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Electronic interactions and nuclear scattering effects in the stopping power of carbon for fragmented H_2^+ projectiles

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Abstract

The stopping power of amorphous carbon for fragmented swift H_2^+ molecular ions has been carried out using a Molecular Dynamics code to follow the trajectory of each fragment proton as it moves through the target. We consider the interaction of each proton with the target electrons, the Coulomb repulsion between both protons and the vicinage effects due to the wake potential created by its partner proton. The nuclear scattering with the target nuclei was also taken into account using a Monte Carlo simulation code. The stopping ratio distribution of the proton fragments has been obtained as a function of the incident energy and target thickness. Comparison of the calculated mean stopping ratio with experimental data shows a good agreement. © 1998 Elsevier Science B.V.

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1. Introduction

During the past couple of decades a large number of papers have been devoted to study, both experimentally [1–6] and theoretically [1,7–9], the interaction of H_2^+ molecular ions with matter. In particular, it has been analysed how the mutual forces felt by each component of the molecular ion affect phenomena such as: energy loss [3,4,8], charge fractions [10], transmission yields [5,11], and secondary-electron emission [12].

In all these phenomena an important role is played by the wake potential that accompanies the motion of a charged projectile [13], in such a manner that each proton of the molecule not only feels its self-induced retarding force, but also the force produced by its partner proton.

The stopping ratio R_2 of a swift H_2^+ molecule is defined as the energy loss of each fragment proton divided by the mean energy loss of a lonely proton with the same velocity as the molecule. Therefore, a value of $R_2 \neq 1$ indicates the existence of interference (or *vicinage*) effects during the propagation of the two protons.

In this paper we will study how the stopping ratio distribution of the transmitted protons resulting from the dissociation of a swift H_2^+ molecule inside a solid is affected by: (a) the self-induced stopping force, the Coulomb repulsion

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and the superposed wake potentials of the two protons moving in a correlated way, and by (b) the nuclear collisions these protons suffer with the target nuclei.

Using the well established dielectric formalism [13] to calculate the response of a medium to the passage of a fast charged projectile, we have evaluated [14,15] the electric field created by a fast proton moving through a target whose dielectric properties were modelled by means of Mermin-type energy loss functions [16], as discussed in detail in [14,15,17].

Due to the axial symmetry of the proton motion (along the positive direction of the z-axis) it is convenient to use the cylindrical coordinates z and ρ (given in the proton's reference frame), which are parallel and perpendicular, respectively, to the proton velocity $\vec{v}$. The electric field induced by the proton in a medium described by the energy loss function $\mathrm{Im}[-1/\epsilon(k,\omega)]$, is written in terms of its components $\mathscr{E}_z$ and $\mathscr{E}_\rho$, as

$$\mathscr{E}_z(z,\rho) = \frac{2}{\pi v^2}\int_0^\infty \frac{\mathrm{d}k}{k}\int_0^{kv} \mathrm{d}\omega\ \omega\ J_0\left(\rho\sqrt{k^2-\omega^2/v^2}\right) \times\left\{\sin\left(\frac{\omega z}{v}\right)\mathrm{Re}\left[\frac{1}{\epsilon(k,\omega)}-1\right] +\cos\left(\frac{\omega z}{v}\right)\mathrm{Im}\left[\frac{1}{\epsilon(k,\omega)}-1\right]\right\}, \quad (1)$$

$$\mathscr{E}_\rho(z,\rho) = \frac{2}{\pi v}\int_0^\infty \frac{\mathrm{d}k}{k}\int_0^{kv} \mathrm{d}\omega\ \sqrt{k^2-\omega^2/v^2}\ J_1\left(\rho\sqrt{k^2-\omega^2/v^2}\right) \times\left\{\cos\left(\frac{\omega z}{v}\right)\mathrm{Re}\left[\frac{1}{\epsilon(k,\omega)}-1\right] -\sin\left(\frac{\omega z}{v}\right)\mathrm{Im}\left[\frac{1}{\epsilon(k,\omega)}-1\right]\right\}, \quad (2)$$

where $J_0(x)$ and $J_1(x)$ are the Bessel function of the zero and first order. Atomic units are used through all this paper.

We present in Fig. 1(a) and (b) the induced electric field $\vec{\mathscr{E}}$ created by a proton travelling in

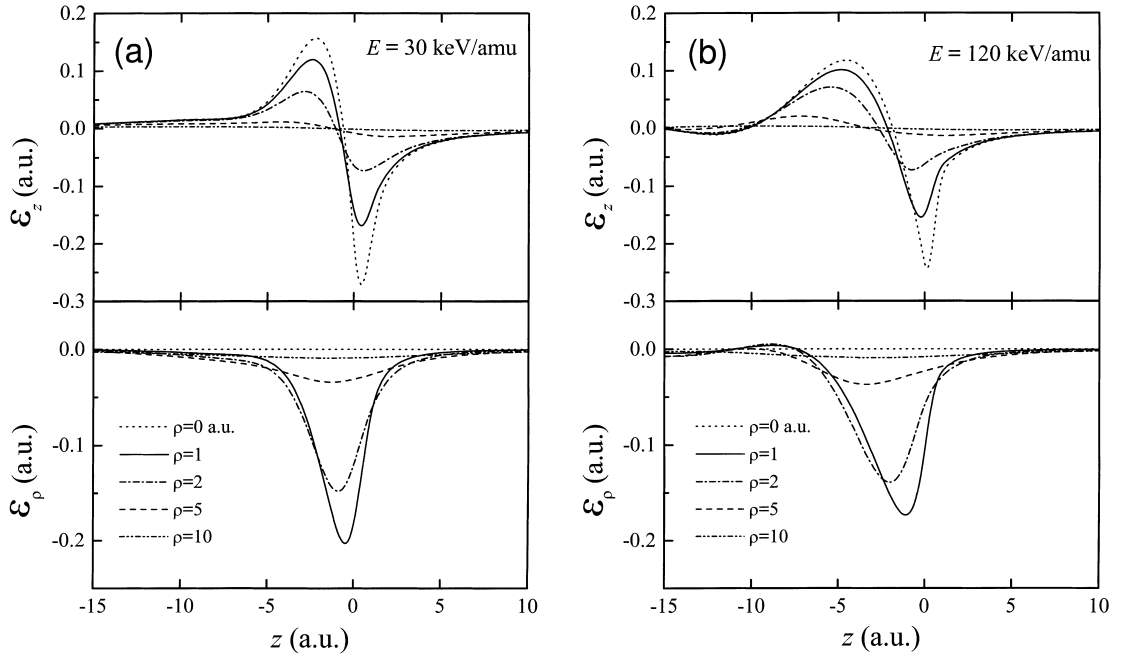

Fig. 1. Wake field created by a proton along the direction of its motion (z-axis) and at the different radial distances ρ that are indicated in the figure. The proton moves in amorphous carbon with energy: (a) 30 keV and (b) 120 keV. The field components $\mathscr{E}_z$ and $\mathscr{E}_\rho$ are parallel and perpendicular, respectively, to the direction of motion.

amorphous carbon, for two different energies, $E = 30$ keV and $E = 120$ keV. The position of the proton corresponds to $z = 0$ and $\rho = 0$. The upper (lower) part of each figure represents the parallel $\mathscr{E}_z$ (perpendicular $\mathscr{E}_\rho$) component of the induced electric field accompanying the swift proton. Due to the symmetry of the problem, it is obvious that there is no transversal field along the proton path of motion, as it is clear by the $\rho = 0$ line shown in the lower half of the figures.

From these figures it is evident that the proton experiences a retarding force due to self-induced field at its position (since $\mathscr{E}_z(0,0) < 0$, $\mathscr{E}_\rho(0,0) = 0$), and that this retarding force (usually called stopping power) depends on the energy (in the case depicted, $|\mathscr{E}_z(0,0)|_{30\ \mathrm{keV}} < |\mathscr{E}_z(0,0)|_{120\ \mathrm{keV}}$). In addition to this self-induced reaction force, the wake field of each proton also disturbs the motion of the companion proton, as a result of which both particles move in a correlated way through the solids. This dynamical correlation is known as vicinage effect and it has two main consequences: one is to produce an additional *accelerating* or *retarding* force acting on the otherwise lonely proton, and the other is to influence the direction of motion of the partner proton. These effects depend both on the relative vector of the fragment protons and on their velocities, as can be seen in the values of $\mathscr{E}_z$ and $\mathscr{E}_\rho$ shown in Fig. 1.

For a typical internuclear distance in the H_2^+ molecule (~ 2 a.u.) and for most orientations of the internuclear axis relative to the direction of motion, Fig. 1(a) shows an accelerating force, while Fig. 1(b) gives a retarding one on the partner proton. Then, it is expected that the energy loss of the molecule would be less for $E = 30$ keV/amu than for $E = 120$ keV/amu.

2. Calculation procedure

We consider now the correlated motion of the two protons, produced by the breakage of the H_2^+ molecule, following the influence of the forces already indicated, namely: the screened Coulomb repulsion [18] with its partner, the stopping force due to the polarization induced in the medium by itself, and the vicinage force due to the wake generated by its partner, viz.,

$$\vec{F} = \vec{F}_{\text{Coulomb repulsion}} + \vec{F}_{\text{self-induced}} + \vec{F}_{\text{vicinage effect}}. \quad (3)$$

Besides this, atomic collisions with the target atoms change the direction of movement of the protons. In the range of energies we are interested in this work, the energy loss due to these collisions is very small.

We describe the evolution of the protons inside the target by means of a Molecular Dynamics (MD) simulation. The stopping forces, as well as the vicinage effects due to the wake of the partner proton, were obtained using the dielectric formalism [15], with an energy loss function modelled by a sum of Mermin-type energy loss functions [16], according to the procedure described in [15,17]. In our calculations we have taken into consideration that the stopping power changes with the instantaneous proton velocity (see [19] for more details).

The plural scattering of the protons due to collisions with the target nuclei was described via a Monte Carlo (MC) simulation, according to the procedure given by Zajfman et al. [20], which is based on the binary collision model developed by Moller et al. [21]. Independent nuclear collisions are assumed for each molecular partner. The cross section to determine the scattering angle at each collision was taken from Meyer's calculations [22] for a Thomas–Fermi potential.

Combining both procedures, MD and MC, we calculate at any instant the coordinates and velocities of the two protons belonging to the H_2^+ molecule.

The fluctuations in the initial geometrical conditions of each H_2^+ molecule were taken into account by choosing randomly the internuclear distance and angular orientation relative to the proton initial velocity; the former was chosen according to the populations of the vibrational states of H_2^+ ions [23], and the latter was randomly picked around the beam direction.

After simulating a given number of histories ($\gtrsim 50\,000$) it is possible to obtain the distribution of energy losses experienced by the two correlated protons at any target thicknesses.

3. Results and discussion

Following the above procedure, and due to the statistical nature of the interactions felt by the protons while they travel through the solid, we obtain the distribution of stopping ratios depicted in Fig. 2, corresponding to three amorphous carbon target thicknesses (284, 567 and 992 a.u.), and for three beam energies ($E = 30$, 60 and 120 keV/amu), which correspond roughly to the experimental situation reported in [24]. It can be appreciated that as energy increases, for a given thickness, the stopping ratio broadens and eventually bifurcates, distinctly displaying that the exiting protons group into two classes: some that are slowed down, and others that are relatively accelerated by the internuclear repulsion. The dependence of R_2 with the thickness, for each energy, shows a wide distribution at the thinner thicknesses, which gradually becomes narrower at thicker targets.

From the stopping ratio distributions we have calculated the mean value, $\overline{R}_2$, for a set of energies and thicknesses where experimental data are available. In Fig. 3 we have plotted $\overline{R}_2$ as a function of

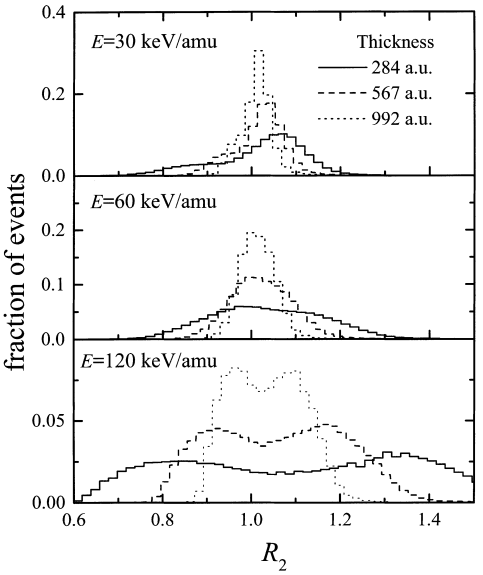

Fig. 2. Distribution of the stopping ratio calculated for different proton energies E and foil thicknesses. The target is amorphous carbon.

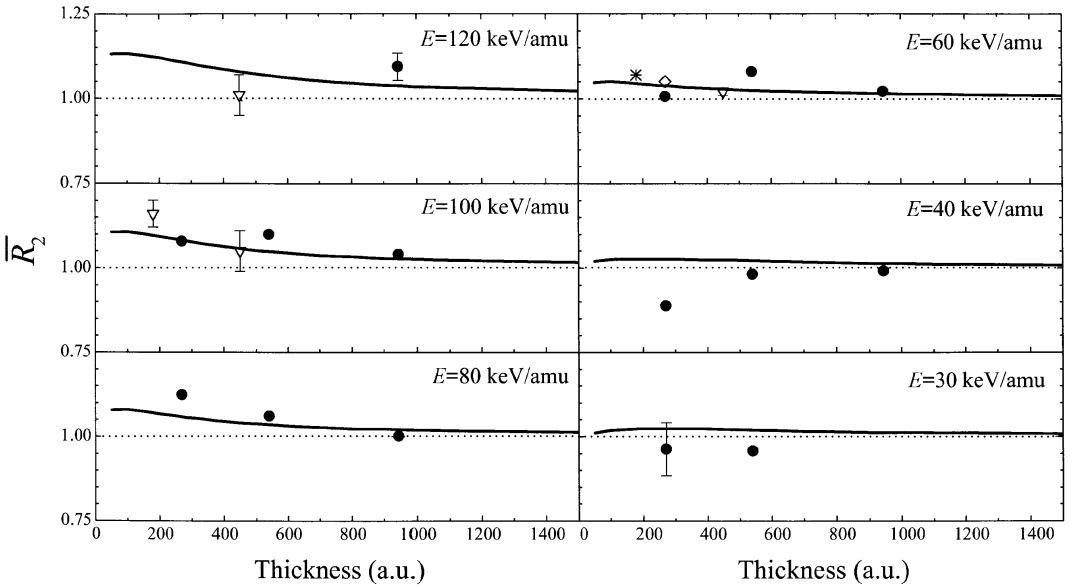

Fig. 3. Mean stopping ratio $\overline{R}_2$ for different proton energies and target thicknesses. The solid line corresponds to our calculations, and the symbols are experimental data by Ray et al. [24] (•), Laubert [4] (▽), Eckardt et al. [3] (◇), and a Monte Carlo simulation by Farizon et al. [25] (∗).

the foil thickness, for the range of energies $E = 30$–120 keV/amu. Solid lines correspond to our calculations, whereas symbols are experimental results [3,4,24] and a simulation [25]. Our results show a reasonably good agreement with the experiments and earlier simulation, most of them lying within the experimental uncertainties. Moreover, the tendency of $\overline{R}_2$ to unity at large thicknesses is well reproduced (being slower as the energy increases); this is so because after a long dwell time the fragment protons are no longer correlated (due to Coulomb repulsion, nuclear scattering, etc.), and the vicinage effect disappears. The same behaviour was found for H_3^+ molecular ions [26]

4. Conclusions

We have developed a code to follow the motion through a solid of a pair of correlated protons originally belonging to a swift H_2^+ molecular ion. This code incorporates Molecular Dynamics and Monte Carlo to give account of electronic interactions (screened Coulomb repulsion, self-induced force and vicinage effects), as well as atomic collisions with the target nuclei. The predicted stopping ratio distribution shows a structure that depends both on beam energy and target thickness, splitting into two peaks at the higher energies. The calculated mean stopping ratio agrees reasonably well with the available experimental data. We plan to use this code to evaluate other magnitudes that are relevant in the passage of fast molecular ions through matter, such as interproton distances and velocities, stopping of aligned pairs, etc.

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