Double impulse effects during a collision of ions and diatomic molecules

M. Nakamura[1] and A. Ichimura[2]

[1] *College of Science and Technology, Nihon University, Funabashi*
[2] *Institute of Space and Astronautical Science, JAXA, Sagamihara*

Presenting Author: mooming@phys.ge.cst.nihon-u.ac.jp

In large angle scattering of ions (atoms) from diatomic molecules at hyperthermal incident energies (1-100 eV), short range repulsive forces play dominant roles in the energy transfer from translational to internal degrees of freedom. In such a collision, the hard-potential model [1-2] or the hard-shell model [3] well describes the mechanism of the energy and angular momentum transfer. These models assume that an impulse is exerted at a point on the hard-shell, which is given by the equipotential surface at the collision energy. If the incident energy is almost exhausted by the first impulse, the 'second impulse' would be possible to occur during a single collision event [4]. In fact, Tanuma *et al.* [5] reported a structure which cannot be explained by these models in the energy-loss spectrum of Na^+- N_2. They presented a possibility of the 'double impulse' effect through an analysis based on the classical trajectory calculation.

In the present work, we investigate the double impulse effect within the framework of the hard-shell model. We calculate systematically trajectories of ions scattered by molecules with varying projectile mass and shell anisotropy at an incident energy of 1 a.u. The shape of the shell is assumed to be a sum of monopole and quadrupole deformations as $r_s(\gamma) = r_0(1 + \beta_2 P_2(\cos\gamma))$. In Figure 1, we draw trajectories of K^+ scattered by N_2 as an example. We take a fixed-in-space molecule before the first impulse and switch the frame rotating with the molecular axis after the impulse. As shown in the right panel of the figure, we see that a trajectory hits the shell again after the first impulse when the anisotropy of the hard-shell is larger ($\beta_2 = 0.4$) . Such an event is not observed in the left panel where the anisotropy is smaller ($\beta_2 = 0.3$). The double impulse effect is observed in the collision where the ion is heavier than the molecule and the anisotropy of the interaction potential is strong.

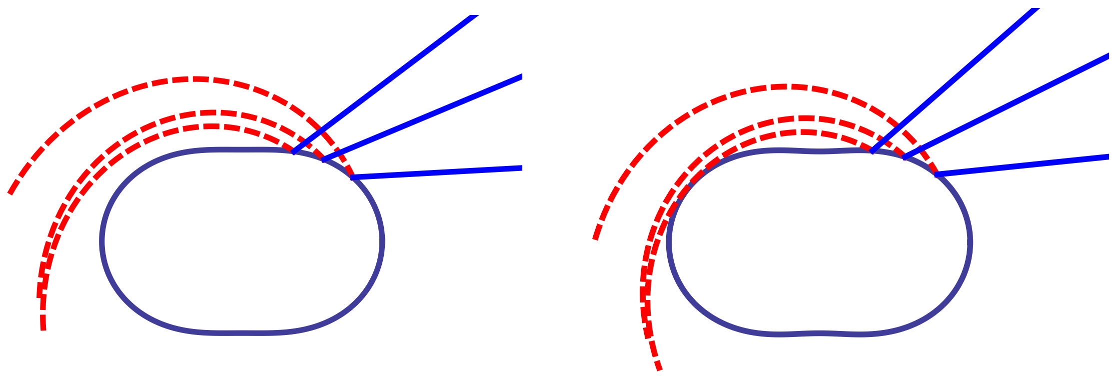

Figure 1: *Trajectories of K^+ scattered from N_2 by the hard-shell model. Solid lines and dashed curves indicate the incident and the scattered orbits, respectively, in a molecular frame. In the left (right) panel, β_2, the anisotropy of the hard-shell is 0.3 (0.4).*

References

[1] A. Ichimura and M. Nakamura, Phys. Rev. A **69**, 022716 (2004)
[2] M. Nakamura and A. Ichimura, Phys. Rev. A **71**, 062701 (2005)
[3] D. Beck *et al.* Z. Phys. A **293** 107 (1979)
[4] D. Beck *et al.* Chem. Phys. **126** 12 (1988)
[5] H. Tanuma *et al.*. Phys. Rev. A**38** 5053 (1988)