§7. Theoretical Study of Elementary Collision Processes Related to Vibrationally Excited Molecules: A Case Study of a Collinear Collision of H with H_2 (v_i)

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One of unresolved problems in a presently pursued fusion reactor such as ITER is how we can efficiently exhaust thermal power and the He ash from the reactor region without degradation of the main plasma burning conditions. The enhancement of longitudinal plasma power and particle flows is considered to be a plausible solution of this problem 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, 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.

We numerically solve the Schrödinger equation[1] describing collision processes between an atom and diatomic molecule with quantum mechanically sufficient accuracy. We have applied our method to a collinear collision of H with $H_2(v_i)$ and their isotopic combinations, and specifically aim at investigating chemical reaction and dissociation of the target molecule in this collision system. The energy dependence of the dissociation and atom exchange 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 H 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. Non-reactive vibrational transition process dominates over the atom exchange reaction and dissociation processes for the initial vibrational states below $v_i \leq 4$ at the total energy up to 10 eV. The probability of the dissociation process for $v_i \leq 4$ is very small, even if the total energy is increased up to 10 eV, which is higher than about 2 times of the dissociation energy. The reaction probability is also small for all the initial vibrational states of H_2 at the total energy above the dissociation threshold. This small reaction probability for the collision of H with $H_2(v_i)$ contrasts with the large one[3] for the collision of He with $H_2^+(v_i)$. This should be understood by taking account of the difference in the non-additive many body interaction potentials between these two collision systems.[4] If the initial vibrational state is above $v_i = 11 \sim 13$ depending on the total energy, the dissociation of H_2 becomes the main process. The probability of the non-reactive vibrational transition process is larger than that of the atom exchange reaction for these initial vibrational states.

A description of our method, further details on these findings, and a full discussion of results shall be published soon.[2] Difference in collision dynamics between He + $H_2^+(v_i)$ and H + $H_2(v_i)$ will be further discussed and reported in detail.[4]

References

1. K.Sakimoto and K.Onda, J.Chem.Phys. **100** (1994) 1171.
2. K. Onda, in preparation.
3. K. Onda and K. Sakimoto, submitted for publication.
4. K. Onda and K. Sakimoto, in preparation.