



Contents lists available at ScienceDirect

Nuclear Instruments and Methods in Physics Research B

journal homepage: www.elsevier.com/locate/nimb

Note on measuring electronic stopping of slow ions

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ARTICLE INFO

Article history:

Received 30 June 2017

Received in revised form 28 July 2017

Accepted 8 August 2017

Keywords:

Electronic stopping

Nuclear stopping

Impact-parameter-dependent energy loss

Reciprocity

Light ions

Heavy ions

ABSTRACT

Extracting stopping cross sections from energy-loss measurements requires careful consideration of the experimental geometry. Standard procedures for separating nuclear from electronic stopping treat electronic energy loss as a friction force, ignoring its dependence on impact parameter. In the present study we find that incorporating this dependence has a major effect on measured stopping cross sections, in particular for light ions at low beam energies. Calculations have been made for transmission geometry, nuclear interactions being quantified by Bohr-Williams theory of multiple scattering on the basis of a Thomas-Fermi-Molière potential, whereas electronic interactions are characterized by Firsov theory or PASS code. Differences between the full and the restricted stopping cross section depend on target thickness and opening angle of the detector and need to be taken into account in comparisons with theory as well as in applications of stopping data. It follows that the reciprocity principle can be violated when checked on restricted instead of full electronic stopping cross sections. Finally, we assert that a seeming gas-solid difference in stopping of low-energy ions is actually a metal-insulator difference. In comparisons with experimental results we mostly consider proton data, where nuclear stopping is only a minor perturbation.

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1. Introduction

A fundamental parameter characterizing the penetration of charged particles through matter is the stopping cross section $S(E)$, which determines the mean energy loss per travelled pathlength,

$$-\frac{dE}{dR} = NS(E) = N \int T d\sigma(E, T), \quad (1)$$

where N is the number of atoms (or molecules) in the medium and $d\sigma(E, T)$ the differential cross section for energy loss (T, dT) at a beam energy E [1]. Stopping cross sections are most frequently measured by analysis of the energy spectrum of an initially monochromatic beam after penetration through a thin film or gas layer of known thickness. Since projectiles experience angular scattering in addition to energy loss, only a fraction of the incident beam particles will typically enter the analysing window. If the energy-loss spectrum of those projectiles is not representative of the entire beam, a correction is necessary. This correction depends on the experimental geometry.

The total energy loss T is made up by contributions due to excitation and ionization of target and projectile atoms, charge exchange, recoils, as well as high-energy effects such as nuclear reactions and bremsstrahlung. Specific stopping cross sections can be assigned to each of these effects. Most common is a splitting into

$$S(E) = S_e(E) + S_n(E), \quad (2)$$

where $S_e(E)$ and $S_n(E)$ stand for energy loss into electronic and nuclear motion, respectively [2]. While this definition is reasonably precise, it is difficult to handle in practice where, instead, $S_n(E)$ is taken to be the stopping cross section for elastic scattering and $S_e(E)$ accounts for all the rest, including corrections to elastic scattering dynamics due to electronic processes.

The two contributions can to some degree be separated due to the fact that nuclear energy loss is accompanied by angular scattering, while collisions with electrons lead to only very small scattering angles. Therefore, the contribution of elastic collisions to the measured energy-loss spectrum can be reduced – although not brought to vanish – if only particles scattered at small angles are allowed to enter the detector.

However, also deflected ions experience electronic energy loss. These ions have undergone a close collision with a target atom. Since electronic energy loss depends on the impact parameter,

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deflected ions will typically have lost electronic energy above average. If this is not corrected for, the extracted mean electronic energy loss may be underestimated.

An influence of this effect on measurements of electronic stopping has been suggested repeatedly and discussed extensively [3–8] but has had very little impact if any on reported stopping cross sections. Specifically, frequently-used tabulations based on experimental data [9,10] ignore this point.

Cross sections for elastic scattering and angular deflection increase with decreasing energy. In order to estimate the significance of the effect, we look primarily at the stopping of slow ions, where there are several more or less wellknown problems:

- Pronounced discrepancies between low-velocity stopping cross sections from different sources [9],
- Significant deviations from the expected linearity with projectile speed of $S_e(E)$ [11],
- Significant deviations from reciprocity,

$$S_e(Z_1 \rightarrow Z_2, v) = S_e(Z_2 \rightarrow Z_1, v), \quad (3)$$

where Z_1 and Z_2 denote atomic numbers of projectile and target, respectively [12], and

- An apparent gas-solid difference in measurements with slow ions [13].

Our study proceeds in two steps. For qualitative orientation we operate with Firsov's expression for impact-parameter-dependent electronic energy loss [14]. More quantitative results are found by combination of our PASS code [15] with classical scattering on a Thomas-Fermi-Molière potential.

2. Single scattering

For transmission through a very thin layer x , the mean detected electronic and nuclear energy loss will be given by

$$\Delta E = Nx \int_{\phi < \phi_0} (T_e + T_n) d\sigma(E, T_e, T_n, \phi), \quad (4)$$

where ϕ is the scattering angle in the laboratory frame and ϕ_0 the opening angle of the scattering cone seen by the detecting device. Reminding that small-angle scattering leads to small nuclear energy loss, one may separate elastic scattering by making ϕ_0 sufficiently small, so that the nuclear contribution vanishes and

$$\begin{aligned} \Delta E &\simeq Nx \int_{\phi < \phi_0} T_e d\sigma(E, T_e, T_n, \phi) \\ &= Nx \left[S_e - \int_{\phi > \phi_0} T_e d\sigma(E, T_e, \phi) \right]. \end{aligned} \quad (5)$$

In other words, for a narrow detector window, the mean energy loss is given by that part of the electronic loss that is not carried away by scattering events exceeding ϕ_0 .

3. Multiple scattering

Eqs. (4) and (5) assume the layer thickness x small enough to ensure single scattering. This assumption is rarely justified. A simple way to correct for multiple scattering was proposed by Fastrup et al. [11], based on Bohr-Williams theory of multiple scattering [16]. In this theory the angular distribution of a beam after penetrating through a layer x is approximated by two regimes, a single-collision regime for $\phi > \phi_1$, in which the angular distribution is given by the differential cross section as $Nx d\sigma_n(E, \phi)$ for single scattering, and a multiple-scattering distribution taken as a gaussian with a width ϕ_1 which, in the notation of [17], is defined by

$$\phi_1^2 = Nx \int_0^{\phi_1} \phi^2 d\sigma_n(E, \phi). \quad (6)$$

It is then assumed that energy loss within ϕ_1 is randomized, so that the contribution of nuclear stopping to the energy loss in the forward direction is expressed by a reduced stopping cross section

$$S_n^{\text{red}}(E) = \int_0^{\phi_1} T_n(E, \phi) d\sigma_n(E, \phi) \quad (7)$$

with

$$T_n(E, \phi) = (M_1/M_2)E\phi^2. \quad (8)$$

Since ϕ_1 depends on the pathlength x according to Eq. (6), also $S_n^{\text{red}}(E)$ depends on the pathlength (or foil thickness).

Eq. (7) has become a standard expression for eliminating the contribution of nuclear stopping to energy losses measured in the transmission geometry. Alternative descriptions are based on Monte Carlo simulation [18] or Bothe-Landau theory [17].

This scheme ignores electronic energy loss due to deflected ions. If the limiting angle ϕ_0 exceeds the multiple-scattering angle ϕ_1 , the missing detector signal will be exclusively due to projectiles scattered outside the multiple-scattering cone, so that the reduced electronic stopping cross section will be given by

$$\begin{aligned} S_e^{\text{red}}(E) &= S_e(E) - \int_{\phi > \phi_0} T_e d\sigma(E, T_e, \phi) \\ &= \int_{\phi < \phi_0} T_e d\sigma(E, T_e, \phi), \quad \phi_0 > \phi_1. \end{aligned} \quad (9)$$

If $\phi_0 < \phi_1$, projectiles reaching the detector window will belong to the multiple-scattering cone, so that

$$S_e^{\text{red}}(E) = \int_{\phi < \phi_1} T_e d\sigma(E, T_e, \phi), \quad \phi_0 < \phi_1. \quad (10)$$

Since ϕ_1 depends on the layer thickness x , also $S_e^{\text{red}}(E)$ must depend on x for $\phi_0 < \phi_1$. Although there is no explicit dependence on x in Eqs. (9) or (10), an implicit dependence is due to the rearrangement of trajectories within the multiple-scattering cone.

Since this treatment rests on the small-angle approximation, second-order effects such as the difference between traveled pathlength and layer thickness are ignored.

4. Elastic scattering

Following common procedure, the trajectory of the projectile is described in terms of classical scattering theory on a Thomas-Fermi-Molière potential

$$V(R) = \frac{Z_1 Z_2 e^2}{R} \sum_j A_j e^{-\alpha_j R/a} \quad (11)$$

with

$$A_j = (0.35, 0.55, 0.10) \quad (12)$$

$$\alpha_j = (0.3, 1.2, 6.0) \quad (13)$$

$$a = 0.8853a_0 \left(Z_1^{2/3} + Z_2^{2/3} \right)^{-1/2} \quad (14)$$

and an impact parameter p relative to the nuclei of the collision partners. For small scattering angles ϕ , elastic scattering theory yields [1]

$$\phi(E, p) = -\frac{1}{pE} \int_p^\infty \frac{dR}{\sqrt{1 - (p/R)^2}} \frac{d}{dR} [RV(R)] \quad (15)$$

$$= \frac{Z_1 Z_2 e^2}{Ea} \sum_j A_j \alpha_j K_1(\alpha_j p/a) \quad (16)$$

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