Numerical study on production processes of vibrationally excited molecules in hydrogen negative ion sources

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(Presented on 2 October 1991)

Production processes of vibrationally excited hydrogen molecules and their effects on H^- production are studied theoretically by using a set of particle balance equations in a steady-state hydrogen plasma. For vibrational excitation, three processes, i.e., fast-electron collisional excitation, neutralization of moleculer ions, and atom-surface recombination, are taken into account. Enhancement of vibrational excitation including vibrational distribution and H^- production is obtained as a function of three different excitation processes.

I. INTRODUCTION

We have recomfirmed semiquantitatively that, according to our recent simulation results,[1-3] most H^- ions are produced by a two-step process[4] which involves dissociative attachment of slow plasma electrons e (electron temperature $T_e = 1$ eV) to highly vibrationally excited hydrogen molecules H_2 (optimum vibrational level $v'' = 7$–9). Therefore, a population in the upper portion of the vibrational spectrum is essential to enhancement of H^- ion production. The distribution of the H_2 molecules within the many vibrational levels of the electronic ground state has been the subject of both theoretical[5,6] and experimental[7,8] investigations.

In this paper, the excitation of $H_2(v'')$ and vibrational distribution are studied numerically by using a set of particle balance equations in a steady-state hydrogen plasma. In particular, the enhancement of the $H_2(v'')$ distribution is discussed as a function of different excitation processes,[9] i.e., fast electron collisional excitation, molecular ions neutralization processes,[10] and wall recombination of atomic hydrogen H.

II. SIMULATION MODEL

To study H^- and $H_2(v'')$ production in a tandem two-chamber system,[2] we divide the single chamber of volume $L\times L\times L$ into two parts. Two chambers of volume $L\times L\times L_1$ (the first) and $L\times L\times L_2$ (the second) are in contact with each other in the region of the magnetic filter, where $L_1 + L_2 = L$. We assume that fast electrons e_f are present only in the first chamber because the magnetic filter impedes e_f from coming into the second chamber. In both regions, there are four ion species (H^-,H^+,H_2^+,H_3^+), two electron species (plasma electrons e and fast primary electrons e_f) and three species of neutral particles [H, H_2, and $H_2(v'')$]. Particles except e_f are assumed to move freely between two chambers without being influenced by the filter. The number of particles passing through the filter is treated in the form of flux nv, where n and v are the particle density and average velocity, respectively.

The present model is an extended version of the previous one.[1,2] Main modifications are as follows:[3,9] (i) Fourteen species of $H_2(v'')$ are considered, i.e., $v'' = 1$–14. (ii) Besides the 28 reaction processes,[1] the following three processes are newly included;

$$H_2 + e \rightarrow H_2(v''=1,2) + e, \tag{1}$$

$$H_2(v''=1,2) + e_f \rightarrow H_2(w'' > v'') + e_f, \tag{2}$$

$$H_2(v'') + H \rightarrow H_2(w'') + H. \tag{3}$$

(iii) The electron energy distribution function is taken to be the sum of two terms: a Maxwellian for e plus a high-energy term for e_f. Reaction rates are calculated for these two electron components, respectively. In this paper, the function for e_f is assumed to be the plateau distribution.

The 19 rate equations for H, $H_2(v'')$, H^-, H^+, H_2^+ and H_3^+ are derived by taking into account the above-mentioned reaction processes and the interaction between two chambers. Besides these, there are two constraints, i.e., the charge neutrality and the particle number conservation. Then, for the tandem two-chamber system, a set of 42 equations are solved numerically as a function of plasma parameters. Details concerning the model will be reported elsewhere in the near future.

III. NUMERICAL RESULTS AND DISCUSSION

Figure 2 shows the effect of e_f collisional excitation of $H_2(v'')$ on H^- production. These results are obtained by varying $n_e(1)$, electron density in the first chamber, on the assumption that other plasma parameters are kept constant, i.e., electron density ratio between two chambers $n_e(2)/n_e(1) = 0.2$, hydrogen gas pressure $p = 5 \times 10^{-3}$ Torr, electron temperature in the first chamber $T_e(1) = 5$ eV and electron temperature in the second chamber $T_e(2) = 1$ eV, and the filter position L_1:L_2 = 28:2 cm. According to the previous results,[2,3] these plasma parameters are chosen to optimize H^- production in the tandem system. Parameter is density ratio of e_f to e for the first chamber $n_{fe}(1)/n_e(1)$, where the shape of the plateau distribution for e_f is kept constant (i.e., energy of e_f, E_{fe}, ranges from 20 to 100 eV). The presence of e_f is essential to H^- production. With increasing $n_{fe}(1)/n_e(1)$, Fig. 1(a) confirms that H^- in the second chamber increases monotonically.[1-3,9] Figure 1(b) shows vibrational distributions at $n_e(1) = 10^{13}$ cm^{-3}, corresponding to H^- in Fig. 1(a). With increasing e_f, vibra-

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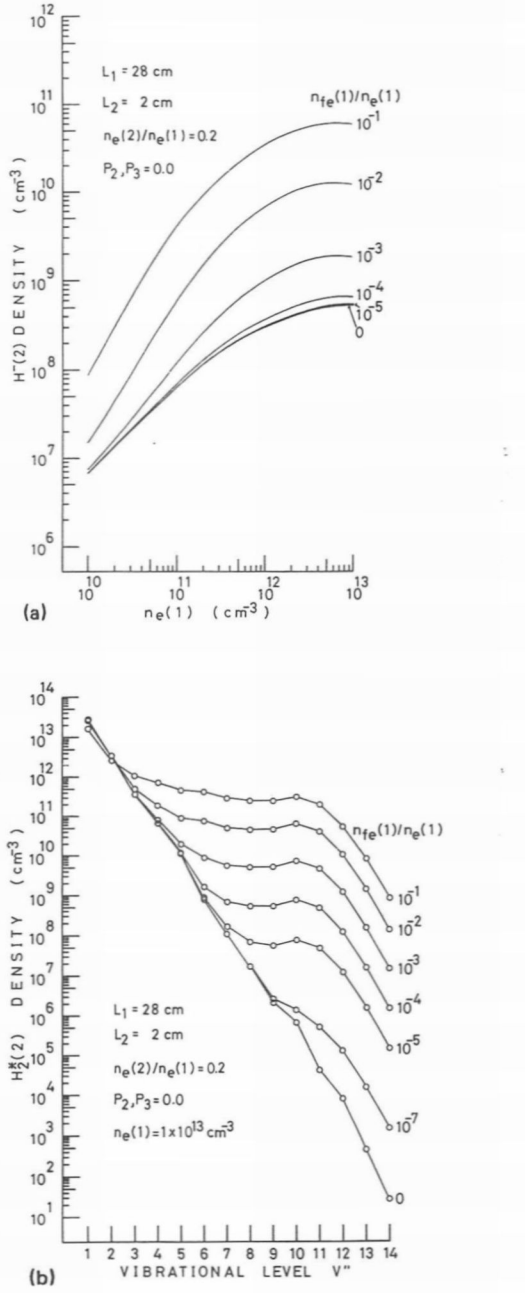

FIG. 1. Effect of fast electrons e_f on H^- and $H_2(v'')$ productions: (a) H^- density in the second chamber $H^-(2)$ vs electron density in the first chamber $n_e(1)$, and (b) $H_2(v'')$ in the second chamber vs v'' at $n_e(1) = 10^{13}$ cm^{-3}. The wall de-excitation collision parameter γ_2 for $H_2(v'')$ is 0.1.

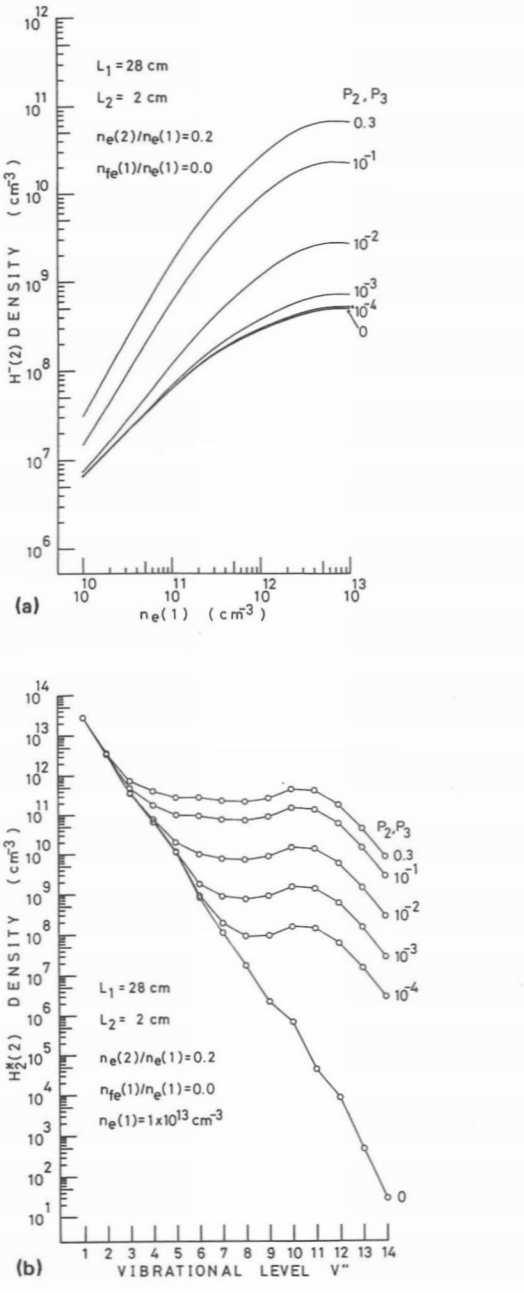

FIG. 2. Effect of neutralization processes of positive ions on H^- and $H_2(v'')$ productions: (a) $H^-(2)$ density vs $n_e(1)$, and (b) $H_2(v'')$ density vs v'' at $n_e(1) = 10^{13}$ cm^{-3}. In this case, e_f is absent and γ_2 is 0.1.

tional distribution becomes plateau-like distribution. Namely, the upper portion of the vibrational spectrum becomes high with e_f. The calculated distribution is found to be qualitatively well in agreement with the experimental results obtained by Eenshuistra and co-workers.[7] It is also noted that vibrational distribution is Boltzmann-like only when e_f is absent.

We have also discussed the effect of the shape of the energy distribution of e_f on $H_2(v'')$ and H^- productions, separately.[9] It is confirmed that H^- yield depends hardly on the shape of energy distribution function of e_f if e_f, whose energy E_{fe}, is nearly equal to or higher than 40 eV, are present.

Figure 2 shows the effect of neutralization of positive ions on H^- and $H_2(v'')$ productions. Parameters are probabilities of finding $H_2(v'')$ in the neutralization processes of molecular ions, i.e., P_2 for H_2^+ and P_3 for H_3^+. Excited molecules caused by the above process are shared equally within 14 vibrational levels. With increasing P_2 and P_3, both $H_2(v'')$ and H^- in the second chamber increase. In the tandem system, the neutralization process could occur

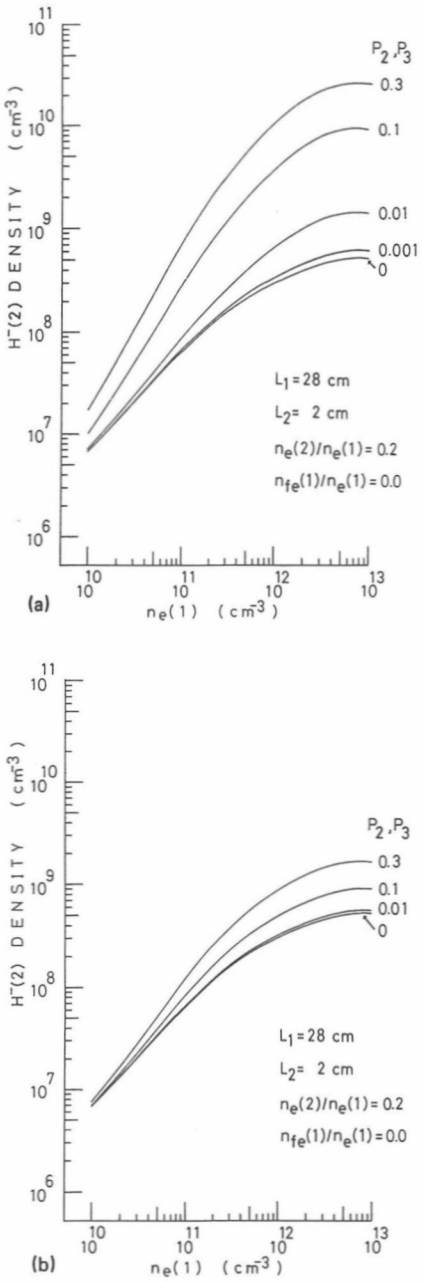

FIG. 3. Effect of neutralization processes of molecular ions on H^- production: $H^-(2)$ density vs $n_e(1)$. Vibrational molecules $H_2(v'')$ produced by neutralization process are shared equally between vibrational levels v'', (a) from 1 to 7, and (b) from 1 to 4, respectively.

in the second chamber, although the collisional excitation caused by e_f cannot take place. Therefore, the neutralization process for the production of $H_2(v'')$ is important to enhance $H^-(2)$. It is also clarified that the neutralization processes make the vibrational distribution superthermal, i.e., plateau formation.

For H^- production, the optimum level V'' of $H_2(v'')$ is 7–9[1] and their potential energy is relatively high, i.e., the energy with $v'' = 7$ is about 3 eV. So, neutralization processes of molecular ions play an important role only when molecular ions could be converted into relatively high energy levels of $H_2(v'')$. It depends on kinetic energy of molecular ions which are converted into $H_2(v'')$.[10] To clarify the relationship between H^- formation and kinetic energy of molecular ions, we calculated H^- density for two different neutralization conditions. Results are shown in Fig. 3. Decreasing the upper limit of the energy level where excited molecules caused by molecular ions are shared, H^- density decreases remarkably.

It is also confirmed that $H_2(v'')$ formation due to wall recombination of H plays an important role for H^- production when high energy levels of $H_2(v'')$ are formed. Therefore, the situation is the same as for the case of neutralization of molecular ions in the previous paragraph. Furthermore, the population of vibrational levels appears not to be Boltzmann, i.e., plateau-type distribution.

The above mentioned two processes for $H_2(v'')$ production, i.e., neutralization of molecular ions and wall recombination of H, depend strongly on wall surface conditions or wall materials.[1,9] Namely, effective life time for neutral particles and then neutral particle densities depend on the wall recombination coefficient γ_1 for H and the wall de-excitation collision parameter γ_2 for $H_2(v'')$, respectively. Detailed discussion on this point will be reported elsewhere.

In summary, findings are as follows: Collisional excitation of $H_2(v'')$ caused by e_f is most important to enhance H^- yield. Besides, $H_2(v'')$ and then H^- productions depend hardly on the shape of energy distribution of e_f if e_f with energies in excess of 40 eV is present. The effect of the neutralization processes of molecular ions for $H_2(v'')$ and H^- productions is remarkable only when molecular ions could be converted into $H_2(v'')$ with high vibrational level. Three different excitation processes (i.e., e_f collisional excitation, neutralization of molecular ions, and wall recombination) generate the plateau distribution for the $H_2(v'')$ vibrational population. Only the thermal electron collisional excitation, i.e., the process (1), makes the vibrational population to be almost Boltzmann.

ACKNOWLEDGMENT

This work was supported in part by a Grant-in-Aid for Scientific Research from the Ministry of Education, Science and Culture of Japan.

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