THEORETICAL ATOMIC PHYSICS FOR FUSION: LOW ENERGY ELASTIC AND INELASTIC ATOMIC AND MOLECULAR COLLISIONS

P. S. Krstić and D. R. Schultz

Atomic and molecular processes that are of critical need in fusion energy research are addressed in this ongoing program of research by calculating the relevant cross sections and rates for which the information is either incomplete or of insufficient accuracy. Speifically, the currently favored concept for power exhaust from a fusion reactor relies heavily on intense impurity radiation cooling at the plasma edge and on dissipation of plasma momentum through elastic and charge-exchange collisions of plasma ions with the neutrals in the divertor chamber. The low plasma temperatures prevailing in the divertor region (as low as a few eV near the divertor plates) support existence of non-dissociated molecular species, neutral atoms and low charge states of impurity ions, defining a medium with very rich and complex atomic physics. The hydrogen atoms and molecules constitute the main portion of the neutral gas. Helium atoms and ions, the ash produced by fusion are also present. The momentum transfer (diffusion) and charge exchange processes of the plasma ions (H^+) colliding with the neutrals (H, H_2, He) in the divertor are responsible for the dissipation of plasma momentum in the region far from divertor plates.

We are performing extensive quantum-mechanical calculations of the elastic, momentum transfer, and charge exchange cross sections for the hydrogen isotope ion-atom systems (e.g., H^+ + D, D^+ + D, D^+ + T) in the energy region below 100 eV. Similar calculations have been performed for the neutral-neutral collision systems (e.g., H + D, D + D, D + T). Momentum transfer cross sections involving collisions of hydrogen atoms, ions and molecules with H_2 in all isotopic combinations have been calculated, with the inclusion of all energetically accessible vibrationally excited channels. The elastic cross sections for other fusion relevant collision systems (e.g., involving He atoms) are being analyzed. Thus we have compiled a comprehensive source for all ion-atom/molecule elastic, momentum transfer and charge exchange differential and integral cross sections, which has been prepared for publication and made accessible through the WWW.

The establishment of the detached plasma regimes in the divertor, which is essential for minimization of plasma-divertor plate interaction and the associated material erosion, can be facilitated by inclusion of a certain fast volume recombination mechanism. One of the reaction schemes proposed is ion conversion, which involves electron capture by protons from vibrationally excited H_2, followed by dissociative recombination of H_2^+ with plasma electrons. The lack of cross section information for many of the processes involving vibrationally excited molecular states does not presently allow construction of a collision-radiative model for the H_2/H gas impeding crucial plasma studies.

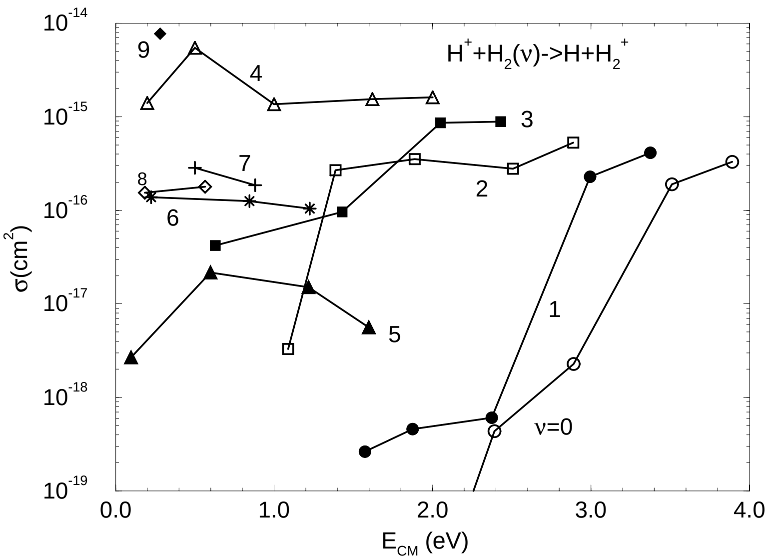

Fig. 1. Cross sections for electron capture by proton from vibrationally excited H_2.

Our preliminary calculations show that the ion conversion recombination mechanism has a relatively large rate coefficient, larger than 4x10^{-9} cm^3/sec for electron temperatures $T_e \leq 5$ eV. Above that energy the dissociative channel by proton impact on $H_2(\nu)$ effectively competes with the ion conversion process. The large rate coefficient of the dissociative reaction by electron impact for $\nu \geq 4$ in the region above 5 eV also indicates that the ion conversion recombination mechanism should be operative only in the regions with $T_e \leq$1-2 eV (close to walls and divertor plates).