Wake effects on the energy loss as a function of the scattering angle for thin-film-transmitted H_2^+ ions

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We calculated the mean energy loss as a function of the exit angle for 100 and 400 keV/amu H_2^+ ions transmitted through thin carbon foils. The results showed that at 100 keV the energy loss exhibited a *maximum* in the forward direction as opposed to that of protons, which had a *minimum* at zero degree ejection angle. Our studies demonstrate that such a difference stems from the wake or polarization forces acting upon the trailing ion in the cluster. [S1050-2947(96)01312-1]

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I. INTRODUCTION

Since first reported by Iferov and co-workers and Ishiwari, Shiom, and Sakamoto [1,2], additional experiments and theoretical works have confirmed that the mean energy loss of protons transmitted through thin solid films becomes greater with an increase of the ejection angle [3–6]. This phenomenon, known as the angular dependence of the energy loss (ADEL), originates from the fact that in a collision with a target atom the energy loss becomes greater with a concomitant increase of the scattering angle. As for ions transmitted through thin films the angle of ejection and that of single collisions are to some extent correlated. It is therefore expected in this respect that the mean energy loss would exhibit a minimum downstream in the beam direction.

Several aspects of the ADEL for protons are objects of continuing investigation (see Refs. [3, 6–10]), nevertheless, one may wonder what would be the case if H_2^+ ions were used in place of protons. For molecular projectiles several possibilities arise. For example, if protons in the cluster moved along the target as two independent particles, then the ADEL would be expected to be similar to that of protons. However, as the wake forces may deflect the center-of-mass of the cluster [11], the correlation between scattering and ejection angles may become weakened or distorted, so that the rationale used for protons may not hold in this case. Moreover in connection with this, the wake forces acting alone may have a different ADEL and therefore the resulting energy loss as a function of the angle could be a sort of combination between that of the wake and that of independent protons.

In this paper we present results of classical trajectory Monte Carlo (CTMC) calculations of ADEL for H_2^+ ions transmitted through thin films. Although a complete description of our CTMC code has been given elsewhere [12], let us briefly mention that our CTMC includes elastic scattering with target atoms, exponential screened Coulomb repulsion between the fragments, energy loss straggling, and wake forces (WK). The wake forces are calculated using the wake potential in the Vager and Gemmell approximation [13],

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

where (z,ρ) represent the coordinates parallel and perpendicular to the beam, respectively. Further, Z is the atomic number of the leading nucleus, γ accounts for the damping of the wake [14], K_0 is the Bessel function of second kind and zeroth order, and $\Theta(x)$ is the unit step function. Similarly, the initial internuclear separations were taken from experiments in Ref. [15].

In the present case, however, we assumed that the energy loss *per collision* depends on the impact parameter as

$$Q(p)=Q_0\exp(-p/p_0), \tag{1}$$

where Q_0 and p_0 are obtained from a fitting to theoretical work in Ref. [16]. Moreover, no correlation between the impact parameter of the leading and that of the trailing ion in the cluster was assumed. Although this point was checked by allowing the two ions to have simultaneous interaction with the same target atom provided $p_2<p_{\max}$, where p_2 is the impact parameter of trailing ion and $p_{\max}$ is the maximum impact parameter in a collision. The results indicated that this type of correlation did not produce an observable effect.

II. RESULTS AND DISCUSSION

As is a common practice, we plot the mean energy loss as a function of ejection angle after subtracting that of the forward direction, i.e., $\delta(\theta)=\langle\Delta E\rangle(\theta)-\langle\Delta E\rangle(0)$. Moreover, the cases of transmitted molecules, dissociation fragments, and protons will be denoted as $\delta_{(H_2^+,H_2^+)}(\theta)$, $\delta_{(H_2^+,H^+)}(\theta)$, and $\delta_{(H^+,H^+)}(\theta)$, respectively. In Figs. 1(a) and 1(b) we plot the results of our calculations for 100 and 400 keV protons transmitted through a 415 Å carbon foil. The corresponding Q_0 and p_0 (in atomic units) resulted in 1.2 and 1.14 for 100 keV and, 1.70 and 0.81 for 400 keV, respectively. In the case of 100 keV experimental results from Ref. [3] were plotted in the same figure as full triangles. As one can see, in the two cases the mean energy loss in-

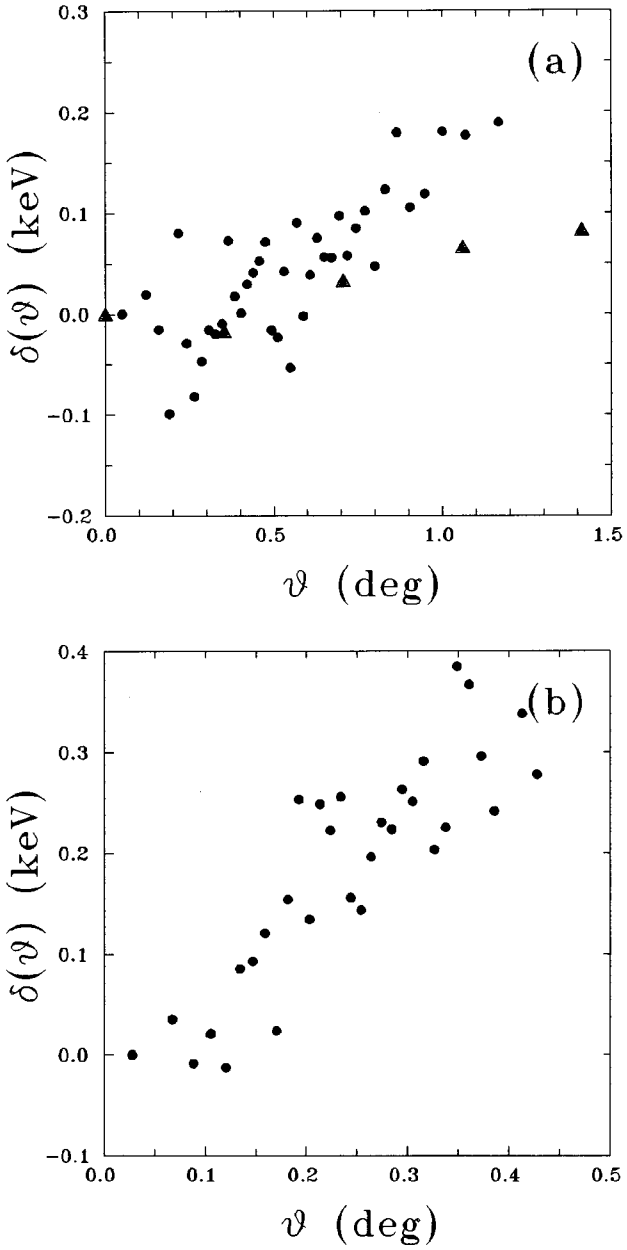

FIG. 1. $\delta_{(H^+,H^+)}(\theta)$ for (a) 100 keV and (b) 400 keV protons traversing a 415 Å carbon foil, respectively. The triangles are experimental results from Ref. [3], whereas circles denote present calculations.

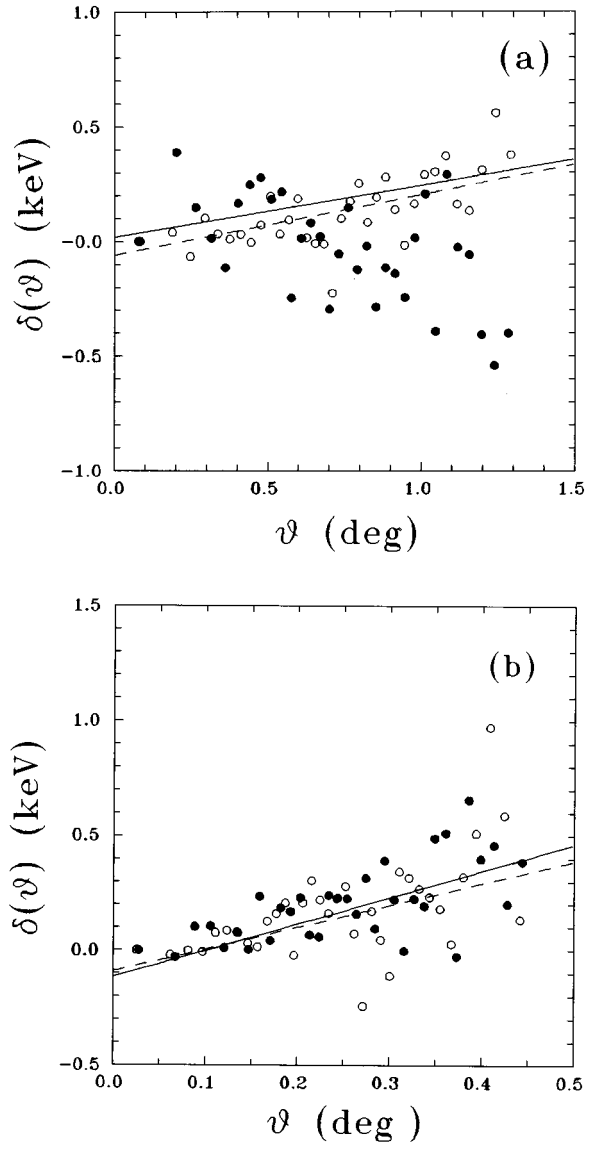

FIG. 2. Calculated $\delta_{(H_2^+,H^+)}(\theta)$ (lines) and $\delta_{(H_2^+,H_2^+)}(\theta)$ (circles) for (a) 100 and (b) 400 keV/amu H_2^+ ions traversing a 415 Å carbon foil, respectively. Both dashed lines and open circles are results of calculating without wake forces, whereas solid lines and filled circles correspond to cases for which the wake forces were included.

creases with an increase of the observation angle and, in the case of 100 keV, calculations compare fairly well with experiments. Only at large angles did calculations appear to be slightly larger than experiments. However, statistical noise at large angles did not allow us to resolve such discrepancies.

In Figs. 2(a) and 2(b) we show the results of calculating the ADEL of transmitted molecules and dissociation fragments under the same conditions as those in Figs. 1(a) and 1(b). In order to avoid a busy plot, however, the results of fragments were replaced by a line representing a fitting to calculations. Observe that the energy loss of the dissociation fragments and protons looks similar irrespective of the bombarding energy, whereas at 100 keV/amu the results for molecules become clearly different. In this case the energy loss becomes largest at $\theta=0$ as opposed to protons, fragments, and even for 400 keV/amu molecules that all have a minimum in the forward direction. Note, however, that after recalculating $\delta_{(H_2^+,H_2^+)}(\theta)$ with the wake forces switched off, the results, plotted as full symbols on the same figure, have the same shape as that of protons, that is, they showed a minimum at $\theta=0$.

These results seem to be not at all unexpected, as recent experiments [17] showed that the ADEL of 50–200 keV H_2^+ ions transmitted through Au films does indeed look different from that of protons. Unfortunately, these cases appear to amount to extremely difficult calculations, since for Au transmission yields and wake forces are both smaller than

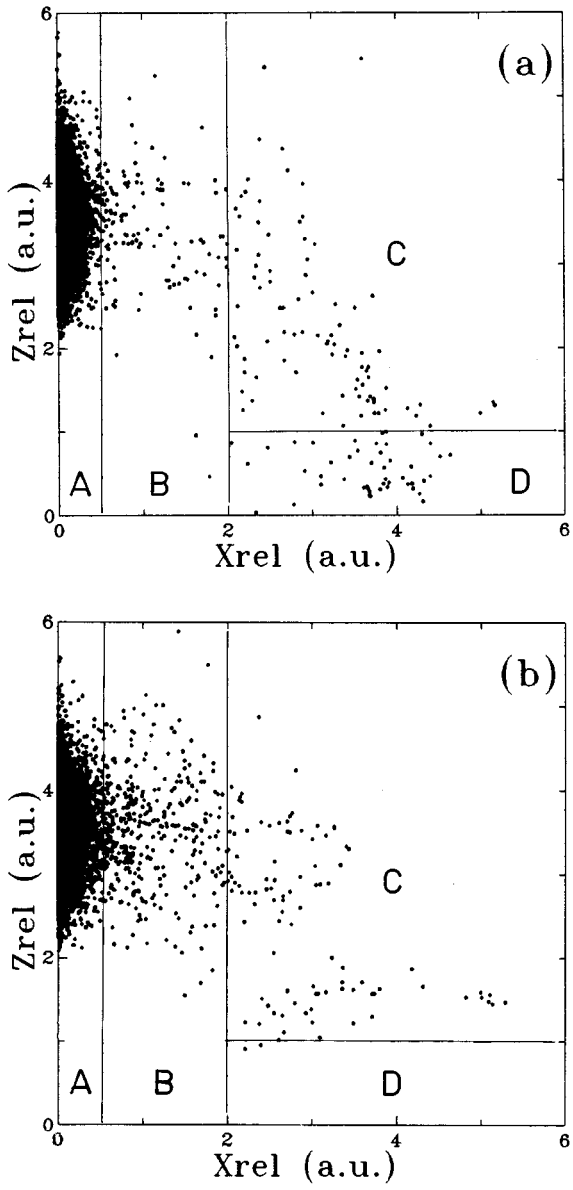

FIG. 3. Relative position of nuclei that led to transmitted molecules in the case of 100 keV/amu, and that were ejected within (a) (0–0.1)° and, (b) (0.5–1.0)° scattering angle. In order to compare between cases (a) and (b) points are grouped into four regions, namely, *A*, *B*, *C*, and *D* (see text).

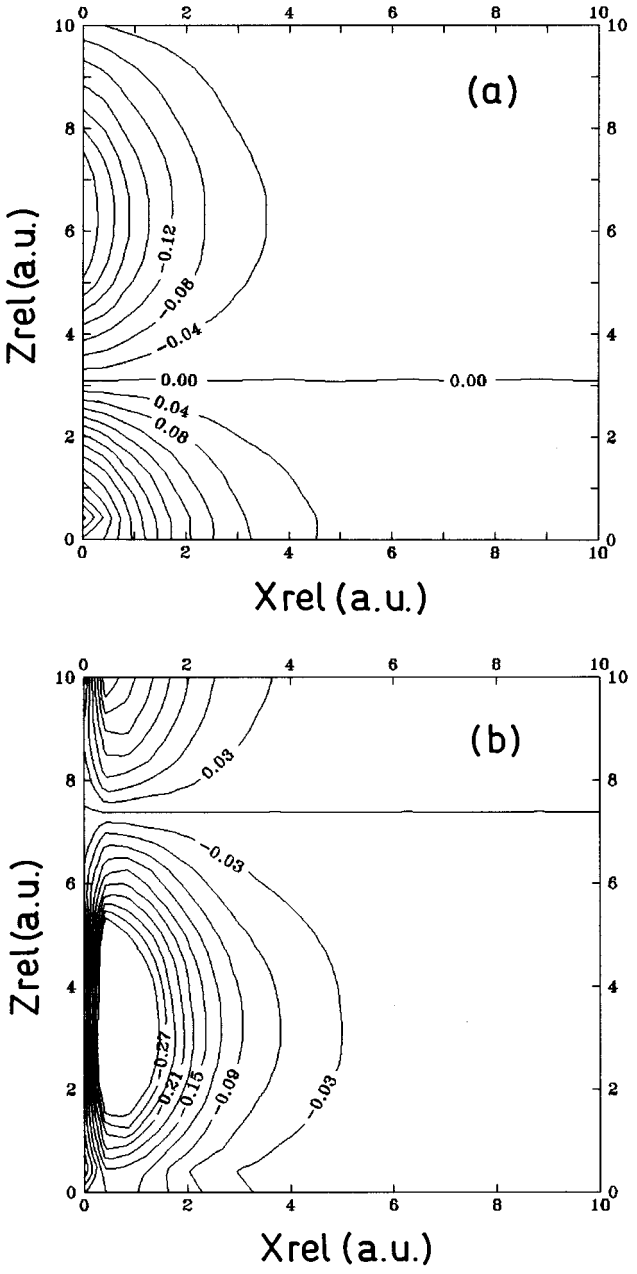

FIG. 4. Contour lines of the wake forces produced by a unit charge (assumed at the origin) moving in a carbon foil with $v=2$ a.u. (100 keV/amu). (a) Force along the beam direction ($F_z^{(w)}$) and, (b) force perpendicular to the beam ($F_\rho^{(w)}$), both in atomic units.

those of carbon. Therefore, obtaining statistically significant ADEL's would demand exceedingly large running times, even for our optimized CTCM code. Moreover in connection with this, it must be recalled that the ADEL amounts to approximately 10% of the total energy loss, and it is not an integrated quantity but a differential one. Therefore one has to calculate the energy loss with an accuracy of 5%, or better along the multiple scattering angular distribution. As a matter of fact, we have found it difficult to calculate the energy loss with a uncertainty better than 5% more or less evenly distributed along 20 channels ranging between zero degrees and two times the half width at half maximum (HWHM) of the angular distribution. The width of the channels were adjusted so as to have approximately 2000 counts per channel. In this manner we could resolve the ADEL fairly well but, nevertheless, the results appeared relatively noisy as one can see in Figs. 1 and 2.

To investigate these results further, we plotted the relative position of the nuclei that had led to molecules in the case of 100 keV/amu [see Figs. 3(a) and 3(b)]. Note that the results for molecules that were ejected within (0–0.1)° are plotted separately from those of (0.5–1.0)°. Moreover, due to symmetry properties in this problem all points were translated into the positive part of the (z,x) coordinates, z being the beam direction. Points on these figures represent the relative position for 2000 histories, along nine equally spaced dwell-

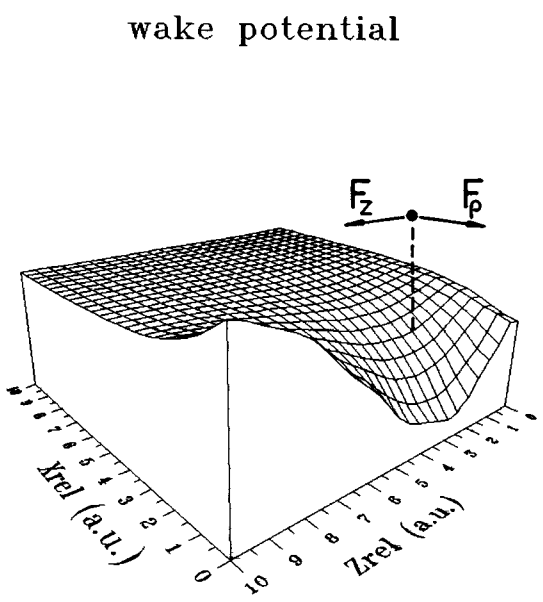

FIG. 5. Parallel ($F_z^{(w)}$) and perpendicular to the beam ($F_\rho^{(w)}$) wake forces, respectively, acting upon the trailing charge in a $E=100$ keV/amu cluster during passage through a carbon target.

time intervals that include both the initial and final separation. Observe that individual trajectories can hardly be identified since successive changes of relative separations are large compared to spatial density.

In the first place, note that in the two cases transmission appears to mainly proceed from nuclei that were within the well of the wake potential. In this regard, it seems that the trailing nuclei were somehow ''trapped'' in the wake well (see Ref. [18] for a longer discussion of this feature). Second, observe that the difference between these two cases, though small, stems from the nuclei that are seen ''off'' the beam direction. In fact, after dividing the (z,x) space into four regions, namely, A, B, C, and D, one can see that regions A and C are almost equally populated in the two cases, whereas in B we counted 173 points in (a) against 497 points in (b). Similarly, for D one finds 107 points at small angles and only two points in the same region for large angles.

By comparing previous results with the lateral ($F_p^{(w)}$) and along-the-beam ($F_z^{(w)}$) wake forces that are plotted in Figs. 4(a) and 4(b) (see also Fig. 5), one can see that clusters ejected at large angles proceeded from regions where, on average, $F_p^{(w)}$ is large and $F_z^{(w)}$ is small. It is thus conceivable that these clusters have undergone both large ejection angles and a small stopping. This was indeed verified by calculating the mean value of these forces for the two cases plotted in Figs. 3(a) and 3(b). Although the difference was small, the $\langle F_p^{(w)}\rangle$ ($\langle F_z^{(w)}\rangle$) corresponding to the cases of large ejection angles were found to be larger (smaller) than those of small angles.

At 400 keV/amu the distribution of the relative initial positions of the transmitted molecules look completely different from those of 100 keV/amu (see Fig. 6). In this case the internuclear axis of transmitted clusters are oriented more or less perpendicular to the beam direction during penetration (see Refs. [18, 19]). In addition, as the minimum in the wake

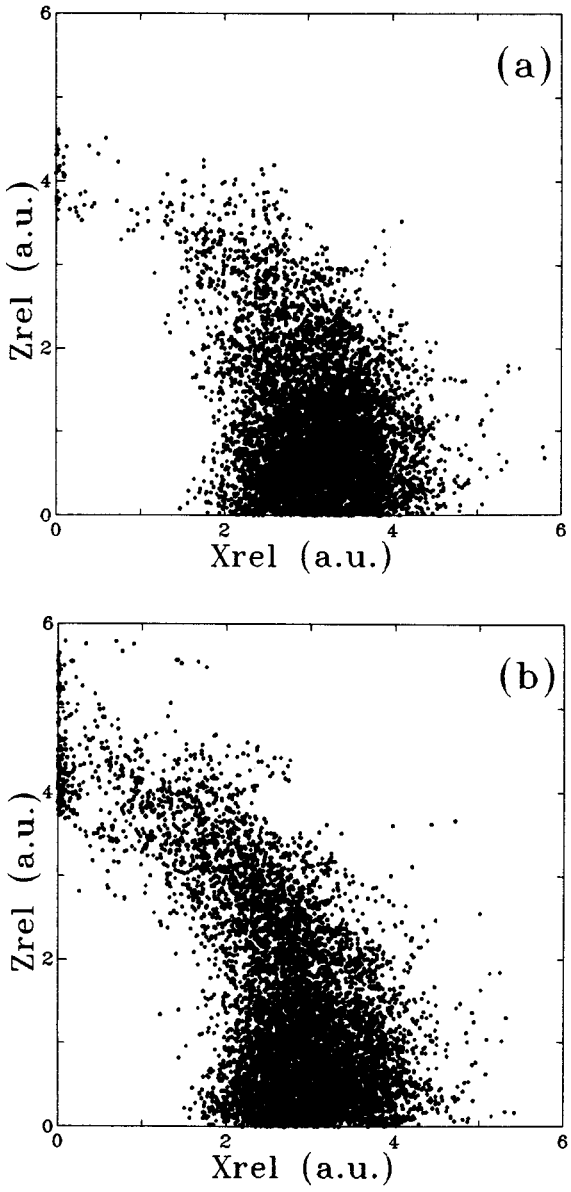

FIG. 6. Relative position of nuclei that led to transmitted molecules for 400 keV/amu bombarding energy and that were ejected within (a) (0–0.1)° and (b) (0.5–1.0)° scattering angle.

potential is further away from the origin, i.e., 7 a.u. [see Figs. 7(a) and 7(b)], the wake forces will act, in all cases, by trying to separate the nuclei by accelerating the trailing ion downstream in the beam direction. Furthermore, as the intensity of the wake force increases as it approaches the z axis, it is clear that transmitted molecules must be ''off'' the beam direction because, there, the wake forces are less efficient in transferring relative kinetic energy and, consequently, less ''destructive'' from the point of view of transmission. Taking into account that lateral forces are also small in these regions, one can readily see that in this case wake forces are less efficient in producing angular deflections. The angular distributions of the transmitted clusters confirm these facts since, at 100 keV the width of the angular distribution for molecules was found to be as wide as that of protons, whereas at 400 keV it became approximately 0.75 times nar-

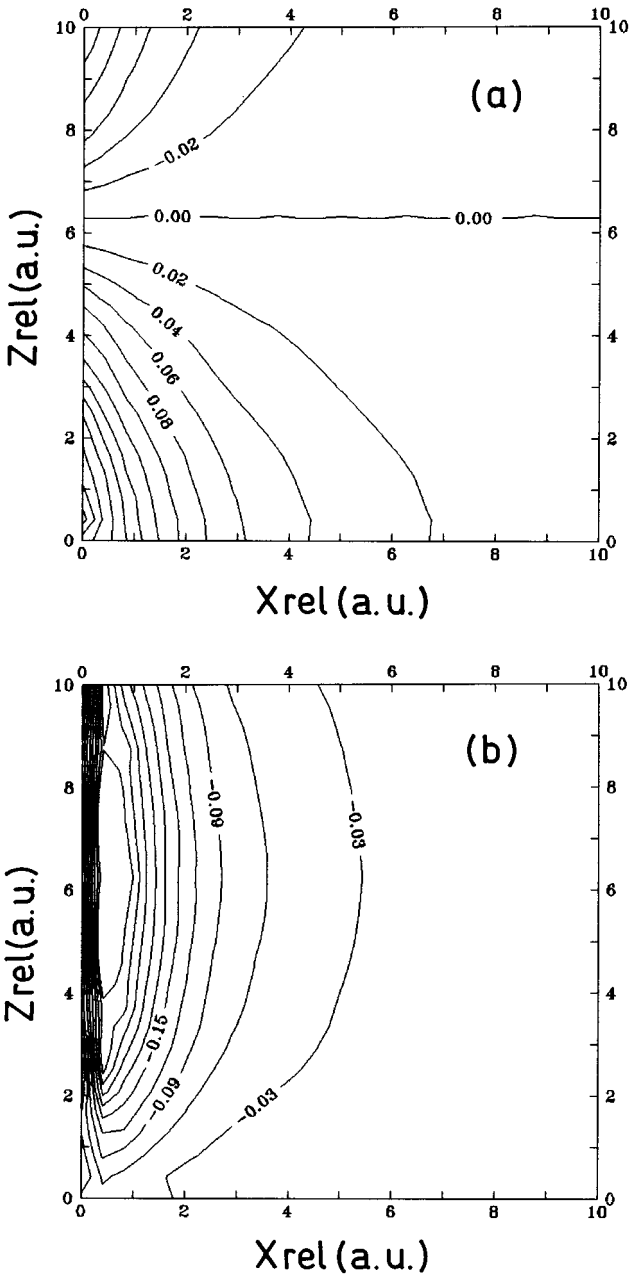

FIG. 7. Same caption as Fig. 4 for $v=4$ a.u. (400 keV/amu).

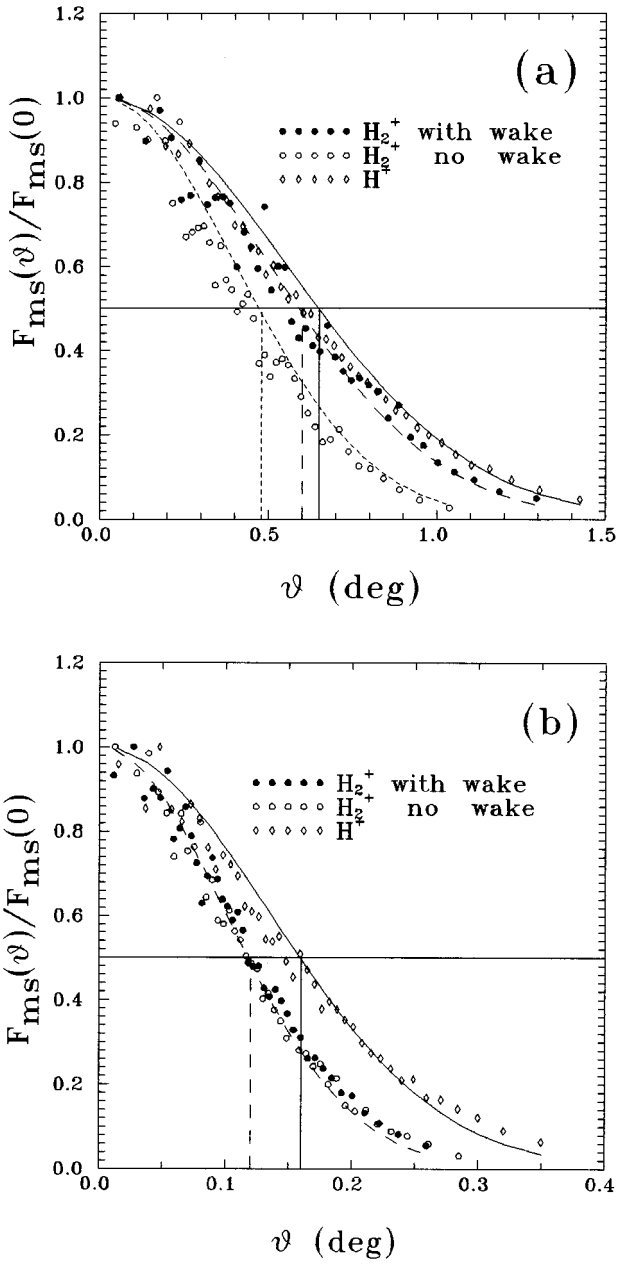

FIG. 8. Multiple scattering angular distribution $F_{ms}(\vartheta)$ for transmitted molecules (open and full circles) and protons (open diamonds). (a) 100 keV/amu and (b) 400 keV/amu. Continuous lines are Gaussian fittings to data, whereas vertical lines indicate the HWHM angle of the distributions.

rower [see Figs. 8(a) and 8(b)].

Observe that at large ejection angles the points extended to both larger z and smaller x values. Therefore, as in this region $F_z^{(w)}$ also becomes larger, then this may account for the larger stopping that is seen at large angles. At small ejection angles, on the contrary, points with large z and small x values are relatively absent. This is related to the fact that $F_p^{(w)}$ increases with a decrease of x, which means that points in this region can seldom be ejected within small angles. As a result, at 400 keV/amu the wake forces become capable of producing a minimum in the mean energy loss down stream of the beam direction, thus reinforcing, but not significantly, that which is caused by $Q(p)$.

III. CONCLUDING REMARKS

Classical trajectory Monte Carlo calculations of the energy loss of transmitted molecules showed that the angular dependence of the energy loss (ADEL) for 100 keV/amu H_2^+ ions transmitted through a 415-Å-thick carbon foil has a maximum around the forward direction. This opposes the ADEL of protons that showed a minimum at zero degree ejection angle. The origin of such a difference was found to be caused by the wake forces, which can produce both deflection and energy loss to the extent that it overrides that of

the impact-parameter-dependent energy loss $Q(p)$. At higher energies the wake effects are seen to change so that the ADEL has, again, a minimum at zero degree. This effect, however, becomes relatively weaker. Therefore, the ADEL of molecules appeared, then, to be nearly identical to that of protons.

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