energy straggling of protons and helium in various gases, and compared the experimental results to theoretical ones calculated by different methods. In their calculations they used the first-order Lenz-Jensen model,[5] an analytical form of the Thomas-Fermi type, for $\rho(r)$. They conclude that the Lindhard-Scharff formulation gives a fair account of the over-all dependence of energy straggling. In a more quantitative comparison of theory and experiment, however, some discrepancy is revealed.

One interesting observation made by Bonderup and Hvelplund was that when one plots $\Omega^2/N\Delta R$ against projectile energy for various gases, energy straggling is found to be greater in air than in Ne at low energy, but greater in Ne at high energy. This crossover cannot be predicted by the theories of Bohr,[1] Lindhard and Scharff,[2] or Bonderup and Hvelplund themselves; all three theories predict that energy straggling will increase with increasing Z_2 at a given energy.

A Z_2 oscillatory structure in the stopping cross section $\Delta E/N\Delta R$ can be described by use of a more realistic atomic model, the Hartree-Fock-Slater charge distribution, as we showed in earlier work.[6,7] Here we combine that model with Bonderup and Hvelplund's formulation to calculate energy straggling. The results reveal the oscillatory structure in energy straggling, and also lead to an explanation of Bonderup and Hvelplund's measurements.[3,4]

III. CALCULATIONS AND RESULTS

In order to calculate the energy straggling by use of Bonderup and Hvelplund's formulation [Eq. (5)], it is necessary to know the atomic charge distribution $\rho(r)$ (the spherically averaged electron density). If $P_{n\lambda}(r)$ is the radial wave function for the $n\lambda$ orbital, then

$$4\pi r^2 \rho(r) = \sum_{n\lambda} \omega_{n\lambda} [P_n(r)]^2 , \tag{7}$$

where $\omega_{n\lambda}$ is the occupation number of the $n\lambda$ orbital. Here $P_{n\lambda}(r)$ is normalized as

$$\int_0^\infty [P_{n\lambda}(r)]^2 dr = 1 . \tag{8}$$

Equations (7) and (8) satisfy the condition of Eq. (6). The normalized radial wave function P_n has been tabulated by Herman and Skillman on the basis of the Hartree-Fock-Slater model.[8] Using this tabulation and Eq. (7), one can obtain $4\pi r^2\rho(r)$ for a given r and a given target element. One can then make a numerical integration of Eq. (5) by using $\rho(r)$. In this way Ω^2/Ω_B^2 is calculated for a given target and a given projectile velocity. Since Ω_B^2 is independent of the velocity of the projectile, it can be calculated easily from Eq. (1).

The result of this calculation,[9] plotted in Fig. 1, gives the Z_2 dependence of $\Omega^2/N\Delta R$ for various projectile energies. The calculation is based on a perturbation treatment. As such, it can be scaled for Z_1^2 as inherent in the treatment. In the low-energy region considered here, however, the calculation applies only to very light ions, such as protons and helium ions. The Bohr formula is energy independent, and $\Omega_B^2 \propto Z_2$, as is also evident from the figure. These results reveal a Z_2 structure, especially at lower energies. At very high energies this calculation approaches the Bohr formula asymptotically. Straggling values calcu-

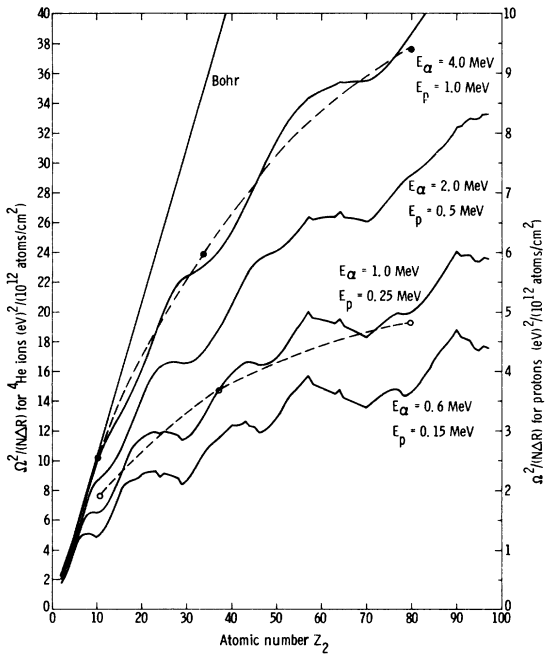

FIG. 1. Energy straggling as calculated for protons (scale on the right) and for ^{4}He ions (scale on the left), for all elements at various energies. Bohr theory gives a linear dependence on Z_2. Straggling values calculated by the Thomas-Fermi model (Ref. 3), given as points and linked with dashed curves, are in good agreement with the values calculated in the present paper. The present calculations are plotted for various energies. The Z_2 structure is more pronounced at lower energies; at higher energies the present calculation approaches the values predicted from Bohr theory.

lated by the Thomas-Fermi model,[3] given as points and linked with dashed curves, are in good agreement with the values calculated in the present paper.

IV. COMPARISON WITH PUBLISHED MEASUREMENTS

There are many measurements of average energy loss, but few of energy straggling. Moreover, the measurements of energy straggling are in general less accurate.

Hvelplund[4] measured average energy loss and energy straggling of atoms with $2 \leq Z_1 \leq 12$ in various gases at 100–500 keV. In Fig. 2 we plot his measurements of energy straggling in helium ions with our calculated curves. The crossing of Ne and N values at low energy, indicated by Hvelplund's measurements, can be explained by the Z_2 oscillatory structure predicted by our calculation. Also, the general agreement in the numerical values is acceptable.

Bonderup and Hvelplund[3] measured the energy straggling of protons in various gases at 100–500 keV. Their results are compared with our calculations and to Bohr theory, in Fig. 3. The crossing of the results for Ne and air is predicted by our calculation at 180 keV. The energy dependence

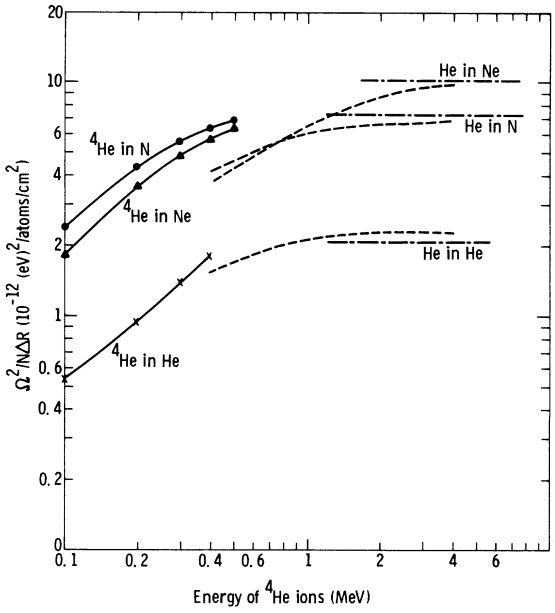

FIG. 2. Comparison of ^{4}He energy straggling in He, N, and Ne. The measurements of Hvelplund (Ref. 4) are given as points and connected as solid curves; the present calculations are given as dashed curves; and values predicted from Bohr theory are given as point-dash lines. The present calculations give the energy dependence of energy straggling, and also predict the crossover of the curves for Ne and N.

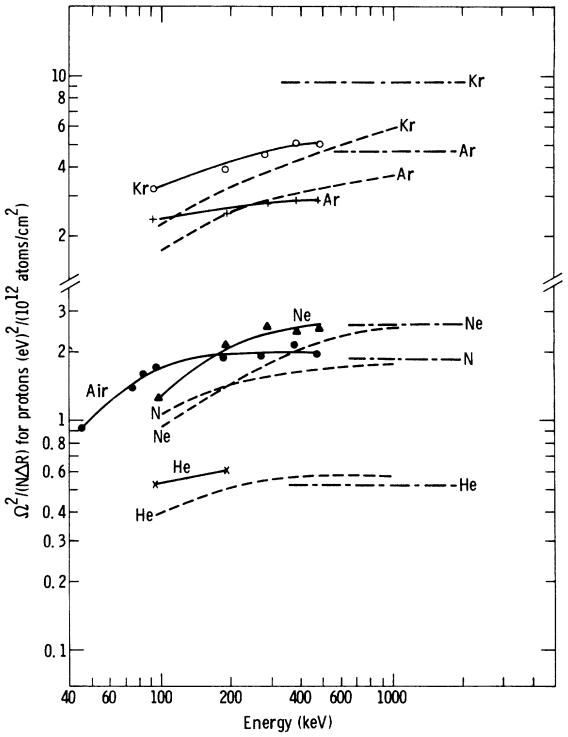

FIG. 3. Energy straggling of protons in various gases. The measurements of Bonderup and Hvelplund are given as points (Ref. 3) and connected with solid curves, the present calculations are given as dashed curves, and values predicted from Bohr theory are given as point-dash lines. The present calculations give the energy dependence of energy straggling, and predict the crossover of the curves for Ne and N at 200 keV for protons; these results agree with the measurements.

of proton straggling observed by Bonderup and Hvelplund is in general agreement with our calculation.

The present results are also compared with Harris and Nicolet's measurement[10] of the energy straggling of He ions at 0.80–2 MeV in Ni, Al, and Au targets. Their Ni measurements are in fair agreement with Bohr's prediction, their Al measurements are 30% above, and their Au measurements are 40% below. A weak energy dependence is seen, which is in qualitative agreement with the theories of Lindhard and Scharff and of Bonderup and Hvelplund, and also with the calculations reported here. The values calculated by all three of these theories are lower than those measured by Harris and Nicolet.

The present calculations have been compared[9] with measurements by Nielson[11]; Madson[12]; Chilton, Cooper, and Harris[13]; Leminen and Anttila[14]; and others. The points in those measurements, however, are so scattered that the experimental

data neither support nor disprove the present calculations.

V. SUMMARY

A Z_2 structure in energy straggling has been predicted by using a Hartree-Fock-Slater model in the formulation given by Bonderup and Hvelplund. The calculated Z_2 structure agrees with Bonderup and Hvelplund's measurements for Ne and N. The present calculations provide a guide to the Z_2 dependence of energy straggling, as well as the energy dependence. Accurate measurements of energy straggling in solids of various Z_2 are needed for comparison.

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