§20. Study of Elementary Collision Processes Related to Vibrationally Excited Molecules

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In a presently pursued fusion reactor such as ITER, one of unresolved problems is how efficiently to exhaust thermal power and the He ash from the reactor region without degradation of the main plasma burning conditions. A plausible solution is sought in the enhancement of longitudinal plasma power and particle flows in the reactor chamber periphery located outside the main plasma torus. This intense directional scrape-off plasma flow concentrates large heat and particle loads on the flux intercepting material surfaces in the divertor chamber. Reduction of these loads can be achieved by using atomic and molecular collision processes in the divertor region. Main components in the divertor chamber are H_2, H, He and their isotopic variance and their ions. It is highly probable that H_2 molecules are in vibrationally excited states. It is thus important to investigate collision processes related to vibrationally excited H_2 molecules.

Our method,[1] by which the Schrödinger equation describing collision processes between an atom and diatomic molecule is numerically solved with quantum mechanically sufficient accuracy, aims specifically at investigating chemical reaction and dissociation of the target molecule, and has been applied to a collinear collision of He and $H_2^+(v_i)$ and their isotopic combinations. The energy dependence of the dissociation and reaction probabilities has been studied at the total energy up to 10 eV, and interesting numerical results have been obtained.[2] In order to understand deeply these results in the physical point of view, we have further investigated the collision process of He and $H_2^+(v_i)$ by dividing the interaction potential into two parts, that is, the one consisting of the sum of two body interaction potentials and the other consisting of the sum of many body interaction potentials except for two body ones.

If we employ the full interaction potential, we have obtained the following results. Probabilities of vibrationally inelastic scatterings without any exception become smaller for all of the initial vibrational states at the total energy from the dissociation threshold to 10 eV. The probability of dissociation process for $v_i \leq 4$ is very small, and the collision almost always ends up with a formation of HeH^+, even if the total energy is increased up to 10 eV. If the initial vibrational state is above $v_i = 11 \sim 13$ depending on the total energy, the dissociation of the H_2^+ ion becomes the main process.

On the other hand, if we take into account only two body part as the inteaction potential, only vibrationally inelastic scatterings dominate over the dissociation of $H_2^+(v_i)$ for the initial vibrational state below $v_i = 4$. The atom rearrangement process is almost completely suppressed for $v_i \leq 4$, and competes with the dissociative one for $v_i = 5 \sim 10$ at the total enegy up to 10 eV.

These results show that the atom exchange reaction has been decisively caused by many body interactions in the collision of He and $H_2^+(v_i)$ for $v_i \leq 4$, and give us an insight into physically understanding mechanism of chemical reactions in collision between an atom and molecule. For $v_i \geq 5$, two body interaction plays almost the same role as many body interaction in atom rearrangement and dissociation of the molecule. Dissociation of the molecule in $11 \leq v_i$ can be caused mainly by two body interaction potential.

A description of our method, further details on these findings, and a full discussion of results shall be published soon.[2]

References
1. K.Sakimoto and K.Onda, J.Chem.Phys. **100** (1994) 1171.
2. K. Onda and K. Sakimoto, in preparation.