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Calculations of Stopping Cross Sections for 0.8- to 2.0-MeV Alpha Particles*

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Calculations of α-particle stopping cross sections based on the theories of Lindhard *et al.* using the Hartree-Fock-Slater atomic-charge distribution provide generally good agreement with previously obtained experimental results. In particular, the calculations are helpful in understanding the structure which results when, for fixed energy of the α particle, the stopping cross section is plotted against the atomic number of the stopping medium.

I. INTRODUCTION

It is plausible to assume that physical properties related to the distribution of the atomic electrons will have a periodic nature due to the shell structure of the atomic electrons. In 1906 Crowther[1] measured the mass absorption coefficient for Pa^{234} β rays and found the absorption to be a periodic function of the atomic number. In 1933 Bothe[2] suggested that Crowther's finding might be due to a periodicity in the characteristic frequencies in the Bohr stopping theory. The first computation to show the periodic structure in the stopping power was made by Westermark,[3] who calculated the energy loss of charged relativistic particles (184 GeV/amu) using the Bethe-Bloch formula and obtained a periodic dependence on the atomic number.

The stopping powers of 23 metallic elements for 19.8-MeV protons were measured by Burkig and MacKenzie.[4] Anomalies were noted from Ca to Fe and from Ta to Th, and the first anomaly was associated with the number of electrons in the $3d$ shell. Recently, Chu and Powers[5] measured α-particle stopping cross sections $\epsilon_\alpha(E_\alpha)$ in 17 solid elements from 400 keV to 2 MeV. An anomalous structure in $\epsilon_\alpha(E_\alpha)$ vs target element Z_2 was observed in the region of the first transition series ($Z_2 = 22$--29), and the amplitude of the anomalous structure was more pronounced at low energy. They attributed this finding to a correlation with the Hartree-Fock-Slater potential. White and Mueller[6] measured the electronic stopping cross section of H^1 and He^4 particles in five solid elements at energies near 100 keV, and an anomalous structure was also obtained. All of the above-mentioned experiments were performed using a given projectile (proton or α particle) to study the Z_2 dependence of ϵ_p or ϵ_α. Numerous experiments have also been performed by using a given target with different ion beams at a fixed velocity to study the Z_{ion} dependence of ϵ_{ion}. In 1963 Ormrod and Duckworth[7] noticed that the electronic stopping cross section has an oscillating dependence on Z_{ion}. This oscillatory dependence (or periodic structure) of ϵ_{ion} on Z_{ion} has been verified in boron, carbon, and aluminum thin films[8–11] and in gaseous targets[12,13] and also has been verified in the channeling of heavy ions in W crystals,[14] Si crystals,[15] and gold crystals.[16] Evidence of an oscillatory behavior of the excitation potential was observed by Andersen *et al.*[17]

Several calculations were made in 1968–69 to explain the above-mentioned experimental results of the oscillation dependence of ϵ_{ion} on Z_{ion}. Most of the calculations were based on the Firsov[18] model or uniform electron-gas model with modification to include an effective atomic number,[19] an ion-size effect,[20,21] or both.[22] Harrison[23] indicated that the periodic dependence of ϵ_{ion} on Z_{ion} was contained in the electron density of the moving ions when the density is determined from the Hartree-Fock-Slater wave function. Chu and Powers[5] indicated that the anomalous structure of ϵ_α vs Z_2 is indirectly related to the Hartree-Fock-Slater atomic potential.

With the above as background, one is encouraged to look for an explanation of the salient structure of the atomic stopping process in terms of the particular electronic structure of the target atoms. In the present paper, the stopping cross section is computed from the spherically averaged electronic charge density obtained from Hartree-Fock-Slater wave functions. The calculation is based on the theories of Lindhard, and co-workers[24–26] and Bonderup.[27]

II. REVIEW OF BASIC THEORY

At sufficiently high energies, the energy loss of a heavy charged particle in matter can be computed using the familiar Golden rule of second-order

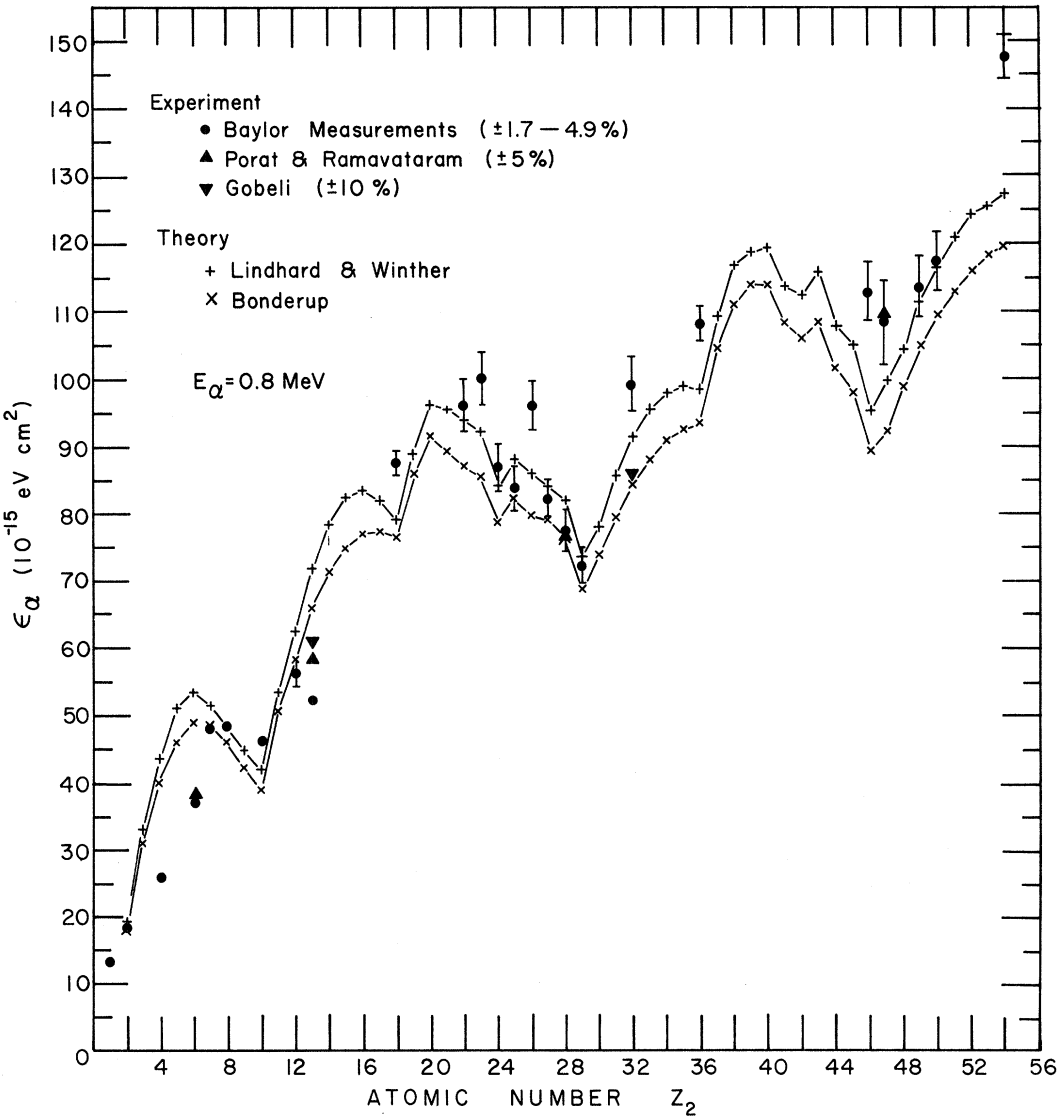

FIG. 1. Stopping cross section ϵ_α of α particles vs the stopping-element atomic number at $E_\alpha = 0.8$ MeV. Present calculations: +, based on Lindhard and Winther (Ref. 26); x, based on Bonderup (Ref. 27). In both calculations Hartree-Fock-Slater wave functions are used to evaluate the atomic charge distribution for the target atom Z_2. Experimental results: ● Measurements made at Baylor University (ϵ_α in solids is given in Ref. 5, ϵ_α in gases is given in Refs. 29 and 30), ▲ Porat and Ramavataram (Ref. 31) and ▼ Gobeli (Ref. 32).

time-dependent perturbation theory. For a particle having charge $Z_1 e$ and moving with velocity $\vec{v}$, dE/dx is given by

$$\frac{dE}{dx} = \frac{1}{v}\frac{dE}{dt}$$

$$= \frac{-Z_1^2 e^2}{v\pi^2}\int \frac{d\vec{k}}{k^2}\int d\omega\, \omega\, \mathrm{Im}\left(\frac{1}{\epsilon(\vec{k},\omega)}\right)\delta(\omega - \vec{k}\cdot\vec{v}), \tag{1}$$

where $\epsilon(\vec{k},\omega)$ is the frequency- and wave-number-dependent dielectric function for the stopping medium. For the case where the stopping medium is a uniform electron gas, Lindhard[24] has studied the stopping problem in considerable detail, making use of the random-phase-approximation (RPA) result for $\epsilon(\vec{k},\omega)$. Since a calculation of dE/dx using a realistic $\epsilon(\vec{k},\omega)$ is prohibitively difficult, Lindhard and Scharff[25] have advocated an approach in which the stopping medium is viewed as a non-uniform electron gas, and the stopping cross section is simply computed by means of an appropriate average. In particular, if, for a particle having charge $Z_1 e$ moving through a uniform electron gas of density n,

$$\frac{dE}{dx} = \frac{-4\pi Z_1^2 e^4}{mv^2} n L(n,v), \tag{2}$$

then for such a particle moving through a medium of N atoms/cm^3, one may approximate the stopping cross section by

$$\epsilon = -\frac{1}{N}\frac{dE}{dx} = \frac{4\pi Z_1^2 e^4}{mv^2}\int_0^\infty \rho(r)\, L(\rho,v)\, 4\pi r^2 dr, \tag{3}$$

where $\rho(r)$ is the spherically averaged electron density for the atom in question, normalized so that

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

The RPA result for $L(\rho,v)$ has been studied in great detail by Lindhard and Winther.[26] Relying in part on the work of Lindhard and Winther, Bonderup[27] has proposed the use of

$$L(\rho,v) = \ln\left(\frac{2mv^2}{\sqrt{2}\hbar\omega_p}\right) - \frac{2T}{mv^2} \tag{5}$$

if the expression on the right-hand side is positive and

$$L(\rho,v) = \frac{1}{2}\left(\frac{\chi^2}{3}\right)^{3/4}\left[\ln\left(\frac{1}{\chi^2}\right) - 1\right]\left(\frac{2mv^2}{\hbar\omega_p}\right)^{3/2} \tag{6}$$

otherwise. In Eqs. (5) and (6), the following definitions are used:

$$\omega_p = (4\pi e^2\rho/m)^{1/2}, \qquad T = \tfrac{3}{5}\hbar^2 k_F^2/2m,$$

$$\chi^2 = e^2 m/\pi\hbar^2 k_F = 1/\pi k_F a_0, \quad k_F = (3\pi^2\rho)^{1/3}.$$

Lindhard and Winther[26] have given asymptotic formulas which accurately represent $L(\rho,v)$ in the low- and high-, but not relativistic, velocity regimes. In the expressions that follow, the velocity of the incident particle is measured by the dimensionless parameter

$$y = 2mv^2/\hbar\omega_p .$$

For low velocities, Lindhard and Winther write

$$L(\rho,v) = (\tfrac{1}{3}\chi^2)^{3/4} C_1(\chi) y^{3/2}, \tag{7}$$

where

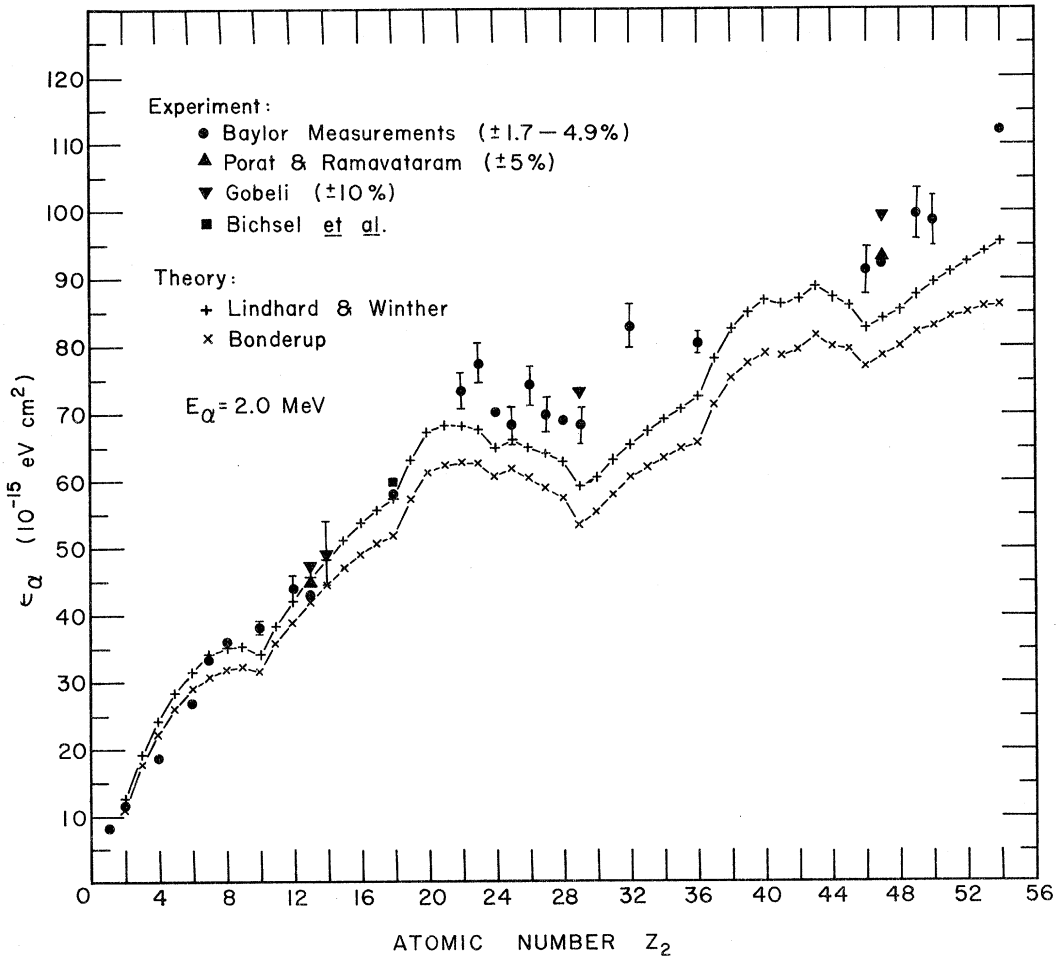

FIG. 2. Same as Fig. 1 except $E_\alpha = 2.0$ MeV. The point ■ for $Z_2 = 18$ is due to Bichsel *et al.* (Ref. 33).

$$C_1(\chi) = \frac{1}{2(1+\frac{1}{3}\chi^2)^2}\left[\ln\left(\frac{1+\frac{2}{3}\chi^2}{\chi^2}\right) - \frac{1-\frac{1}{3}\chi^2}{1+\frac{2}{3}\chi^2}\right]. \quad (8)$$

For high velocities, they write

$$L(\rho, v) = \ln y - \frac{3^{3/2}}{5\chi}\frac{1}{y} - \frac{9}{14\chi^2 y^2} \ . \quad (9)$$

III. NUMERICAL CALCULATIONS AND RESULTS

In order to compute the stopping cross section from Eqs. (3), (5), and (6) or from Eqs. (3), (7), and (9), it is necessary to know $\rho(r)$, the spherically averaged electron density. If $P_{n\lambda}(r)$ is the radial wave function for the $n\lambda$ orbital, then

$$\sigma(r) = 4\pi r^2 \rho(r) = \sum_{n\lambda} \omega_{n\lambda}[P_{n\lambda}(r)]^2, \quad (10)$$

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

$$\int_0^\infty [P_{n\lambda}(r)]^2 dr = 1 \ . \quad (11)$$

The radial wave functions, computed in the Hartree-Fock-Slater approximation, can be obtained from the tabulation of Herman and Skillman.[28] It is convenient to measure r in Bohr units and to introduce $x = r/b$, where b is the Thomas-Fermi parameter, $b = 0.885\,341\,38 Z_2^{-1/3}$. Also, we introduce $s(x) = \sigma(bx)$ and $v_0 = e^2/\hbar$. Equation (3) can now be rewritten as

$$\epsilon = \frac{4\pi Z_1^2 b(\hbar^2/m)}{(v/v_0)^2}\int_0^\infty s(x) L(s, v/v_0) dx \ . \quad (12)$$

Every factor in Eq. (12) is dimensionless with the exception of $\hbar^2/m$ which has the value $0.761\,952\,8 \times 10^{-15}$ eV cm^2.

The stopping cross section of α particles is numerically integrated using the expression for $L(s, v/v_0)$ given by Bonderup and also that of Lindhard and Winther. The calculations have been made for 0.8 and 2.0 MeV ($v/v_0 = 2.84$ and 4.49) and are shown in Figs. 1 and 2, respectively. The most striking feature of these calculations is the considerable structure in both the first ($Z_2 = 21-28$) and second ($Z_2 = 39-46$) transition series. The calculations provide generally good agreement with the previously obtained experimental results. Moreover, there are marked changes in the slope of the curve at points where Z_2 corresponds to a closed-shell atom, i.e., $Z_2 = 10$, 18, 36, and 54. Thus, the over-all structure of the curve can be intuitively understood in terms of the effects of unfilled d and f shells and the effect of adding a new s shell. The present calculations provide considerable insight into the possible origins of the structure of the experimental $\epsilon_\alpha(E_\alpha)$-vs-$Z_2$ curves.

An experiment to measure ϵ_α as a function of $Z_2 \simeq 30-50$ is underway at Baylor University to test for a possible anomaly in the second transition series.

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