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Progress in understanding heavy-ion stopping

P. Sigmund [a,*], A. Schinner [b]

[a] Department of Physics, Chemistry and Pharmacy, University of Southern Denmark, DK-5230 Odense M, Denmark
[b] Institut für Experimentalphysik, Johannes Kepler Universität, A-4040 Linz, Austria

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ABSTRACT

We report some highlights of our work with heavy-ion stopping in the energy range where Bethe stopping theory breaks down. Main tools are our binary stopping theory (PASS code), the reciprocity principle, and Paul's data base. Comparisons are made between PASS and three alternative theoretical schemes (CasP, HISTOP and SLPA). In addition to equilibrium stopping we discuss frozen-charge stopping, deviations from linear velocity dependence below the Bragg peak, application of the reciprocity principle in low-velocity stopping, modeling of equilibrium charges, and the significance of the so-called effective charge.

1. Introduction

Research on the penetration of heavy ions in matter dates back to early studies of the scattering and stopping of fission fragments [1]. The subject received renewed interest with the application of accelerators in the study of atomic collisions and material properties [2,3], ion implantation [4], ion-beam modification [5], ion-beam analysis [6,7] and ion-beam therapy [8].

While the penetration of protons and alpha particles is well described by Bethe's [9] theory of the stopping of point charges over a wide range of beam energies, penetration theory for heavier particles increases in complexity with increasing atomic number Z_1 for several reasons:

- The Coulomb force is not necessarily a weak perturbation,
- The projectile cannot necessarily be treated as a point charge, and
- Energy may be lost in charge-changing collisions.

Fig. 1 shows a comparison of measured electronic stopping forces with well-known formulae by Bohr [10] and Bethe [9],

$$-\frac{dE}{dx} = \frac{4\pi Z_1^2 Z_2 e^4}{m v^2} NL; \quad L = \begin{cases} \ln \frac{2mv^2}{\hbar\omega} & \text{Bethe} \\ \ln \frac{Cmv^3}{Z_1 e^2 \omega} & \text{Bohr,} \end{cases} \tag{1}$$

where $Z_1,\ Z_2$ are atomic numbers of the ion and the target, respectively, v the ion speed, ω is an effective resonance frequency of the target electrons, N the number of target atoms per volume, and $C = 1.1229$. It is seen that within the energy range depicted in the graph, the Bohr formula comes closest to the experimental data down to $\sim$0.5 MeV/u. This is consistent with the wellknown Bohr criterion [11],

$$\frac{2Z_1 e^2}{\hbar v} \gtrsim 1 \tag{2}$$

for the validity of a classical-orbit description of ion–electron scattering, the basis of Bohr's theory. The opposite limit, $Z_1e^2/\hbar v \lesssim 1$, is known to define the range of validity of the Born approximation, the basis of Bethe's theory [11].

Due to the logarithmic form of (1), both expressions drop below zero at some apparent threshold. This is an artifact of the mathematics involved, since energy is transferred from the ion to the target in both theories, and not in the reverse direction. For the Bohr theory this is easily repaired by avoiding asymptotic expansion in $1/v$ [12] (solid line). The same can be done for the Bethe formula, but whereas the solid line in Fig. 1 represents a universal result when plotted in appropriate units (L versus $mv^3/Z_1e^2\omega$), the corresponding result for the Bethe theory depends on the target and therefore has not been included.

Fig. 1 suggests that, over a wide energy range around the Bragg peak, Bohr theory should be a better starting point for understanding heavy-ion stopping than Bethe theory. This has led to a series of studies beginning with Ref. [14]. The present note summarizes some highlights of this development. The presentation is based

* Corresponding author.
E-mail address: sigmund@sdu.dk (P. Sigmund).

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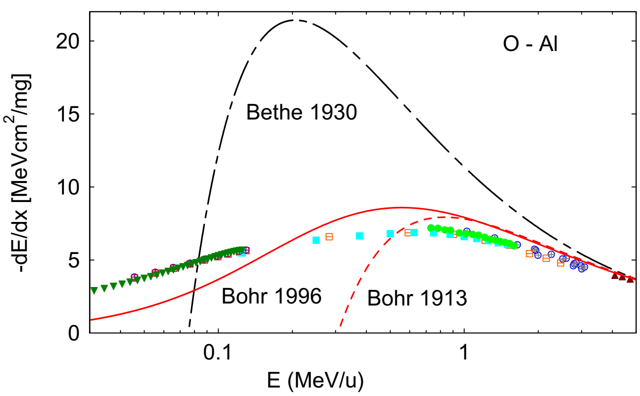

Fig. 1. Stopping force on oxygen ions in aluminum. Dashed line: Bohr formula [10]; Dot-dashed line: Bethe formula [9]; Solid line: Bohr theory avoiding asymptotic expansion [12]. Experimental data (symbols) compiled by Paul [13].

mainly on our own work, but comparisons with alternative theoretical schemes are made, and emphasis is laid on comparisons with experimental findings.

Although considerable progress has been made in straggling [15,16], the present paper focuses on mean energy loss.

2. Qualitative orientation

Bohr and Bethe stopping theory, as expressed by (1), ignore several important physical phenomena,

- *Screening of the Coulomb interaction* by electrons bound to the projectile. According to Bohr [1], electrons with orbital speeds v_e less than the projectile speed v tend to be stripped. Since both Bohr and Bethe theory consider the projectile as a point charge, a screening correction must be expected for

$$v \lesssim v_0 Z_1^{2/3}, \tag{3}$$

where we characterize projectile electrons by their Thomas–Fermi speed $v_{\mathrm{TF}} = v_0 Z_1^{2/3}$, v_0 denoting the Bohr speed.
- *Orbital motion of target electrons* is ignored in Bohr theory. Although this effect (shell correction), is inherent in Bethe theory, its contribution to the stopping cross section is not taken into account in the asymptotic formula (1). Such a correction must be expected for

$$v \lesssim v_0 Z_2^{2/3}, \tag{4}$$

where the Thomas–Fermi speed $v_0 Z_2^{2/3}$ characterizes the target atom.

Thus, if v decreases from the high-speed limit where (1) applies, screening will be the dominating correction to be taken into account if $Z_1 \gg Z_2$, while the shell correction will dominate for $Z_1 \ll Z_2$.

Consider now a situation where projectile screening is important, i.e., (3) applies. Then the Bohr parameter (2)

$$\frac{2Z_1 e^2}{\hbar v} \gtrsim \frac{2Z_1 e^2}{\hbar v_0 Z_1^{2/3}} = 2Z_1^{1/3} \tag{5}$$

will be greater than 1 for all values of Z_1. Therefore, in the presence of substantial projectile screening, the Born approximation, and hence Bethe theory, cannot be expected to provide a valid theoretical basis. This finding, emphasized by Bohr in 1948 [11], has been ignored in numerous theoretical studies over half a century.

- Another important effect, studied primarily in light-ion stopping, is *charge asymmetry* or *Barkas–Andersen effect*, characterized by the factor [17,18]

$$\frac{Z_1 e^2 \omega}{m v^3}. \tag{6}$$

If we approximate $\hbar\omega \sim Z_2 m v_0^2/2$ according to Bloch [19], we find that charge asymmetry becomes important for

$$v \lesssim (Z_1 Z_2/2)^{1/3} v_0, \tag{7}$$

indicating that this correction is intermediate between screening and shell correction, (3) and (4), respectively.

3. Theoretical schemes

Table 1 lists theoretical schemes which have been developed to estimate stopping cross sections for heavy ions in cold matter.[1] As noted in the last column, three of the listed schemes are high-speed theories incorporating effects that extend the range of validity towards lower velocities. The opposite holds for the scheme listed in the third row.

All these schemes incorporate features that are not taken into account in Bethe or Bohr stopping theory. While not ab initio theories, none of them employs adjustable parameters fitted to measured or tabulated stopping forces. Moreover, none of them make use of the (still) popular effective-charge concept. A brief discussion of the inadequacy of this type of description, based on Ref. [24], has been included in an Appendix A.

Table 2 lists effects entering the various schemes:

- Binding forces on target electrons enter explicitly into binary theory and PCA/UCA (Perturbed convolution approximation/ Unitary convolution approximation) but not into the free-electron model TCS-EFRS (Transport cross section-extended Friedel sum rule). In SLPA (Shellwise local plasma approximation) the effect is taken into account implicitly via a local-density approximation (LDA).
- All models allow for orbital motion of target electrons (shell correction), static screening of the projectile by bound electrons, and variation of the ion charge.
- Charge asymmetry (Barkas–Andersen effect) is inherent in all schemes, although the case of CasP is special, as will be discussed below.
- Projectile excitation enters PASS and SLPA. In CasP, projectile excitation can be computed but is not part of the default option.
- Charge exchange is included in CasP, although not in the default version. Binary theory incorporates an estimate requiring charge equilibrium.
- Only the CasP code is available on the internet.

There are significant differences in the way how the above effects are treated in these theoretical schemes. Some of those aspects have been discussed in Ref. [25], but for details we refer to the original papers and various followups.

Fig. 2 shows a comparison of measured stopping cross sections with predictions of PASS and CasP for the O–Al system. This ion-target combination is exceptionally well covered with experimental data in good mutual agreement over an energy interval of six orders of magnitude. While the agreement with PASS data is close to perfect, CasP data lie below experiment from ~1 MeV/u down. The Bohr speed v_0 has been marked to emphasize the fact that neither PASS nor CasP can be expected to cover lower velocities. The

[1] The term ‘cold matter’ is meant to indicate that high-temperature-plasma targets require separate consideration.