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Stopping Powers of Solids for Low-Energy Protons*

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Electron gas models are useful approximations for describing the valence electron response of a solid to the passage of a charged particle. A simple free-electron gas model was used by Fermi and Teller[1] to estimate the time required for a "mesotron" to be stopped in various solids. More recent work has employed the Lindhard dielectric response function,[2] or approximations thereto, for calculations of the valence electron contributions to energy loss per unit pathlength for protons. Such calculations have generally shown rather poor agreement with experimental data for low-energy protons (velocity small compared to the Fermi velocity, $v \ll v_F$). The purpose of this paper is to draw attention to a recent calculation of the stopping power for slow protons using a density-functional formalism.[3] These new results have been shown to give good agreement with experimental data and thus should provide valuable theoretical guidance in estimating stopping powers of solids for which no experimental data are available.

The density-functional approach was used to calculate the self-consistent potential of a static proton in an electron gas.[3] The energy loss rate for a slowly moving proton of speed v calculated from this potential is shown as curve ENR in Fig. 1 in the form "stopping power/v" as a function of r_s. All quantities are in atomic units and r_s is related to the valence electron density n_o through $4\pi r_s^3/3 = 1/n_o$. For comparison we show

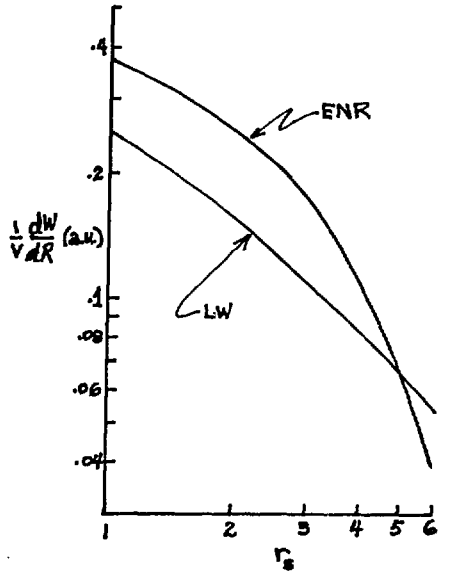

Figure 1

the Lindhard-Winther result[5] (curve LW) given by

$$\frac{1}{v}\frac{dW}{dR}\Big]_{LW} = \frac{2}{3\pi}\left[\ln\left(\frac{1+2\chi^2/3}{\chi^2}\right) - \frac{1-\chi^2/3}{1+2\chi^2/3}\right](1-\chi^2/3)^{-2}$$

with $\chi^2 = 0.166 r_s$. This form is a very good approximation to the values predicted numerically using the exact Lindhard dielectric response function for an electron gas. The dramatic increase of the non-linear, density-functional results over those of the linear response theory is shown in Fig. 2. For many solids commonly used in experiments ($1.5 \lesssim r_s \lesssim 2.5$) the new results show increases of ~65% over the Lindhard-Winther predictions.

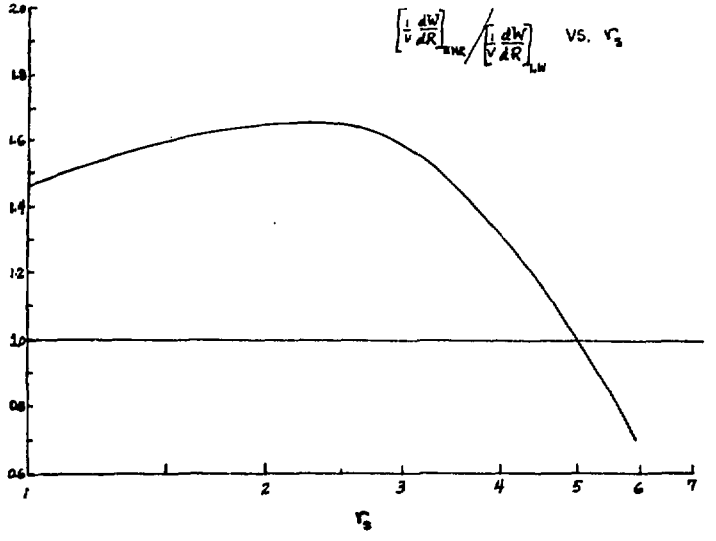

Figure 2

Comparisons of the density-functional predictions with experimental data were recently made by Mann and Brandt.[4] They collected data on targets covering a wide range of atomic numbers and plotted reduced stopping powers S_p/f_{LW}, where $S_p = dW/dR$ and $f_{LW} = (v_F/v)(dW/dR)]_{LW}$, as a function of v/v_F. The values of r_s were taken from Isaacson's tables.[6]

Their comparisons are shown in Fig. 3 with the density-functional results given by the curve ENR and the Lindhard-Winther prediction by LW. The curve FR is a theoretical prediction by Ferrell and Ritchie[7] in which electrons at the Fermi surface are viewed as scattering from the screened potential of a proton. As a guide to the comparison of data with theory, short-dash lines are included giving a $\pm 15\%$ variation around the line ENR. Mann and Brandt conclude that, within the uncertainties in the data: (1) the density-functional predictions give good agreement with the data, (2) the linear dependence on velocity holds up to $v \approx v_F$, and (3) a proton effective charge less than 1 is not required.

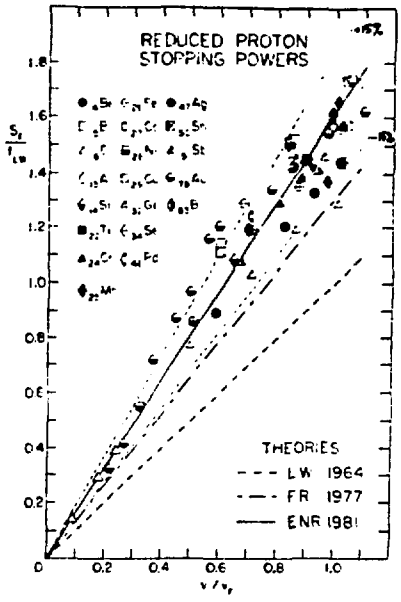

Figure 3

Additional comparisons of theory and experiment may be made using results compiled by Anderson and Ziegler in a book on stopping powers.[8] They collected experimental data for a wide range of energies and employed simple analytic forms to obtain

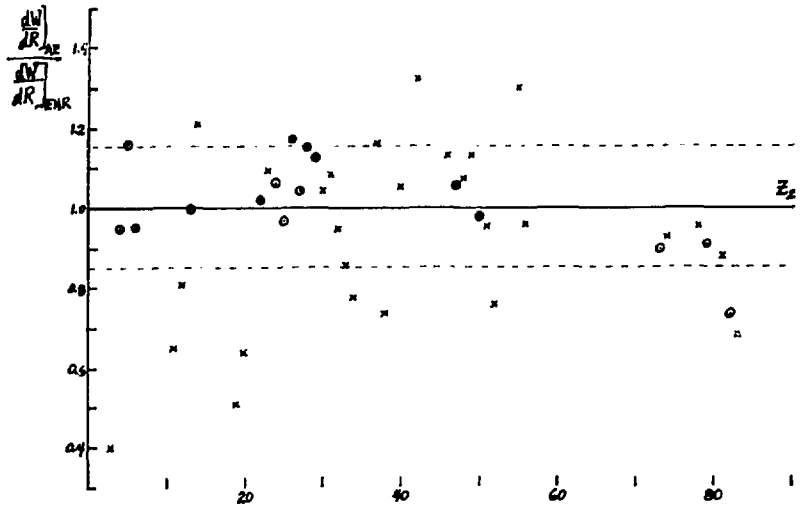

Figure 4

a "best-fit" for several elemental solids. For energies below 10 keV, a simple, velocity-proportional expression for stopping power is given. These data-based fits are compared with the density-functional results as a stopping power ratio. The ratios are shown by circles in Fig. 4 for 16 elements specified by their atomic number Z_2. With the exception of Pb(Z_2 = 82) the agreement is similar to that shown in Fig. 3 since many of the same data sets are employed in References 4 and 8.

Anderson and Ziegler used an interpolation scheme, described in Ref. 8, to predict stopping powers of materials for which no data were available. Comparisons for several solids are shown as "x's" in Fig. 4. Substantial variations about the density-functional predictions are seen.

In conclusion, the recent density-functional calculation of the stopping power of an electron gas for low-velocity protons is well-supported by experimental data. These theoretical results should be useful for estimating stopping powers of solids for which no reliable experimental data are available.

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