Wake forces and the transmission yield of H_2^+ through thin carbon foils

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The transmission of 0.05–1.0 MeV/amu H_2^+ molecular ions has been calculated as a function of dwell time in carbon foils. The results indicate that wake forces may have a notorious influence upon the transmission yields. Experimental results, however, are lacking within the range of dwell time and bombarding energy where wake effects are expected to become noticeable.

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I. INTRODUCTION

Due to the unique possibility offered by molecular ions to investigate the perturbation induced by fast charged particles in solid matter, a number of experiments using molecular beams were triggered late in the 1970s and during the 1980s. Among them the transmission yield of H_2^+ molecular ions through thin C films was measured by several groups around the world [1], as it offered the unique possibility of observing charged atomic particles that arrive at and emerge from the foil as bound clusters.

The theoretical activity on this matter, however, was substantially smaller. This is due in part to the exceedingly difficult problem posed by the motion of the nuclei during penetration. The first attempt to calculate the transmission yield of H_2^+ was carried out by Cue *et al.* [2]. They used what is known as the incoherent approximation, according to which multiple scattering and Coulomb repulsion are treated in a separate manner. That is, the nuclei are first subjected to only the Coulomb repulsion. Afterward, during the same period of time, multiple scattering is turned "on" while the Coulomb repulsion is "off." These results, therefore, are expected to fail at large dwell times, where the interplay between the Coulomb repulsion and multiple scattering may have a large influence upon the recombination probability. Using the Monte Carlo method, Zajfman [3] could readily have Coulomb repulsion and multiple scattering coherently included. Due to the exceedingly small transmission yields, however, Zafjman's results were limited to dwell times not greater than 8 fsec. Moreover, both Cue *et al.* and Zajfman have not taken into account the wake forces in their calculations.

In this paper we present results of the transmission yield for H_2^+ ions through thin C foils calculated using Monte Carlo simulations. These calculations incorporate multiple scattering, energy-loss straggling, Coulomb repulsion, and the wake forces, all of them handled in a coherent manner. Our Monte Carlo (MC) code, which was described in detail elsewhere [4], is quite similar to that in Ref. [3]; the latter however differs from ours in its inclusion of both the wake forces and an advance MC technique that speeds up simulations. Such a technique enables the calculation of transmission yields for dwell times as large as 20 fsec within reasonable running times, even on a 486 personal computer. As we shall see in the following sections, our results indicate that wake forces might have a notorious influence upon the transmission yield. Surprisingly enough, however, available experimental results do not appear conclusive, since they are lacking within the range of bombarding energy and dwell times where wake effects may become noticeable.

II. MONTE CARLO SIMULATION

Although a detailed description of our Monte Carlo simulation program can be found elsewhere [4], we shall briefly describe the most essential ingredients in our simulations. In the first place the initial positions of the nuclei in the incoming molecular ion are selected; to this end we assume that all orientations are equally populated and that the internuclear separation obeys a distribution function like that in Ref. [5]. Then, right at penetration, the molecular ions lose their bound electrons and become subjected to (i) elastic scattering with targets atoms, (ii) energy-loss straggling, (iii) screened Coulomb repulsion, and eventually, (iv) the wake forces.

For computational reasons, the dwell time in the foil is divided into a finite number of time steps. At the beginning of each one, the nuclei undergo both angular scattering and energy-loss straggling. These two processes are assumed to be instantaneous, so that, after scattering and straggling effects are added, the nuclei find themselves moving in their own screened Coulomb field (and, eventually, the wake forces) during the whole time step. The screening by target electrons is approximate by an exponential function of the distance with a screening length obtained as $\lambda_s = v/\omega_p$, where v is the ion velocity and ω_p is the plasma frequency of the electron gas in the solid [6,7]. Similarly the wake potential is approximated, in atomic units, as [8,9]

$$\Phi^{(w)}(z,\rho)=\frac{2Z}{\lambda_x}\sin(z/\lambda_s)(K_0)(\sqrt{\rho^2+v^{-2}}/\lambda_s) \times\exp(z\gamma/2v)\Theta(-z)\ , \quad (1)$$

where (z,p) represent the coordinates parallel and perpendicular to the beam, respectively. Further, Z is the atomic number of the leading nucleus, γ describes the damping of the wake [7], K_0 is the Bessel function of the

second kind and zeroth order, and $\Theta(x)$ is the unit step function.

The motion in the field of the Coulomb and wake potential is handled by an adaptive step-size integration procedure. Here the two-body problem is reduced to a *single* particle representing the relative motion of the nuclei. Analogously, the scattering angle in the laboratory frame of reference, ψ, is obtained as [10]

$$\psi=\frac{2M_1}{(M_1+M_2)\sqrt{1+[1+b(1+b)](2\epsilon b)^2}}\ , \tag{2}$$

with $b=p/a$, where p is the impact parameter, a is the screening radius, ϵ is the reduced energy, and M_1 and M_2 are the ion and target masses, respectively. In each time step two impact parameters are selected, one for each nucleus. The solid is assumed random and the correlation that might exist between the two impact parameters is ignored. Furthermore, angular deflections are assumed to change only the velocity of the nuclei on the plane perpendicular to the beam direction. Similarly, the energy-loss straggling is included by adding a Gaussian-distributed random velocity along the beam direction. The mean value of such a distribution is zero with a standard deviation obtained from the energy-loss straggling data in Ref. [11].

Once the nuclei leave the target, the probability of having a bound molecule is obtained as

$$P_b=\begin{cases}\sigma_c^g/\sigma & \text{if } E_k+U_g(R)\le 0\\ 0 & \text{otherwise,}\end{cases} \tag{3}$$

where E_k is the relative kinetic energy and $U_g(R)$ is the potential energy of the nuclei in the $1s\sigma_g$ electronic state; similarly, σ_c^g is the electron-capture cross section in the mentioned state, which can be approximated by the expression

$$\sigma_c^g=Z_g^5(R)\sigma_c(v)\ , \tag{4}$$

where $\sigma=\sigma_c^g+\sigma_l$; σ_l and σ_c are the electron loss and capture cross section for atomic hydrogen at the same velocity, respectively. The function $Z_g(R)$ represents the effective charge of the two nuclei for the capture into the mentioned bound state of the hydrogen molecule [12].

The transmission yield is finally obtained as the mean value of P_b over a number of such histories. This result is then divided by $2\sigma_c/(\sigma_c+\sigma_l)$ in order to have the relative yield, i.e., $Y(H_2^+)/(2\phi_o)$.

Our MC code is also equipped with a computational technique that increases the efficiency of simulations. It is basically based on the possibility of terminating before completion trajectories that can be anticipatingly termed "bad," while initiating new histories out of those, which, in a similar way, can be assumed to have "good" chances of producing molecules. To compensate for such an artificially enlarged probability of success, a *weight* is assigned to each one of those split trajectories so that the mean yield will suffer no bias. The interested reader is referred to Ref. [4] for more details.

III. RESULTS AND DISCUSSIONS

In Fig. 1 we show the results of experiments together with previous calculations in Refs. [2,3] and those of our own MC calculations. Despite the fact these calculations, including ours, *do not* incorporate the wake forces, the agreement between theory and experiment is however remarkable. Only at large dwell times do the data appear to be slightly smaller than calculations. Further, the "universal" character displayed by the experimental curve [2] is also supported *remarkably* well by our MC calculations, which, it is worth noting, cover a wide energy range, i.e., from 0.05 to 1.0 MeV/amu. According to these results one would be led to conclude that wake effects are either negligible *or* they should become apparent within a range of dwell time and/or bombarding energy different from those in Fig. 1.

In this regard the results of our MC calculations, including wake forces, shown in Fig. 2 appear quite revealing. In the first place, one can see that wake forces break down the "universal" character of the yield curve mentioned above. Second, a sort of envelope curve emerges that drops faster than the no-wake results and, naturally, sets a lower limit for the yield as a function of dwell time. At small dwell time all yields seem to follow such an envelope curve. However, at a dwell time that increases with increasing energy the yields branch off from such a curve to finally approach, or become even larger than the nonwake results at larger dwell times.

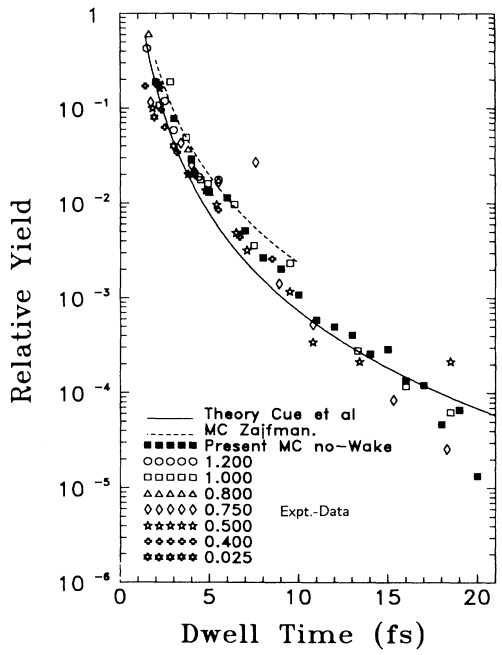

FIG. 1. Relative transmission yield for H_2^+ ions as a function of dwell time in carbon foils. Experiments are indicated by open symbols. Calculations with no wake: our Monte Carlo calculation for 0.05 to 1.0 MeV/amu (full symbols); Monte Carlo calculations of Zajfman [3] (short dashed curve), and the analytical approximation of Cue *et al.* [2] (full curve). Bombarding energies are in MeV/amu.

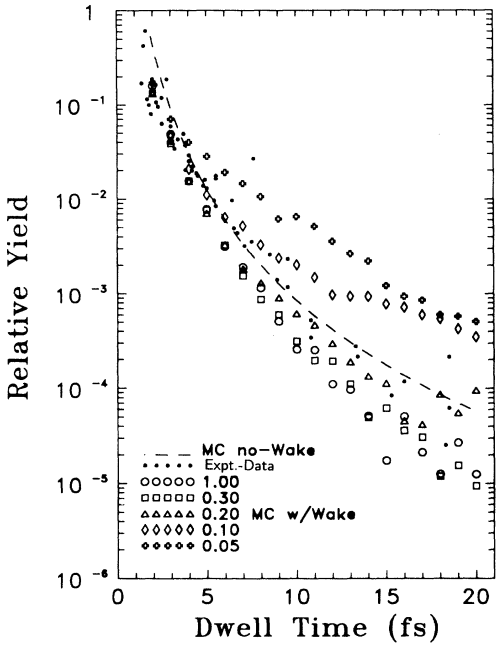

FIG. 2. Relative transmission yield for H_2^+ ions as a function of dwell time in carbon foils. Experiments (solid circles); our Monte Carlo calculations with wake forces (open symbols). For reference, results of our MC calculation without wake in Fig. 1 are replaced by a best-fit broken line. Bombarding energies are indicated in MeV/amu.

A detailed investigation of the origin of these results is still on the way to being finished. They can be explained, at least qualitatively, by figuring the relative motion of the nuclei in the field of the Coulomb and the Coulomb plus the wake forces, respectively. In fact, in Fig. 3 we plot the potential that "sees" the reduced nucleus, i.e., the one that substitutes the two nuclei when dealing with relative positions. Observe that, as far as the motion of the reduced nucleus is concerned, the potential is symmetric against transformation $z \rightarrow -z$, or more physical, against the interchange of the leading and trailing nuclei.

It is obvious that if the wake forces were not present, the nuclei would irreparably "explode" with an intensity that depends on the initial separation. This, together with multiple scattering and energy-loss straggling, is responsible for the monotonic decrease of the relative transmission yield, which can be observed in Fig. 1. In cases where the wake force is "on," our analysis however should be carried out in two parts: At small dwell times, where the nuclei do not appreciably displace, the wake force is *always* working against the recombination of molecules. In fact, looking at contour lines in Fig. 3 one can readily see that the wake potential extends the force field to much larger distances compared to that of the Coulomb repulsion. This implies that, independent of the potential sign, there will be more nuclei subjected to much larger accelerations than the no-wake cases. For example, if there were no wake, all nuclei at separation distances larger than 3 a.u. would see practically no force, whereas if the wake potential were turned on, the same nuclei would find themselves well within the field of the wake. In this regard and contrary to a preestablished idea, the wake appears to affect the nonaligned nuclei as much as the well-aligned ones. Previous arguments may explain the origin of the much stronger decay of the transmission yield with dwell time that one can observe in Fig. 2, particularly at small dwell time and high bombarding energies.

At larger dwell times the possibility for the nuclei of being "trapped" in the well of the wake potential reverses the situation described above. It must be said that for "trapped" nuclei we mean those that have had the possibility of being reflected by the wall of the potential well at least once during dwell time. On analyzing this effect, however, one must look at such a smaller part of the nuclear population from which bound clusters may proceed, rather than at the whole distribution. In fact, despite the potential well's tendency to increase (on average) the kinetic energy of the particles, for " trapped" particles the velocity will necessarily reduce during reflection from the potential well. In this regard, the wake well is clearly

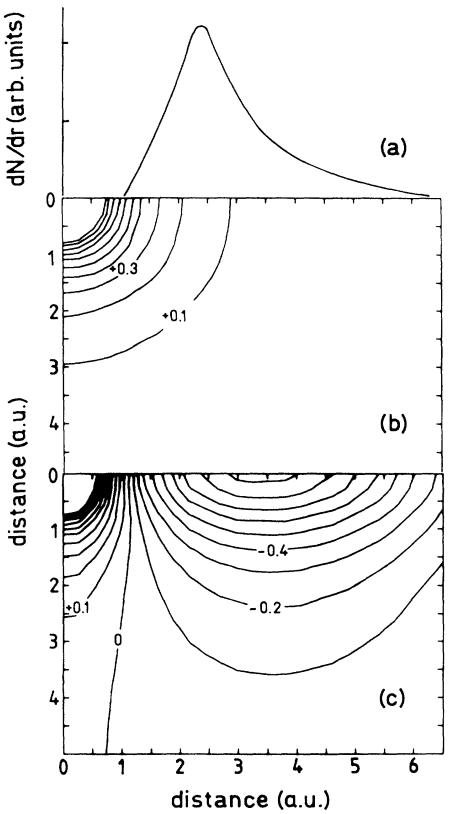

FIG. 3. (a) Separation distribution of the nucleus in the incoming molecules and contour lines of (b) screened Coulomb and (c) screened Coulomb plus wake potential. In the last two plots a unit positive charge is assumed to be exactly at the origin. The wake potential is obtained following the approximation in Ref. [8]. Both the Coulomb and wake potentials are in atomic units and correspond to 0.1 MeV/amu bombarding energy. Distances are in atomic units in all plots except the number of nuclei per unit separation, which is in arbitrary units.

provided with additional means for reducing the nuclei velocity which, otherwise, would solely depend on a "lucky" compensation from among the Coulomb explosion, energy-loss straggling, and multiple scattering.

Now, as the shape of the wake potential depends on the ion velocity, the wake effect previously described will therefore change with the bombarding energy. In fact, the nearest minima of the wake potential are symmetrically located at approximately $z=\pm\pi v/2\omega_p$. Hence, at large energies the wake well will be far away from the most populated part in the initial separation; then a larger dwell time will be required before particles can be trapped into the wake well (see Fig. 3). With a reduction of the ion velocity, on the contrary, the wake minima become nearer the initial separation and, therefore, trapping may start acting sooner or even immediately after penetration. This appears to be the reason for the increase of the yield at larger dwell times and lower bombarding energies.

The obvious question here is: How can it be that such a notorious effect was not observed before? In the first place, it must be mentioned that transmission yields in Fig. 1 are not *actually* at odds with our results. In fact, if one carefully observes Fig. 1 it can be seen that they were all obtained for either high bombarding energies or dwell times where the "splitting" of the yield with energy did not become notorious. Moreover, for data obtained at extremely low energy, as those in Ref. [13], the wake effects as described above cannot be observed unless the measurements extend up to 5 fsec, or beyond. Second, it must be taken into account that measuring the transmission yield implies *absolute* determinations of the fraction of molecules that survive after traversing the foil. Hence, the data in Fig. 1 might well be accompanied by considerable "systematic" errors. In this regard, the change of slope shown by the yields of low bombarding energies appears as a hallmark of the wake forces, which can be determined, even with not-so-accurate absolute determinations.

IV. CONCLUDING REMARKS

In summary, the results of our MC calculations show that wake forces may have a noticeable influence upon the relative transmission yield for H_2^+ ions through C foils. Regrettably enough, it appears that available experimental data cannot resolve the difference between wake and no-wake calculations. In this regard, measurements of the transmission yields between 0.05 and 0.2 MeV/amu and 5 to 20 fsec seem crucial, since according to our results these are the ranges of dwell time and bombarding energy where the wake forces might show the largest effect. For example, the relative transmission yield for a 10 $\mu g/cm^2$ C foil can be measured within the energy range 0.05–0.20 MeV/amu; hence according to Fig. 2 the relative yields should be nearly the same if wake forces are there. Otherwise it should notoriously increase with increasing energy.

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