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Projectile polarization effects in the energy loss of swift ions in solids

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Abstract

We have evaluated the energy loss of swift hydrogen ions moving through a solid target, paying special attention to the effect due to the polarization of the projectile. Our calculation is done in the framework of the dielectric formalism, taking into account the contribution to the energy loss due to the charge fraction of protons and hydrogen atoms, the electronic capture and loss processes, and the polarization of the projectile. The electronic structure of the projectile is described by a hydrogen-like model screened by the target electrons. We have found that the polarization of the projectile is a non-negligible contribution to the energy loss of the hydrogen atoms in the energy range around the maximum of the stopping power. The calculated stopping power (accounting for all the above mentioned effects) agrees satisfactorily well with the experimental data in a wide projectile velocity region.

1. Introduction

When swift ions move through solid targets they can capture or loss electrons, which results in a change of their charge state. After a transient time, a dynamical equilibrium between all the possible projectile charge states is reached. In this context, there is a probability to find a concrete charge state of the atomic ion inside the solid, so we can assign a charge fraction to each possible atomic charge state. This charge fraction depends on the projectile nature and velocity, but also on the target composition [1–5].

During the motion through the solid, the swift ion is decelerated due to the energy it loses mainly in the electronic excitations induced in the medium [6]. We evaluate the energy loss of atomic ions using the dielectric formalism and considering the screening of the projectile electronic cloud due to the target electrons. Moreover, we take into account in our calculations the charge fraction of the atomic ions and the energy loss due to electronic capture and loss processes.

The purpose of this work is to analyze the contribution to the energy loss of swift atomic ions moving through solid targets due to the polarization of the projectile. We will particularize to the case of swift protons incident on aluminum, however our model could be applied to other projectiles and targets.

The paper is organized as follows: in Section 2 we introduce the model we use to do the calculations, whose main results are compared with experimental data in Section 3. Finally, in Section 4 we present the conclusions of this work. In what

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follows we will use atomic units, except where otherwise stated. [1]

2. Model

In the case of swift protons moving through a solid target, there are two charge states (+1 and 0) for which the charge fractions are important in the velocity region we will discuss [1–5]. Therefore, the stopping power of the target for the system H^+/H^0 can be written as

$$S_{1,0} = \phi_1 S_1 + \phi_0 S_0 + S_{C\&L}, \tag{1}$$

where ϕ_1 and ϕ_0 are the charge fraction of protons or hydrogen atoms, respectively; analogously, S_1 and S_0 are the stopping power of the target for protons or hydrogen atoms. $S_{C\&L}$ is the stopping power that corresponds to the energy loss due to the electronic capture and loss processes. We obtain the value of ϕ_0 by a fitting to the available data [1–5] and $\phi_1 = 1 - \phi_0$. In the dielectric formalism the stopping power of a target for protons with velocity v is given by

$$S_1 = \frac{2}{\pi v^2}\int_0^\infty \frac{\mathrm{d}k}{k}\int_0^{kv} \mathrm{d}\omega\,\omega\,\mathrm{Im}\left[\frac{-1}{\epsilon(k,\omega)}\right] \tag{2}$$

and for hydrogen atoms

$$S_0 = \frac{2}{\pi v^2}\int_0^\infty \frac{\mathrm{d}k}{k}[1-\rho(k)]^2\int_0^{kv} \mathrm{d}\omega\,\omega\,\mathrm{Im}\left[\frac{-1}{\epsilon(k,\omega)}\right]. \tag{3}$$

$\mathrm{Im}[-1/\epsilon(k,\omega)]$ is the energy loss function of the stopping medium characterized by a dielectric constant $\epsilon(k,\omega)$, which is a function of the momentum, k, and energy, ω, transferred to excitations of the target electrons. The Fourier transform of the hydrogen atom electronic density is $\rho(k)$; to describe the electronic cloud that surrounds the hydrogen atom we have used a hydrogen-like model [7] screened by the target valence electrons. We have considered this screening by replacing the projectile nuclear charge Z by an effective nuclear charge $Z_{\mathrm{eff}} = Z\exp(-\langle r\rangle/a)$, where a is the screening length [8] and $\langle r\rangle$ is the average value of the electron–nucleus distance (i.e. 3/2 a.u. for a hydrogen atom). In our calculations we have considered an aluminum target, characterized by an energy loss function constructed according to the model presented in Ref. [6], but with the inner shell electrons described by their generalized oscillator strengths [9].

In order to evaluate the stopping power due to the electronic capture and loss processes $S_{C\&L}$, we use the following expression [10]:

$$S_{C\&L} = n\frac{\sigma_{01}\sigma_{10}}{\sigma_{01}+\sigma_{10}}(I_0 + E), \tag{4}$$

where n is the atomic density of the target (aluminum, in our case), σ_{10} and σ_{01} are the capture and loss cross sections [11], respectively, I_0 is the first ionisation energy of the target, and E is the energy of the electron bound to the projectile.

There is still other important contribution that is not considered in the previous calculations: the polarization of the projectile, which appears due to the electric field induced by the projectile in the target. This self-induced electric field modifies the position of the projectile electronic cloud by displacing its center of charge a distance d from the projectile nucleus. Taking into account this charge distribution, the stopping power of a target for the hydrogen atom could be easily evaluated in a first approach as

$$\begin{aligned} S_0^{\mathrm{pol}} = {} & S_1 + \frac{2}{\pi v^2}\int_0^\infty \frac{\mathrm{d}k}{k}\rho^2(k)\int_0^{kv}\mathrm{d}\omega\,\omega\,\mathrm{Im}\left[\frac{-1}{\epsilon(k,\omega)}\right] \\ & - \frac{4}{\pi v^2}\int_0^\infty \frac{\mathrm{d}k}{k}\rho(k) \\ & \times \int_0^{kv}\mathrm{d}\omega\,\omega\,\mathrm{Im}\left[\frac{-1}{\epsilon(k,\omega)}\right]\cos\left(\frac{\omega d}{v}\right). \end{aligned} \tag{5}$$

We have used the superindex "pol" in the above expression to recall that it corresponds to a polarized hydrogen atom.

The distance d between the nucleus and the centre of the electronic cloud is calculated as $d = \alpha\mathscr{E}$ where α is the projectile polarizability (we use the value $\alpha = 4.5$ a.u. stated in [12] for the polarizability of an hydrogen atom) and $\mathscr{E}$ is the self-induced electric field,

[1] Atomic units are defined by the condition $m_e = e = \hbar = 1$, where m_e is the mass of the electron and e is the elementary charge.

$$\mathscr{E} = \frac{2}{\pi v^2}\int_0^\infty \frac{\mathrm{d}k}{k}[1-\rho(k)]^2\int_0^{kv}\mathrm{d}\omega\,\omega\,\mathrm{Im}\left[\frac{-1}{\epsilon(k,\omega)}\right]. \tag{6}$$

Eq. (5) assumes that the self-induced electric field only separates the nucleus and the electronic cloud and does not modify its size and shape. It is interesting to note the similarities between Eq. (5) and the stopping power for an aligned molecular ion [13,14], made of a positive and a negative charge, both with the same magnitude; the first term in Eq. (5) corresponds to the stopping power for a proton, the second term is the stopping power for the electronic cloud, and the last term comes from the interference between the electronic excitations produced by the proton and the electronic cloud separated a distance d; typical values of d are 0.67 and 0.46 a.u. for $v = 1$ and 4 a.u., respectively.

3. Results and discussion

In Fig. 1 we present the calculated stopping power of aluminum for hydrogen atoms as a function of the velocity. The solid line represents our calculation considering the polarization of the projectile and the screening due to the target electrons, the dashed line shows our calculation when only the screening effects are considered in Eq. (3), and the dotted line depicts our calculation, using Eq. (3), without including additional effects. There are clear differences between the three calculations presented in this figure. It can be observed that the stopping power increases when considering the screening effect, because in this case the atomic electron is less bound and then $\langle r\rangle > 3/2$ a.u. On the other hand, the inclusion of the polarization effect also increases the stopping power, the differences being more important near the maximum. The three curves in Fig. 1 will coincide at high velocities, because both the self-induced electric field (responsible of the polarization) and the screening decrease when v is large.

The total stopping power of aluminum for the H^+/H^0 system, calculated by means of Eq. (1) and considering Eqs. (2), (4) and (5), is represented in Fig. 2 by a solid line. In this Figure we also show all the contributions to the total stopping power. At high velocities the stopping power for protons is the main contribution to the total stopping power, because $\phi_0 \to 0$ at these velocities. However, the stopping power for hydrogen atoms (dashed line) is more important at low velocities, where the charge fraction ϕ_0 of hydrogen atoms is greater. The polarization and the screening of the projectile only affect the stopping power for hydrogen atoms, so these effects (dotted line) modify the total stopping power around the maximum and at low velocities, like the contribution due to the electronic capture and loss processes (dash-dotted line).

Finally, in Fig. 3 we compare our calculations of the stopping power of aluminum for the H^+/H^0 system with experimental data [15–30]. The thick line is our calculation of the total stopping power taking into account the changes of the charge state

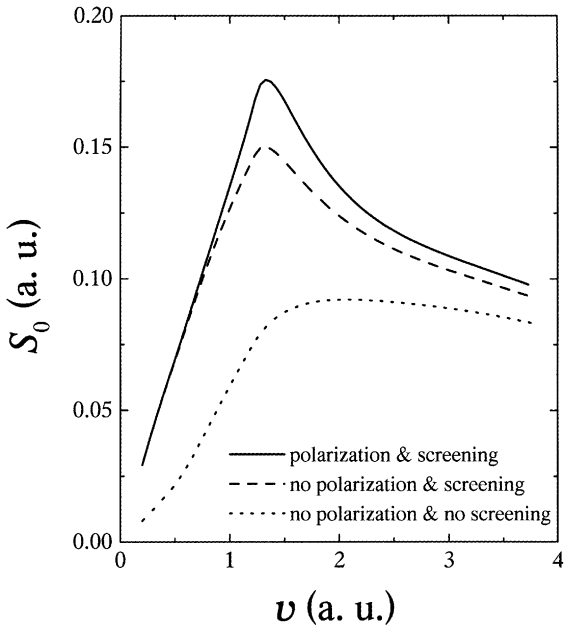

Fig. 1. Stopping power of aluminum for hydrogen atoms, as a function of the projectile velocity. The solid line represents our calculation considering the polarization and screening effects, the dashed line shows our calculation only considering the screening effects, and the dotted line corresponds to Eq. (3) without considering additional effects.

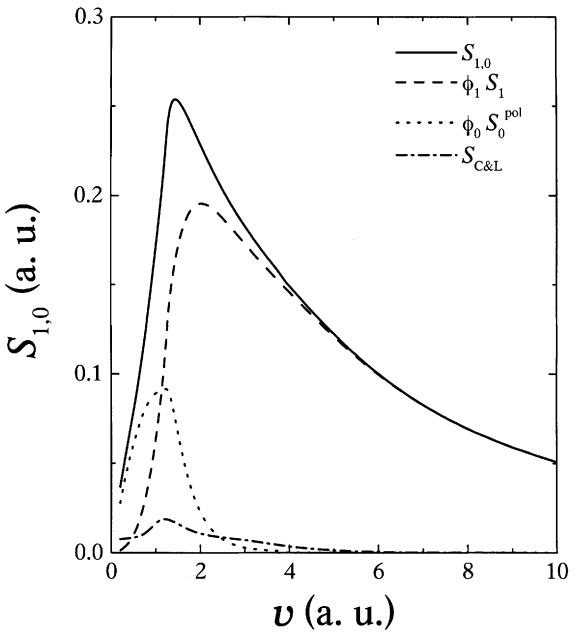

Fig. 2. Stopping power of aluminum for the system H^+/H^0, as a function of the projectile velocity. The solid line represents our calculation of the total stopping power. The dashed and dotted lines are our calculation of the stopping power for protons or hydrogen atoms, respectively, considering their charge fraction. The dash-dotted line is the capture and loss processes contribution to the total stopping power.

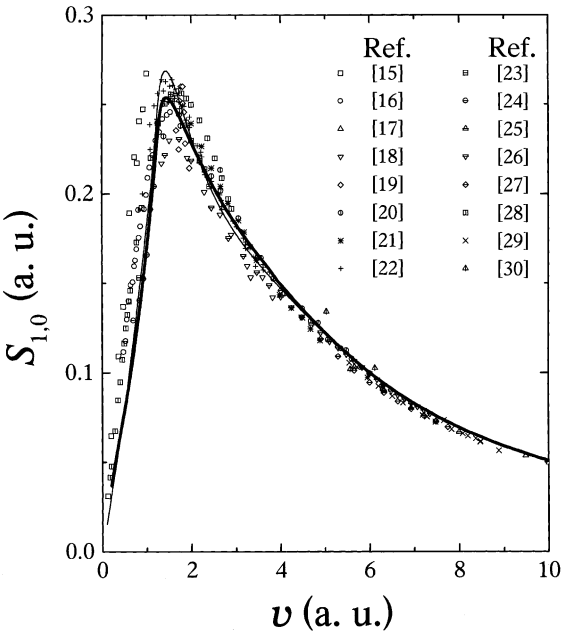

Fig. 3. Stopping power of aluminum for the system H^+/H^0 as a function of the projectile velocity. The thick line represents our calculation of the total stopping power and the thin line is the stopping power for protons. Symbols represent experimental data [15–30].

of the projectile, Eqs. (1), (2), (4) and (5), and the thin line is our calculation of the stopping power considering that the projectiles are frozen protons that do not undergo capture and loss processes, Eq. (2). It is interesting to note that the differences between both calculations are negligible, except around the maximum of the stopping power, where the calculation for frozen protons in aluminum overestimates the stopping power. Although both types of calculations compare reasonably well with the experimental data, the more complete model we have developed in this work seems to ponderate better the dispersion of the data around the maximum value of the stopping power.

4. Conclusion

The polarization of the hydrogen atom is a non-negligible contribution to the stopping power for the H^+/H^0 system in the velocity region around the maximum. The calculated stopping power for H^+ looks like the calculated stopping power for the H^+/H^0 system. In both cases, comparison with experimental data is satisfactorily good, except at very low velocities, where non-linear effects should be included for a proper description.

This work seems to suggest that a decomposition of the energy loss in the different contributions to the projectile energy loss will give approximately the same result than a simpler calculation considering the projectile in a frozen state. The generalization of this conclusion to other projectile–target combination is not conclusive and would need further work. However, the polarization effect should be considered when the above mentioned decomposition is done and it could be important when evaluating the energy loss of projectiles that have a high polarizability, like lithium.

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