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Electron-Impact Collision Cross Sections Involving H_2 and N_2 Vibrationally and Electronically Excited Molecules

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Abstract

Calculated collision cross sections for allowed and forbidden transitions induced by electron impact in electronically and vibrationally excited H_2 and N_2 molecules are presented. Total and state-to-state cross sections are shown and compared with other theoretical and experimental data.

Keywords:

electron-molecule collision, state-to-state cross section, excited state

1. Introduction

Many molecular plasmas, generated from gaseous systems constituted of diatomic molecules, and in non equilibrium conditions can present strong deviations from Boltzmann distribution. In such cases the presence of excited diatomic species in non negligible concentration, can give rise to a complex microscopic physics, characterized by collision processes where each molecular quantum state behaves as an independent chemical species. In these conditions, the role played by the excited states can be of paramount importance and may strongly affect the evolution of the plasma.

Typical example is given by the edge and divertor plasmas in nuclear fusion. In the external region of the tokamak thorus, in fact, and in the divertor chamber, the hydrogen plasma is relatively cold (1−10 eV) so that the formation of large concentration of molecules in highly excited quantum states is allowed. On the other hand, the large degree of ionization of the gas produces a high electron density, so that among the possible collision processes that may occur in the system a central role is played by the electron impacts with excited (mainly vibrationally and electronically) H_2 molecules.

Hereby, the need of the knowledge in theoretical simulations, as well as in experimental measurements, of electron-impact cross sections and rates for molecular transitions connecting vibrational levels of different electronic states (states-to-states cross sections).

A further example of plasma systems where the role of the excited molecular states cannot be neglect, is represented by the N_2 plasmas, widely studied in many field of scientific and technological interest (nitrogen discharges, atmosphere, re-entry problems...). Also for these systems, kinetic modeling and diagnostic requires large sets of state-to-state cross sections data and rates for electron-molecule collisions [1] involving excited vibrational and electronic states.

In this communication we present very recent state-to-state cross sections data, calculated by using the so-called impact parameter method and Born approximation, for a number of "allowed" and "forbidden" transitions of H_2 molecules, involved in the experimental determination of electron and vibrational temperature of divertor plasma [2,3], and for the electron impact induced transition to the diabatic $b^1\Pi_u$ state of N_2 molecule (Birge-Hopfield system). This last process significantly contribute to the formation of atomic nitrogen through direct and predissociative mechanisms.

2. e - H_2

2.1 Allowed transitions

In Figs. 1(a) – (c), are shown the total excitation cross sections (summed over the final vibrational ladder), as a function of the incident energy and for different initial vibrational quantum number v_i, for the triplet-triplet transitions $a^3\Sigma_g^+ \rightarrow d^3\Pi_u$, $c^3\Pi_u \rightarrow h^3\Sigma_g^+$ and $c^3\Pi_u \rightarrow g^3\Sigma_g^+$. In figure 1(d) is given an example of state-to-state cross sections for the $a^3\Sigma_g^+ \rightarrow d^3\Pi_u$ transition as a function of the final vibrational quantum number v_f. The incident energy is set to 10 eV and the three curves refer to v_i = 0, 6, 13. The particular behavior shown by these curves is mainly due to the Franck-

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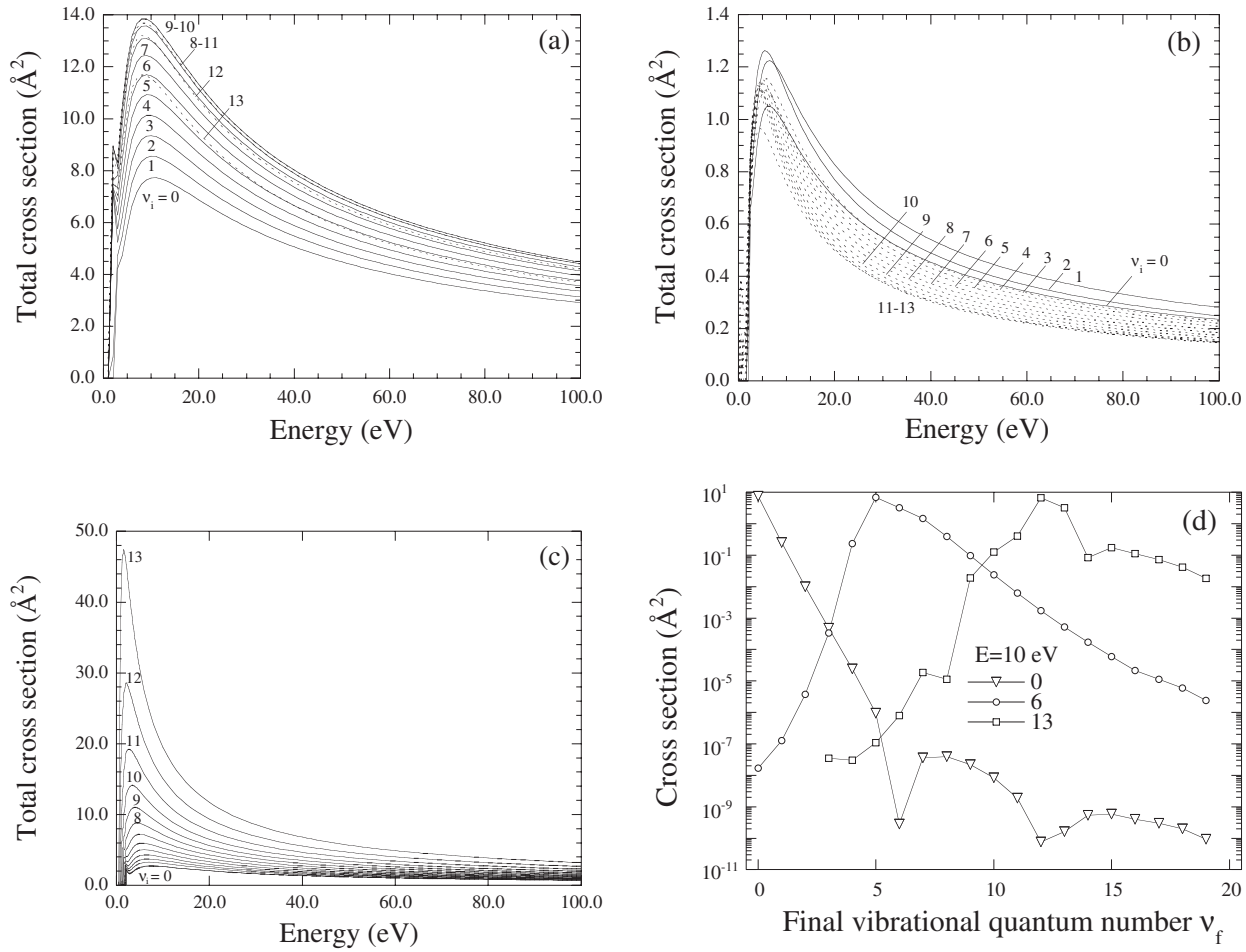

Fig. 1 Total excitation cross sections as a function of energy for the process (a) $H_2(a^3\Sigma_g^+, \nu_i) + e \rightarrow H_2(d^3\Pi_u) + e$; (b) $H_2(c^3\Pi_u, \nu_i) + e \rightarrow H_2(g^3\Sigma_g^+) + e$; (c) $H_2(c^3\Pi_u, \nu_i) + e \rightarrow H_2(h^3\Sigma_g^+) + e$. (d) State-to-state cross sections for the process $H_2(a^3\Sigma_g^+, \nu_i) + e \rightarrow H_2(d^3\Pi_u, \nu_f) + e$ as a function of final vibrational quantum number, at the incident energy $E = 10$ eV, for $\nu_i = 0$, 6 and 13.

Condon factors governing the $\nu_i \rightarrow \nu_f$ excitation.

2.2 Forbidden transitions

Figure 2(a) and 2(b) shows the total excitation cross sections, calculated with the Born approximation, for the following singlet-triplet (forbidden) transitions $X^1\Sigma_g^+ \rightarrow a^3\Sigma_g^+$ and $X^1\Sigma_g^+ \rightarrow d^3\Pi_u$

The present data agree quite well, in the region of high incident energies where the Born approximation is valid, with the experimental data available for $\nu_i = 0$ [4].

2.3 e-N_2

Total excitation cross sections for the $X^1\Sigma_g^+ \rightarrow b^1\Pi_u$ transition for different initial vibrational states are presented in Fig. 3(a). The vibrational dependence can be studied plotting the total cross section, at a fixed incident energy, versus the initial vibrational quantum number (see Fig. 3(b)): the cross section shows a regular decreasing behavior with ν_i. In the same figure also the $\nu_i - \nu_f$ excitation and the dissociative components are displayed. The excitation to the bound vibrational levels of the b state is the main process up to $\nu_i = 6$ then the corresponding cross section rapidly decreases and the direct dissociation through the vibrational continuum becomes the dominant contribution. As already pointed out the interest for this process is due to its importance in the atomic nitrogen production. Actually the present results show that the vibrational excitation of the N_2 molecule greatly enhances the direct dissociation probability, especially for high vibrational quantum numbers. However also the excitation to bound levels can lead to dissociation through predissociative mechanism. This channel in fact represents the main contribution to dissociation for $\nu_i \leq 7$. For higher ν_i direct dissociation becomes dominant (see Fig. 3(b)). Experimental results of Zipf and Gorman [5] for $\nu = 0$ are in good agreement with the present results.

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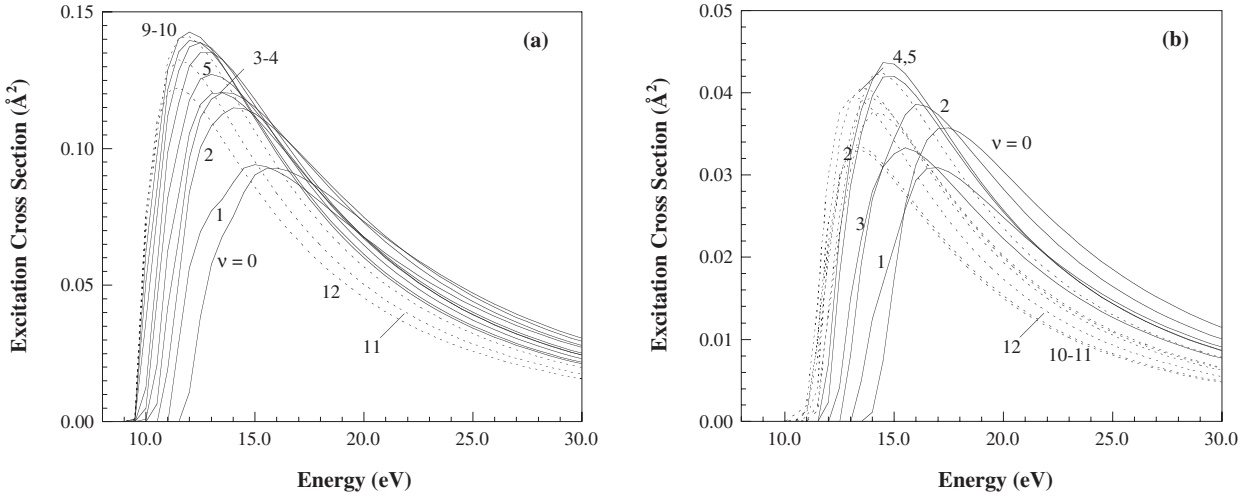

Fig. 2 Cross sections as a function of energy for the process
(a) $H_2(X^1\Sigma_g^+, \nu_i) + e \rightarrow H_2(a^3\Sigma_g^+) + e$;
(b) $H_2(X^1\Sigma_g^+, \nu_i) + e \rightarrow H_2(d^3\Pi_u) + e$.

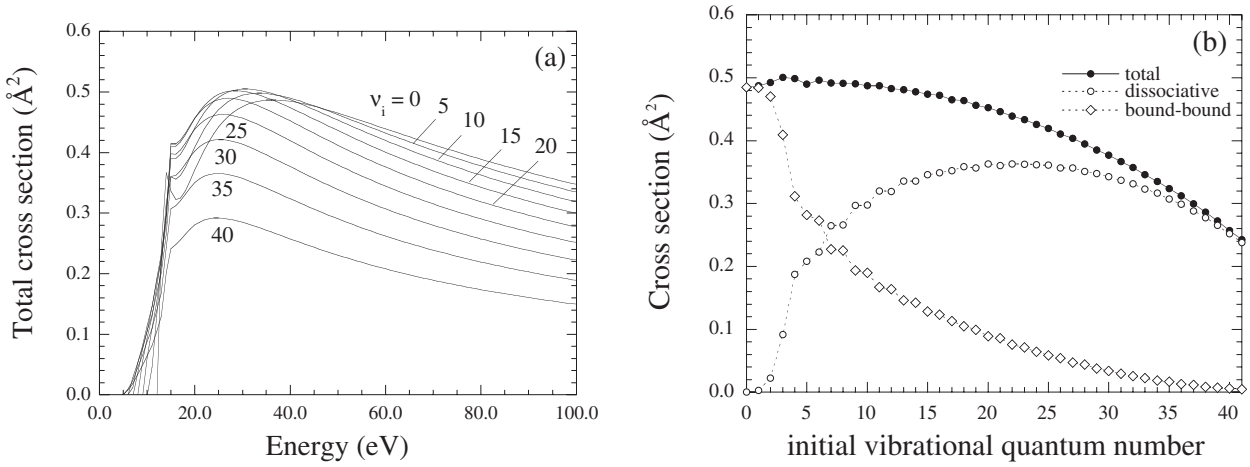

Fig. 3 (a) Total excitation cross sections as a function of energy for the process $N_2(X^1\Sigma_g^+, \nu_i) + e \rightarrow N_2(b^1\Pi_u) + e$.
(b) Dependence on the initial vibrational quantum number, ν_i, at $E = 40$ eV, of total, dissociative and $\nu_i - \nu_f$ cross sections for the same process.

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