§11. Study on Vibrational Transition and Dissociation in He + H$_2$

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It is essential to have reliable collision data relevant to divertor plasma, when one intends to design efficient gas cooling divertors. Some important collision processes are those between H$_2$ molecules and H, He, H$_2$, or their ions. It is highly probable that H$_2$ in divertor plasma are in vibrationally excited states. There is few studies on collision processes related to vibrationally excited H$_2$. In order to understand collision dynamics of vibrationally excited molecules with atoms or molecules and to supply such collision data, we have started investigation of those collision processes.[1]

Here we have investigated vibrational transition and dissociation of H$_2$ caused by He impact in the range of the total energy 0.5 - 7.5 eV. All vibrational states of H$_2$ have been taken into account as an initial state. Our collision system is restricted to T shape configuration, that is, the He approaches along the line bisecting the H$_2$ internuclear distance and all the particles remain in a plane during collisions. We have approximated the dissociative continuum states by a set of discrete states which are defined by confining a vibrational motion of H$_2$ in a box. We applied the standard close coupling method to solve Schrödinger equation of our collision system.

Figure 1 shows representative probabilities of elastic scattering, vibrational transition, which is the sum of excitation and de-excitation, and dissociation processes as a function of the total energy. The initial vibrational state is chosen to be n = 6. Vibrationally inelastic scattering is dominant over the elastic scattering at the total energy above 4.5 eV. Dissociation probabilities for n = 1 -10 are shown as a function of the total energy in Fig. 2. Increasing vibrational energy is more efficient than increasing collision energy to dissociate H$_2$. Dissociation from n = 0 is neg-

ligibly small, though the total energy is far beyond the dissociation energy. Detailed results and discussion are presented in our papers.[2]
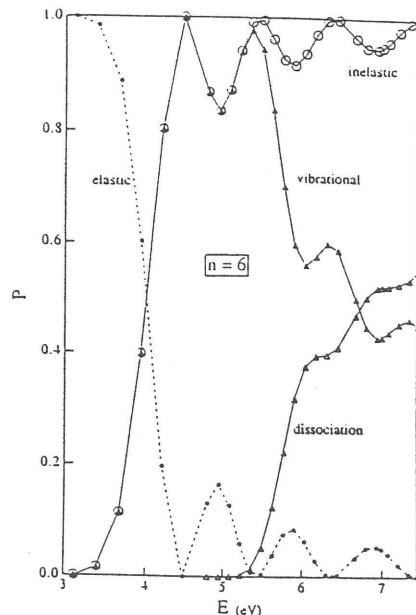

Fig. 1. Probabilities for the elastic (closed circles), inelastic (open circles), vibrational transition (closed triangles), and dissociation (open triangles) processes as a function of the total energy.
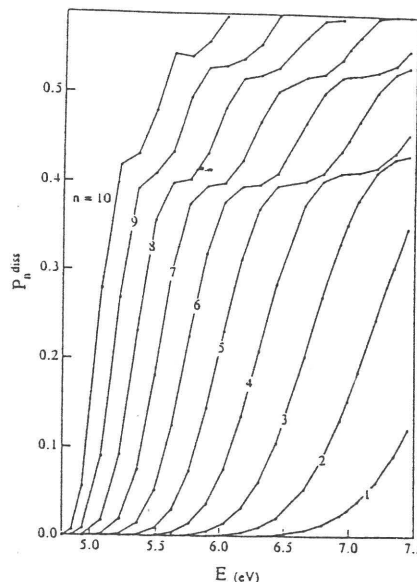

Fig. 2. Dissociation probabilities for n = 1 - 10 as a function of the total energy.

References
1) K. Onda, J. Phys. B **24** (1991) 4509.
2) K. Nobusada, K. Sakimoto, and K. Onda, Chem. Phys. Letters **216** (1993) 613; submitted for publication.