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Collision Database for Low-T Hydrogen Plasmas

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Abstract

A comprehensive cross section database for collision processes between constituents of a low-temperature, low-density hydrogen plasma e, H^+, H, H^-, H_2, H_2^+, H_3^+ is established. The processes involving electronically and/or vibrationally excited reactants or reaction products are also included in the database. The presented data information is based on critical assessment of the available experimental and theoretical data, and on the use of well established scaling relationships or relatively simple theoretical models for generation of cross sections when such were not found in the literature. All derived cross sections are represented by analytic fit functions that have physically correct energy behavior at both low (near threshold) and high collision energies. The database, however, still contains gaps for certain important state-selective collision processes required for constructing a complete H/H_2 collision-radiative model.

Keywords:

collision process, cross section, hydrogen plasma

1. Introduction

The understanding of spectroscopic, transport and other properties of low-temperature hydrogen plasmas requires detailed knowledge of collision and radiative processes that take place in such plasmas. The constituents of pure hydrogen plasmas with temperature in the range 0.01 – 300 eV and densities below $\sim 10^{15}$ cm^{-3} include e, H^+, H, H^-, H_2, H_2^+, H_3^+, where H and H_2 may be in electronically excited states, and H_2 (and H_2^*), H_2^+ and H_3^+ may be ro-vibrationally excited. The large number of states associated with the internal degrees og freedom of neutral and molecular hydrogen species makes the collision kinetics of hydrogen plasmas extremely complex. On the other hand, the role of excited species in a hydrogen plasma is obviously of paramount importance, as evidenced by the spectroscopic observations (frequently also used as plasma diagnostic tools [1,2]), and collision processes of excited species with plasma electrons, protons and ground state atomic and molecular species must be included in the collision kinetics scheme to determine their populations. Another feature of electronically or (ro-)vibrationally excited species is that the cross sections for many of their collision processes are significantly larger than those for corresponding processes involving ground state species. Moreover, the thresholds of inelastic processes and all related collision characteristics (e.g., energy and angular distributions of reaction products) have a strong dependence on the excited state energies and consequently, significantly affect the plasma energy and momentum transport [3].

In the present contribution we describe a H/H_2 collision database that includes cross section information for collision processes of both ground state and electronically and vibrationally excited hydrogen plasma constituents. A detailed account of this database is given elsewhere [4]. We should mention that the earlier attempts to construct a H/H_2 collision database either do not adequately describe the processes with vibrationally excited molecular species [5], or do not include all important collision processes and the most accurate cross section information [6,7].

2. Collision processes in low-T hydrogen plasmas

2.1 Collision processes of H ($n \geqslant 1$)

The collision processes of ground state ($n = 1$) and excited ($n > 1$) hydrogen atom with plasma electrons and protons include: excitation, ionization, transitions between excited states, radiative and three-body recombination, and charge transfer (in the proton impact case). The proton impact excitation and ionization processes have small cross sections in the energy region pertinent to low-T plasmas (as defined above), except for the high-n states. However, due to its resonance

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character, the charge transfer is a powerful process at low collision energies for all n, and scales like n^4 for $n \geqslant 4$.

Of neutral-neutral collision processes the most important for the low-T plasma kinetics are those involving H($n = 1$) and H($n \geqslant 2$). Among them, the processes of mixing the angular momentum states, excitation transfer and associative and non-associative ionization show cross sections that in the low energy region are sufficiently large to produce rate coefficients comparable to those of electron impact inelastic processes.

2.2 Collision processes of H_2 ($N\,^{1,3}\Lambda_{g,u}; v$)

Most of the available cross section data for electron and proton impact processes of H_2 are those involving the ground electronic state X $^1\Sigma_g^+$, vibrationally unexcited ($v = 0$). Theoretical cross section calculations for electron impact excitation (to higher electronic states) and ionization, however, do exist for $v \geqslant 1$. Electron impact induced transitions between electronically (and vibrationally) excited states, or for ionization from electronically (and vibrationally) states are very sparse and usually performed using rather crude approximations (such as the Gryzinski-Bartky-Bauer classical model, see [4]). Besides excitation and ionization, other electron impact processes included in the database are: vibrational excitation of ground electronic state of H_2 (via formation of resonant H_2^- resonant states, or by radiative decay of exited electronic states), dissociative attachment and dissociative excitation and ionization of H_2(X;v) in all v-states. The cross section information for electron impact dissociative processes involving electronically excited states of H_2, is presently missing in the literature. There is also very little information on the non-radiative decay processes of excited electronic states (auto-ionization, pre-dissociation).

Most important low-energy proton impact processes of H_2(X;v) are: vibrational excitation and electron transfer. The latter becomes exothermic (and even quasi-resonant) for $v \geqslant 4$, characterized by a large cross section. In the thermal energy region, the particle exchange process becomes also important. The electron transfer in proton collisions with electronically excited H_2 should have large cross section for certain vibrational levels (due to an energy quasi-resonance), but this process has not been studied so far.

2.3 Collision processes of H^-, H_2^+ and H_3^+

The most important low-energy processes of H^- negative ion with electrons and protons are the electron detachment and the mutual neutralization (electron capture), respectively. The electron capture process dominantly populates the $n = 2$ and $n = 3$ states of H (produced on the basis of proton reactant). The resonant charge transfer and associative detachment in H^- +H collisions are also characterized by a large cross sections at low energies.

The predominant low-energy process of H_2^+ (v) with electrons is the dissociative recombination, resulting in production of H($n \geqslant 2$) excited atoms. The cross section magnitude, as well as the n-distribution of excited reaction products are sensitive to the value of initial vibrational state of H_2^+. At energies above 10 eV, the dissociative excitation starts to compete with dissociative recombination, and eventually becomes dominant at energies above 20 eV. The low-energy collisions of H_2^+ (v_i) with H_2(X;v) are dominated by charge transfer and H_3^+(v_3) formation (particle exchange) processes. While the former is theoretically studied fairly exhaustively, the information on v_i–v_3 and v–v_3 selectivity of the latter is still rather limited. This information is, however, critical for the cross section magnitude and quantum state of reaction products of processes of H_3^+ (v_3) with other plasma constituents (notably with e and H^-).

Dominant low-energy collision process of H_3^+ (v_3) with electrons is the dissociative recombination, producing either three H atoms or H + H_2 (v). While the total cross section of this process for $v_3 = 0$ is experimentally well established, including the energy dependence of branching ratio 3H/(H + H_2), large discrepancies in experimental data exist regarding its v_3 dependence. Very little is known also regarding the quantum states of atomic products, as well as the v-distribution of H_2. The cross sections of collision processes of H_3^+ (v_3) with H_2 (v) in the thermal energy region are also not well known, neither are the cross sections of the mutual recombination of H_3^+ and H_2^+ with H^-.

3. Data assessment and presentation

The cross section data information available in the literature for each considered collision process, either experimental or theoretical, was critically assessed and a preferred (or "recommended", when the information was abundant) cross section was derived with an assigned accuracy in various energy regions. When only one set of data was found in the literature for a given process, that set was taken to represent the cross section with its accuracy assigned by the author(s), or, in case of theoretical data, derived on the basis of accuracy of the method used in the calculations for a particular energy region.

The cross sections for many processes involving excited initial states are known to obey certain scaling relationships (at least in well defined energy regions) that follow from the general theory or particular theoretical models. Such scaling relationships were used to generate cross section for processes for which no data information was found in the literature. Finally, to fill in certain gaps in the available data, or make appropriate inter-/extrapolations, the predictions of certain relatively simple models, known to provide a reasonable description of corresponding physical process, were used.

All cross sections derived by applying the above prescriptions have been represented by analytic fit functions, the form of which was chosen to preserve the known (or expected on general theoretical grounds) the near threshold (when such exists) and high energy cross section behavior. An example of such analytic fit function is given below for the dipole allowed electron impact excitation cross sections of singlet states of H_2 from its ground electronic and vibrational state:

$$\sigma_{exc}\left(X^1\Sigma_g^+(v=0) \to N^1\Lambda_u\right) = \frac{5.984}{\Delta E x} \cdot \left(1 - \frac{1}{x}\right)^{\alpha} \cdot \left(A_1 + \frac{A_2}{x} + \frac{A_3}{x^2} + A_4 \ln(x)\right) (\times 10^{-16}\mathrm{cm}^2) \quad (1)$$

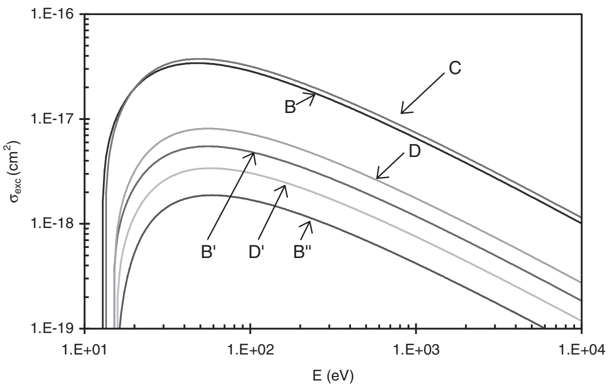

Fig. 1 Total electron impact excitation cross sections of *B*, *C*, *D*, *B'*, *D'*, *B"* singlet electronic states of H_2 from the H_2 ($X^1\Sigma_g^+$; $v=0$) ground state.

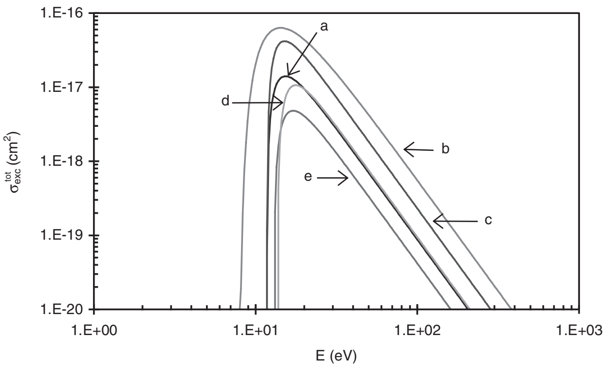

Fig. 2 Total electron impact excitation cross section of a, b, c, d and e triplet states of H_2 from its ($X^1\Sigma_g^+$; $v=0$) ground state.

where $x = E/\Delta E$, ΔE is the threshold energy, and A_i are the fitting parameters. Similarly, for the electron impact induced transitions to triplet excited states of H_2 from its ground electronic and vibrational state, the fit function was chosen in the form:

$$\sigma_{exc}^{tot}\left(X^1\Sigma_g^+(v=0) \to N^3\Lambda_\sigma\right) = \frac{A}{x^3} \cdot \left(1 - \frac{1}{x^\beta}\right)^{\gamma} (\times 10^{-16}\mathrm{cm}^2) \quad (2)$$

The excitation cross sections for the lowest singlet and triplet states of H_2 given by the above fit functions are shown in Figs. 1 and 2, respectively. The fits represent the derived cross sections with an rms deviation of 2–3%.

4. Conclusions

We have presented the content of a cross section database for collision processes taking place in low-temperature, low-density hydrogen plasmas. The processes mentioned in this presentation are only those that play a major role in the kinetics of ionizing and recombining plasmas. The scope of the database is, however, considerably broader and includes processes important for the description of hydrogen neutral beams propagating through a hydrogen plasma. The present article addresses also the question of completeness of the H/H_2 collision database, emphasizing the existing gaps in the database and in the present knowledge as well, regarding certain important collision processes in low-*T* hydrogen plasmas. These gaps are particularly serious for the processes involving electronically (and vibrationally) excited H_2 states and for the state-selective processes involving the formation and destruction of H_3^+ ion.

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