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Energy loss for electronically elastic atom-molecule collisions in the keV energy range

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An analytical expression is obtained for the average energy loss of atomic projectiles scattered by homonuclear diatomic molecules in the absence of electronic excitations.

Recent experimental works[1,2] have confirmed the theoretical prediction[3,4] that the most probable energy loss T_0 of an atomic projectile scattered by a diatomic homonuclear molecular target without transferring energy to the electronic system is given by

$$T_0=\frac{EM_p\phi^2}{M_T}f(E\theta)\ , \qquad (1)$$

where E, M_p, and ϕ are the energy, mass, and scattering angle in the laboratory system of the projectile, respectively, M_T is the mass of each nucleus on the molecule, and f is an unknown function which depends only on the variable $E\phi$. This function has two well-defined limits; as $E\phi$ decreases, f tends to one half, while for large $E\phi$, f tends to one. This can be easily understood: for large $E\phi$, scattering is so violent that the collision takes place mainly with one atom of the molecule; then obviously, $T_0 \simeq E\phi^2 M_P/M_T$. On the other hand, for small $E\phi$ a "molecular effect" occurs: The projectile is deflected simultaneously by both atoms on the molecule as if they were a structureless particle having an effective mass close to $2M_T$.

Let us recall briefly that Eq. (1) is derived by assuming that the scattering time is short enough such that the motion of the molecular nuclei can be neglected. In addition, it is assumed that there are no electronic excitations and the scattering angles are sufficiently small that the change on the projectile direction of motion can be approximated by a vector perpendicular to the incoming trajectory. Finally, it is shown[3] that the moments of the energy loss obey expressions of the type

$$\overline{T}^n=(EM_p\phi^2/M_T)^n f_n(E\phi),\quad n=1,2,\ldots \qquad (2)$$

and Eq. (1) follows immediately from Eq. (2).

According to Eq. (1) if we plot the quantity $T_0M_T/(EM_p\phi^2)$ as a function of the parameter $E\phi$ we must obtain the f function for the given projectile-target combination; this is experimentally observed.[1,2] Furthermore, it is found that such a function depends on the charge state of the projectile.

We present in this note a simple way to evaluate the function $f_1(E\phi)$ in Eq. (2), and by using the fact that the energy-loss spectrum has a well-defined maximum,[3] we will compare the $\overline{T}^1$ values of our theory with the measured T_0. The calculation is based on the binary interaction between the projectile and each nucleus according to a screened Coulomb potential. We assume that during the collision the nuclei of the molecule remain fixed, that there are no electronic excitations, and that the scattering angles are small. Therefore, we can consider the scattering process projected into a plane perpendicular to the beam direction as shown in Fig. 1. Here 1 and 2 indicate the nuclei of the molecule and their projected separation b; p_1 and p_2 are the impact parameters relative to nuclei 1 and 2, respectively, and ϕ_1 and ϕ_2 are the corresponding scattering angles.[5]

We consider that after the collision the projectile direction of motion is changed by an amount

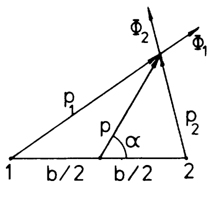

FIG. 1. Schematic diagram showing the scattering process projected into a plane perpendicular to the beam direction.

$$\vec{\phi}_+ = \vec{\phi}_1 + \vec{\phi}_2 \tag{3}$$

normal to the incoming trajectory, and that it has lost an energy given by

$$T = T_1 + T_2 \ , \tag{4}$$

where T_1 and T_2 are the energies transferred to the nuclei 1 and 2, respectively. Sigmund[3,4] has shown that under these approximations the average energy lost in an electronically elastic ion-molecule scattering, at a given deflection angle ϕ, is

$$\bar{T} = \frac{\langle \int d\vec{p}\, \delta(\vec{\phi}^{\,2} - \vec{\phi}_+^{\,2})(T_1 + T_2) \rangle}{\langle \int d\vec{p}\, \delta(\vec{\phi}^{\,2} - \vec{\phi}_+^{\,2}) \rangle} \ , \tag{5}$$

where $\vec{p}$ is the impact parameter of the process relative to a given origin. The brackets mean that the average is performed over all possible molecular orientations, i.e., molecules are oriented at random.

For small scattering angles

$$T_i = \frac{M_p E \phi_i^2}{M_T} \quad (i = 1,2) \ . \tag{6}$$

Therefore

$$\bar{T} = \frac{M_p E \vec{\phi}^{\,2}}{2M_T} \left[1 + \frac{\langle \int d\vec{p}\, \delta(\vec{\phi}^{\,2} - \vec{\phi}_+^{\,2}) \vec{\phi}_-^{\,2} \rangle}{\vec{\phi}^{\,2} \langle \int d\vec{p}\, \delta(\vec{\phi}^{\,2} - \vec{\phi}_+^{\,2}) \rangle} \right] , \tag{7}$$

where

$$\vec{\phi}_- = \vec{\phi}_1 - \vec{\phi}_2 \ . \tag{8}$$

When $\phi << 1$, the impact parameters can be either $p_1 \sim p_2 > > b/2$ or $p_1 \sim p_2 \sim b/2$. It can be shown that the contribution to Eq. (7) of those trajectories having $p_1 \sim p_2 \sim b/2$ is small compared to that of $p_1 \sim p_2 >> b/2$. Therefore we only consider large impact parameters.

Let us introduce the interatomic potential

$$V(r) = \frac{Z_p Z_T e^2}{r} \varphi \left[\frac{r}{a} \right] , \tag{9}$$

where Z_p and Z_T are the atomic numbers of the projectile and target, respectively, e is the electron charge, a is the screening length, and φ is the screening function. Following Lindhard *et al.*[6] we will use the power-law approximation

$$\varphi(r/a) = \frac{k_s}{s} (a/r)^{s-1} \ . \tag{10}$$

The numerical factor k_s is obtained from the fitting of the power law (10) to the interatomic potential. Therefore, it will depend on the screening function and the interval of interatomic distances which dominates the scattering.

According to Ref. 6 we have

$$\phi_i(p_i) = C_s / p_i^s \quad (i = 1,2) \tag{11}$$

where

$$C_s = \frac{\gamma_s k_s a^{s-1} Z_p Z_T e^2}{E} \ , \tag{12}$$

and $\gamma_s = B(\frac{1}{2}, s/2 + \frac{1}{2})$; $B(x,y)$ being the beta function.

Thus if we expand ϕ_+^2 and ϕ_-^2 in a power series of the variable $b/(2p)$, where p is the impact parameter relative to the center of mass of the molecule, and conserve the first nonzero term, we obtain

$$\phi_+^2 \sim 4C_s / p^{2s} \tag{13a}$$

and

$$\phi_-^2 \sim \phi_+^2 [1 + (s^2 - 1) \cos^2\alpha] b^2 / (4p^2) \ , \tag{13b}$$

where α is the angle between p and b.

For a spherically symmetric distribution of molecular orientations, the distribution of the projection of the internuclear vector on the plane perpendicular to the beam is given by

$$N(b)db = \frac{b\, db}{D^2[(1 - b^2/D^2)]^{1/2}} \ , \tag{14}$$

where D is the internuclear distance. Hence we calculate

$$\frac{\bar{T}}{M_p E \phi^2 / M_T} = \frac{1}{2} + \frac{D^2(s^2+1)}{24} \left[\frac{\phi_+}{2C_s} \right]^{2/s} . \tag{15}$$

By defining $\tau = E\phi$ and

$$\tau_0 = \frac{Z_p Z_T e^2}{a} 2k_s \gamma_s \left[\frac{24}{(s^2+1)} \left[\frac{a}{D} \right]^2 \right]^{s/2} \tag{16}$$

we finally obtain

$$\bar{T} / (M_p E \phi^2 / M_T) = \tfrac{1}{2} + (\tau/\tau_0)^{2/s} \tag{17}$$

which gives us an explicit expression for $f_1(\tau)$.

It is worthwhile to notice that τ is related to the $t^{1/2}$ Lindhard's[6] parameter by

$$t^{1/2} \simeq \tau a / (2 Z_p Z_T e^2) \ . \tag{18}$$

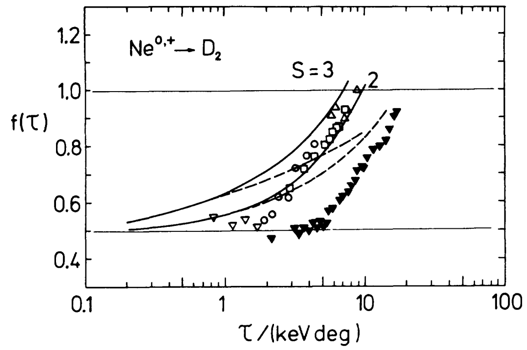

FIG. 2. f function from experiment (Ref. 2): Ne^0 on D_2 at ▽ 0.5; ○ 1.0; □ 1.5; and △ 2.0 keV, and ▼ Ne^+ on D_2 at 3.5-keV bombardment energy. Theory: (——) analytical approximation [Eq. (17)] and (— — —) exact numerical calculation [Eq. (7)] for different s power potentials, respectively.

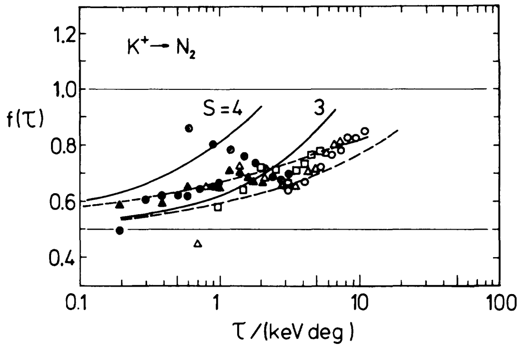

FIG. 3. f function from experimental (Ref. 8): K^+ on N_2 at ○ 1.0; △ 0.7; □ 0.5; ⊙ 0.3; ◬ 0.2, and ● 0.1-keV bombardment energy. Theory: (——) analytical approximation [Eq. (17)] and (— — —) exact numerical calculation [Eq. (7)] for different s power potentials, respectively.

As was pointed out in Ref. 6, $t^{1/2}$ is a measure of the distance of approach between the two collision partners; therefore, its value determines which s should be appropriate.[6] For instance, the experimental results of Refs. 1 and 2 lie in the $10^{-2}<t^{1/2}<2.10^{-1}$ range, then $2 \lesssim s \lesssim 3$ is suitable. In addition, we choose $k_s=0.831$ and 5.22 for $s=2$ and 3, respectively, corresponding to a Thomas-Fermi Coulomb screened potential.[6] We show in Fig. 2 the comparison of our results given by Eq. (17) and experimental data.[1] As was pointed out, we approximate $f(\tau)$ by $f_1(\tau)$. Our calculation shows that the weaker the screening, the stronger the molecular effect due to the larger probability that the projectile can be deflected by both atoms on the molecule. On the other hand, if there were no screening it would be unlikely for the projectile to interact with one nucleus without being significantly influenced by the other. The preceeding discussion gives a clue to understand the difference between the Ne^0 and Ne^+ cases. The lack of one electron when Ne^+ is the projectile could affect the interatomic potential,[7] that is, the screening function. Therefore we must expect that for highly ionized projectiles the $f(\tau)$ function will deviate from 0.5 at much larger τ values.

In Fig. 3 we show the results from Ref. 8 for K^+ on N_2. In this case $t^{1/2}$ ranges from 1.4×10^{-4} to 7×10^{-3}, therefore a larger s value should be appropriate, that is $3 \lesssim s \lesssim 4$. At those high s values the Lenz-Jensen screening function may be more suitable than Thomas-Fermi to describe the interatomic potential;[6,9] hence, we choose $k_s=3.06$ and 20.5 for $s=3$ and 4, respectively.[9]

We have evaluated Eq. (7) numerically in order to check the analytical expression given by Eq. (17). The results are depicted in Figs. 2 and 3. Such a numerical calculation takes full account of all possible impact parameters, even though at small τ there is no deviation from our approximate solution (17); at large τ, however, discrepancies become important. It is due to our assumption given below Eq. (8) which fails at large τ; that is, as τ increases it is not always true that there are two impact parameter regions, viz., $p_1 \sim p_2 \sim b/2$ and $p_1 \sim p_2 >> b/2$. On the contrary, at not too small projected separation b (i.e., $b \sim D$) large values of τ arise from $p_1 \sim b$, and $p_2 << b/2$, and vice versa. In those cases the truncated expansions in (13) are unreliable.

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