Available online at www.sciencedirect.com
ScienceDirect
Nuclear Instruments and Methods in Physics Research B 256 (2007) 137–140
NIM B
Beam Interactions with Materials & Atoms
www.elsevier.com/locate/nimb

Alignment effects in the interaction of H_2^+ molecules with thin foils

Cristian D. Denton [a,*], Isabel Abril [a], Rafael Garcia-Molina [b], Santiago Heredia-Avalos [b]

[a] Departament de Física Aplicada, Universitat d'Alacant, Apartat 99, E-03080 Alacant, Spain
[b] Departamento de Física – CIOyN, Universidad de Murcia, Apartado 4021, E-30080 Murcia, Spain

Available online 24 January 2007

Abstract

We use a simulation code to study the alignment of the proton fragments of a H_2^+ molecule after traversing thin foils. The simulation code follows in detail the motion of the molecular constituents from the entrance until the exit of the target, taking into account the following interactions by each projectile: (i) Coulomb repulsion, (ii) wake force, (iii) stopping force and (iv) elastic scattering with the target nuclei. We compare the results of our simulation with two different experimental situations where the aligning effects of the wake forces become evident.

PACS: 34.50.Bw; 36.40.−c; 61.48.+c

Keywords: Stopping force; Energy loss; Molecular beams; Wake force

1. Introduction

The interaction of swift molecules with solids has been widely study since the pioneering work of Brandt et al. [1]. In that paper it was established for the first time the existence of the vicinage effects in the energy loss of neighbor projectiles; that is, the energy loss of the molecular fragments when they travel close to each other is different than that of the same fragments moving independently. These vicinage effects are caused by the electronic excitations induced in the target by each molecular fragment, or said in other words the effect of the wake forces acting on the molecular partner [2]. Apart from this effect on the energy loss, the wake forces tends to align (or disalign, depending on the relative distance between the molecular components) the molecular fragments toward the direction of motion. On the other hand the angular spread caused by the elastic scattering with the target nuclei competes with the previous effect, tending to destroy this alignment effect.

While a great number of papers has considered the effects of the wake forces on the energy loss of the fragments dissociated from a molecular beam [1–5], only a few have discussed the consequences of the wake on the motion of the fragments [6,7].

The aim of this paper is to study in a quantitative way, using a computer simulation, the alignment of the fragments of a H_2^+ molecule after traversing a thin foil. In order to do so we will study two different experimental situations [8,9] where the alignment effects of the wake can be clearly stated.

Our paper is structured in the following way: Section 2 shows the details of our simulation code, in Section 3 we describe the experimental works discussed here and compare them with the results obtained in our simulations. The summary and conclusions of the paper appear in Section 4. Atomic units are used except when otherwise stated.

2. Simulation code

We assume that the swift H_2^+ molecule loses its binding electron in the first atomic layers of the foil. The following motion of the resulting proton fragments is governed by

* Corresponding author.
E-mail address: denton@ua.es (C.D. Denton).

0168-583X/$ - see front matter © 2006 Elsevier B.V. All rights reserved.
doi:10.1016/j.nimb.2006.11.104

four main interactions: the stopping force due to excitation of target electrons, the elastic scattering with the target nuclei, the mutual Coulomb repulsion between the fragments (inside or outside the foil) and finally the wake forces produced by the electronic excitations induced in the target by each partner fragment. In the energy range we are considering here ($E \geqslant 0.5$ MeV/u) the fragments of the molecule can be considered fully stripped, so capture and loss processes can be neglected.

Our simulation code uses a finite difference algorithm to follow the trajectories of both protons of a H_2^+ molecule through the foil and in the vacuum until reaching the detector [10–12]. The interaction felt by the fragments are modelled in the following way.

The inelastic energy loss is treated using the linear dielectric formalism. Within this model the stopping force (or stopping power), which represents the mean energy loss per unit path length, takes the form:

$$S_p(v) = \frac{2Z_1^2}{\pi v^2}\int_0^\infty \frac{dk}{k}\int_0^{kv} d\omega\,\omega\,\mathrm{Im}\left[\frac{-1}{\epsilon(k,\omega)}\right], \quad (1)$$

v being the velocity of the projectile, $Z_1 = 1$ its atomic number and $\mathrm{Im}[-1/\epsilon(k,\ \omega)]$ the energy loss function (ELF) of the target.

The ELF of the material gives information about the probability of the different electronic excitations the target can sustain. We have modelled it by fitting the experimental optical ELF, corresponding to the outer electrons, with a sum of Mermin type ELF, whereas the ELF of the inner electrons is described with hydrogenic generalized oscillator strenghts, as described in [12–15]. In our simulations we choose the stopping force at each time step from a Gaussian distribution whose mean value is the stopping power and whose variance is related to the energy loss straggling per unit path length [12,16], both calculated within the dielectric formalism. Higher moments of the energy loss distribution have not been considered in the simulations because they do not affect the calculations presented in this paper, as will be justified later.

The wake force is also calculated within the same formalism as the stopping force. The components of the force induced by one proton i of the molecule and acting on the other j can be expressed in cylindrical coordinates relative to the motion of proton i as:

$$F_z = \frac{2Z_1^2}{\pi v^2}\int_0^\infty \frac{dk}{k}\int_0^{kv} d\omega\,\omega J_0\left(\rho\sqrt{k^2-\omega^2/v^2}\right) \times\left\{\sin\left(\frac{\omega z}{v}\right)\mathrm{Re}\left[\frac{1}{\epsilon(k,\omega)}-1\right]+\cos\left(\frac{\omega z}{v}\right)\mathrm{Im}\left[\frac{1}{\epsilon(k,\omega)}-1\right]\right\}, \quad (2)$$

$$F_\rho = \frac{2Z_1^2}{\pi v}\int_0^\infty \frac{dk}{k}\int_0^{kv} d\omega J_1\left(\rho\sqrt{k^2-\omega^2/v^2}\right)\sqrt{k^2-\omega^2/v^2} \times\left\{\cos\left(\frac{\omega z}{v}\right)\mathrm{Re}\left[\frac{1}{\epsilon(k,\omega)}-1\right]-\sin\left(\frac{\omega z}{v}\right)\mathrm{Im}\left[\frac{1}{\epsilon(k,\omega)}-1\right]\right\}, \quad (3)$$

where z and ρ are the cylindrical coordinates of proton j relative to proton i; J_0 and J_1 are the Bessel functions of zero and first order. For the energies considered in this work the direction of the motion of both fragments is approximately the same in practice, therefore F_z affects the energy loss of fragment undergoing the wake, giving rise to the vicinage effects in the energy loss already mentioned. On the other side, the perpendicular component of the wake force F_ρ tends to change the separation ρ between both fragments in the direction perpendicular to their motion, aligning (or disaligning) both fragments (depending on the sign of F_ρ), with the ion beam direction. Both components of the wake force are much more important behind the particle generating the wake ($z < 0$) and becomes negligible if both particles are far away [17].

The elastic multiple scattering of the dissociated fragments with the target nuclei is considered introducing a Monte Carlo algorithm [18] in our code. The angles of scattering and the distance between successive collisions depend on the energy of each projectile and the atomic density of the target. The interaction potential between the projectile and the target atoms was assumed to be the Universal ZBL potential [19].

3. Results and discussion

3.1. Aligning effects of the wake

In [8] a beam of 0.5 MeV/u H_2^+ of is used to bombard amorphous carbon foils of different thicknesses, ranging from 2 μg/cm^2 up to 30 μg/cm^2. A detector, whose acceptance angle is 0.04° measures the number of aligned pairs or isolated protons arriving at the detector. The solid dots in Fig. 1 depict the experimental ratio between the number of aligned pairs and the number of isolated protons reaching the detector, as a function of the foil thickness. The

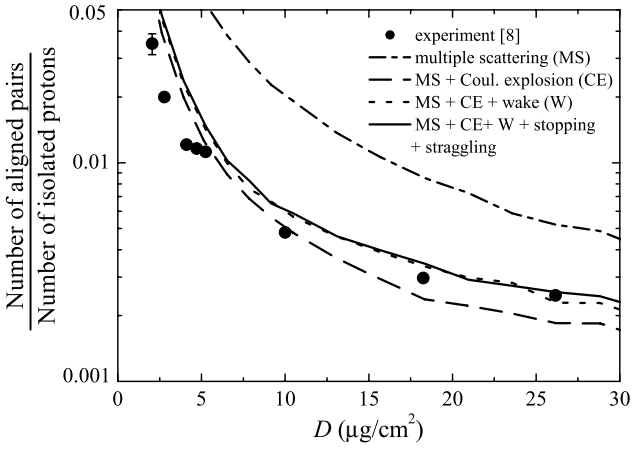

Fig. 1. Number of aligned pairs relative to the number of isolated protons reaching a 0.04° detector, after a 0.5 MeV/u H_2^+ molecule traverses an amorphous carbon foil of thickness D. Solid dots are experimental data [8]; different type of lines represent our simulations when the indicated interactions are taken into account.

lines appearing in Fig. 1 are the results of our simulation when different interactions are considered. Dashed-dotted line represents the case where only elastic multiple scattering is included in the simulation. This interaction changes the direction of motion of the protons, increasing its effect as the thickness of the foil is larger; therefore it reduces the probability that two aligned fragments could reach the detector. The inclusion of the Coulomb explosion inside and outside the foil (dashed line) tends also to disalign the fragments, reducing the number of aligned pairs. Only the inclusion of the wake force (dotted line), which is aligning in the range of separations between the fragments covered by this experiment, tends to align the fragments toward the direction of motion, thus increasing the number of proton pairs reaching the detector. This effect is more noticeable for larger thicknesses. The final inclusion of the stopping power and energy loss straggling (full line) does not change very much the results as the stopping force does not affect the direction of motion of the fragments, only their energy loss; therefore the effect of considering higher moments of the energy loss distribution could be neglected. The curve containing all the above mentioned interactions fits satisfactorily well the experimental data.

3.2. Oscillatory nature of the wake

Ref. [9] describes a two foil experiment where a 14 MeV/u H_2^+ beam is directed toward the foils, which are separated by a distance ranging from 2 μm to 30 μm. The first foil is a very thin amorphous carbon target and its purpose is to strip the electron from the molecular ion. The resulting protons experience Coulomb repulsion while travelling in vacuum until reaching the second target, which is a 20 μg/cm^2 foil of aluminium. Depending on the distance L between the foils, the interproton distance d at the entrance of the second foil will change, due to Coulomb repulsion. An energy detector in the beam direction accepting only particles lying within 0.01 mrad allows to determine the number of trailing protons (N_1) or leading protons (N_2), by analyzing their energy spectrum. Due to the stringent acceptance angle only particles practically aligned with the beam direction will reach the detector. Studying the relative differences between N_1 and N_2 as a function of the foils distance L it is possible to test the aligning effect of the wake force and, besides, show its oscillatory spatial dependence.

In our simulation we assume that the first foil (carbon) only strips the binding electron of the H_2^+ molecular ion and that the pure Coulomb explosion in vacuum increases the distance between the protons. The interproton separation d at the entrance of the second foil (aluminium) can be calculated from the following equation [1,20],

$$\frac{t}{t_0} = \sqrt{\xi(\xi-1)} + \ln\left[\sqrt{\xi} + \sqrt{\xi-1}\right], \tag{4}$$

where $t = L/v$, v being the projectile velocity; $\xi = d/d_0$, $d_0 \sim 2.4$ a.u. is the initial interproton distance [1], $t_0 = \left[M_1 d_0^3/(4Z_1^2)\right]^{\frac{1}{2}}$, and M_1 is the proton mass. The evolution of the proton fragments in the second foil (aluminium) until reaching the detector is studied through the computer simulation code described previously and in more details in [11,12].

In Fig. 2 we have represented the quantity $(N_1 - N_2)/N_2$ as a function of the distance between the foils L. The gray dots with error bars correspond to the experimental results [9] while the black dots (joined by a line to guide the eye) are our calculations. A large number of histories ($\sim 3 \times 10^8$) is necessary to obtain a good statistics due to the stringent acceptance angle of the detector. We observe that even when there is a disagreement in the absolute value of $(N_1 - N_2)/N_2$, the calculations are able to assess the main features of the experimental results, namely the wavelength and the position of minima and maxima, as well as their relative amplitude; all these magnitudes are well described by the simulations and can be understood by properly taking into account the wake forces in the analysis.

Fig. 3 depicts the wake forces induced in an aluminium target by a 14 MeV/u proton and acting on a neighbour proton, for a relative distance between both protons given by $\rho = 5$ a.u. and variable z. The perpendicular force F_ρ is the one responsible for the alignment. We observe that depending on the range of z it can be aligning ($F_\rho < 0$) or disaligning ($F_\rho > 0$). The first maximum of F_ρ corresponds to $z \sim -180$ a.u. and in this case F_ρ tends to disalign the trailing protons, then reducing N_1 and hence giving a minimum in the $(N_1 - N_2)/N_2$ data. The leading protons are not affected by the wake force generated by a trailing proton as F_ρ is practically negligible ahead the trailing proton ($z > 0$). The corresponding distance between the protons in this case can be seen to agree with the first minimum of

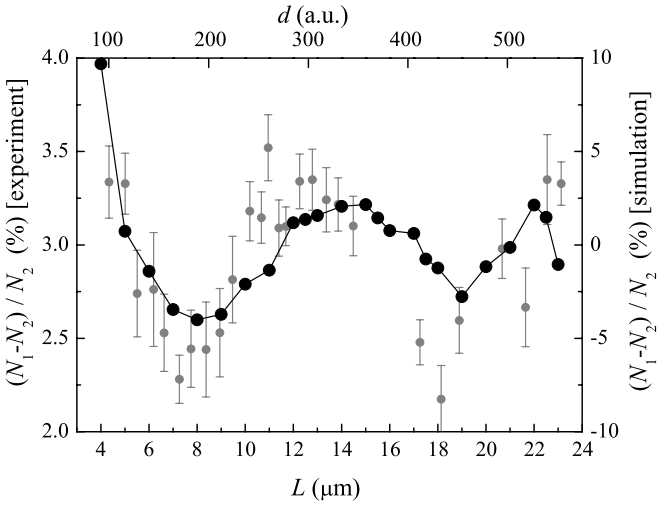

Fig. 2. $(N_1 - N_2)/N_2$ as a function of the distance L between the foils in the experiment [9]. The gray dots are the experimental data while the black dots correspond to the results of our simulation, which are connected by lines to guide the eye. The calculated separation d between the protons at the entrance of the second foil (aluminium) is indicated in the top axis.

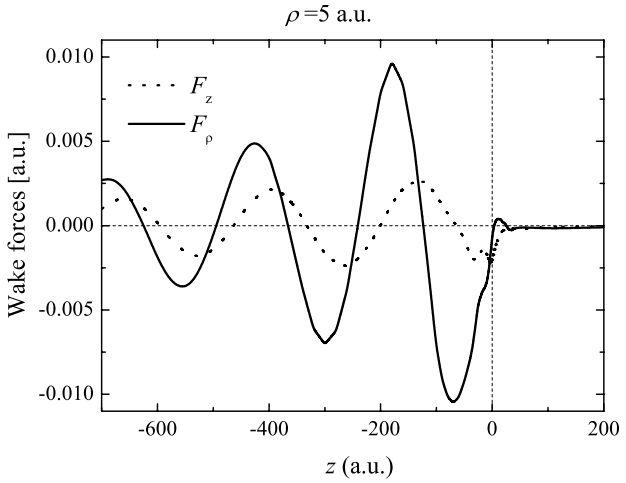

Fig. 3. Components of the wake forces generated in an aluminium target by a 14 MeV/u proton acting on another proton located at the cylindrical coordinates ρ and z relative to the first proton.

$(N_1 - N_2)/N_2$. The next maxima (or minima) of F_ρ also agree with the next minima (or maxima) of $(N_1 - N_2)/N_2$.

4. Conclusions

Many works have been devoted to study the effect of the wake force on the energy loss of the molecular components. However its effect on the spatial distribution of the fragments has not been analyzed so much in the literature [6,7]. In this work we have studied, by means of computer simulations, the aligning effects of the wake force in the dissociated fragments from a H_2^+ molecule traversing thin foils. The results of our simulation are compared with the data of two experimental situations.

In the first experiment the detection of aligned pairs was measured [8]. The perpendicular wake force F_ρ, which is responsible for the alignment of the fragments of the molecule is negative in all cases and so it tends to align the trailing proton towards the direction of the leading proton. The inclusion of this wake force enhances the detection of aligned pairs, being necessary to obtain a agreement with the experimental results.

In the second experiment the number of trailing and leading protons coming from a H_2^+ molecule was measured [9]. As the relative distance between the protons can be adjusted before they enter a target where the wake effects take place, this experiment can test the nature of the wake forces at different distances. Here F_ρ can be aligning or disaligning depending on the relative distance between both protons. The changes in the number of trailing protons can be correlated to the form of F_ρ. The general features of the experimental data, namely the position of maxima and minima, are well reproduced by our simulation.

Acknowledgments

This work has been supported financially by the Spanish Ministerio de Educación y Ciencia (Projects BFM2003-04457-C02-01 and BFM2003-04457-C02-02). SHA thanks the Fundación CajaMurcia for financial support and CDD thank the Spanish Ministerio de Educación y Ciencia for support under the Ramón y Cajal Program.

References

[1] W. Brandt, A. Ratkowski, R.H. Ritchie, Phys. Rev. Lett. 33 (1974) 1325.
[2] N.R. Arista, Nucl. Instr. and Meth. B 164–165 (2000) 108.
[3] E. Ray, R. Kirsch, H.H. Mikkelsen, J.C. Poizat, J. Remillieux, Nucl. Instr. and Meth. B 69 (1992) 133.
[4] C.D. Denton, F.J. Pérez-Pérez, I. Abril, R. Garcia-Molina, N.R. Arista, Europhys. Lett. 35 (1996) 499.
[5] R. Garcia-Molina, C.D. Denton, F.J. Pérez-Pérez, I. Abril, N.R. Arista, Phys. Stat. Sol. (b) 219 (2000) 23.
[6] L. Lammich, H. Buhr, H. Kreckel, S. Krohn, M. Lange, D. Schwalm, R. Wester, A. Wolf, D. Zajfman, Z. Vager, I. Abril, S. Heredia-Avalos, R. Garcia-Molina, Phys. Rev. A 69 (2004) 062904.
[7] R. Garcia-Molina, I. Abril, S. Heredia-Avalos, L. Lammich, H. Buhr, H. Kreckel, S. Krohn, D. Strasser, R. Wester, A. Wolf, D. Zajfman, D. Schwalm, Nucl. Instr. and Meth. B 230 (2005) 41.
[8] Y. Susuki, M. Fritz, K. Kimura, M. Mannami, R. Garcia-Molina, I. Abril, Phys. Rev. A 62 (2000) 012902.
[9] G.J. Kumbartzki, H. Neuburger, H.P. Kohl, W. Polster, Nucl. Instr. and Meth. 194 (1982) 291.
[10] C.D. Denton, R. Garcia-Molina, I. Abril, N.R. Arista, Nucl. Instr. Phys. Rev. A 62 (2000) 012901.
[11] R. Garcia-Molina, C.D. Denton, I. Abril, N.R. Arista, Phys. Rev. A 62 (2000) 012901.
[12] R. Garcia-Molina, I. Abril, C.D. Denton, S. Heredia-Avalos, Nucl. Instr. and Meth. B 249 (2006) 6.
[13] I. Abril, R. Garcia-Molina, C.D. Denton, F.J. Pérez-Pérez, N.R. Arista, Phys. Rev. A 58 (1998) 357.
[14] J.C. Moreno-Marín, I. Abril, R. Garcia-Molina, Nucl. Instr. and Meth. B 193 (2002) 30.
[15] S. Heredia-Avalos, R. Garcia-Molina, J.M. Fernández-Varea, I. Abril, Phys. Rev. A 72 (2005) 052902.
[16] R. Garcia-Molina, M.D. Barriga-Carrasco, Phys. Rev. A 68 (2003) 054901.
[17] M.D. Barriga-Carrasco, R. Garcia-Molina, Phys. Rev. A 68 (2003) 062902.
[18] W. Moller, G. Pospiech, G. Schrieder, Nucl. Instr. Meth. 130 (1975) 265.
[19] W. Eckstein, Computer Simulation of Ion–Solid Interactions, Springer-Verlag, Berlin, 1991.
[20] M.P. Carpenter, R.W. Dunford, D.S. Gemmell, T. Graber, R.V.F. Janssens, E.P. Kanter, J.A. Nolen Jr., Z. Vager, Phys. Rev A 55 (1997) 2090.