In large-angle scatterings of an ion by molecule, a short-range repulsive force plays a dominant role. Since the collision time is much shorter than the rotational period, we can specify an orientation angle $\theta$ between two Jacobi coordinates at an instant of a collision. When the collision energy is sufficiently low (less than a few eV), only rotational excitation is possible since the vibrational period is much faster than the collision time. The rotational energy transfer from the translational motion is essentially determined by the orientation angle $\theta$. This stereodynamic effect on rotational excitation has been observed as a double peak (rotational rainbow) structure in energy-loss spectra.

If the collision energy becomes higher, the collision time is shorter than the vibrational period. In such a case, the sum of rotational and vibrational excitation energies is expressed as a function of the orientation angle. The energy loss spectrum thus reflects the stereodynamic effects in both rotational and vibrational excitations. We have proposed a model to incorporate such an ideal situation [1]. Through the model, it is found that a stereodynamic effect in vibrational excitation manifests itself as a shift of the peak positions in the double peak structure.

We make an analysis of energy-loss spectra of Li$^+$ scattered from N$_2$ in the collision energy of 8 - 100 eV in the center-of-mass system [2]. We calculate the energy-loss spectra from our model and the classical trajectory calculation and compare with experiments. We find through a systematic analysis that, when the collision energy is as low as 10 eV, only rotational excitation is observed in the energy-loss spectra, vibrational excitation being negligible [3]. When the collision energy is as high as 100 eV, on the other hand, vibrational excitation also contributes to the experimental spectra, where the stereodynamic effects appear in both rotational and vibrational excitations [4].

References