

Effects of the energy distribution of fast electrons on H_2 vibrational excitation in a tandem negative ion source

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The population distribution of vibrationally excited hydrogen molecules $H_2(v'')$, and the H^- production are investigated theoretically by solving numerically a set of particle balance equations in a steady-state pure hydrogen plasma. In particular, the enhancement of the $H_2(v'')$ distribution is discussed for different energy distributions of fast electrons e_f . Whether the energy distribution for e_f is a delta function type or a plateau type, collisional excitation of $H_2(v'')$ caused by e_f is very effective to enhance the H^- production and a resultant vibrational distribution becomes the plateau distribution. Besides these, if e_f with energies higher than 30–40 eV are present, both $H_2(v'')$ excitation and then H^- yield hardly depend on the form of the energy distribution of e_f .

I. INTRODUCTION

High current H^-/D^- ion sources are of interest to the fusion community for the preparation of neutral beams, as H^- but not H^+ can be efficiently neutralized at beam energies in excess of 150 keV. A volume source is one of the candidates for generating such a beam. According to our recent simulation results,^{1,2} most of the H^- ions are produced by a two-step process³ which involves dissociative attachment of slow plasma electrons e (with electron temperature $kT_e \approx 1$ eV) to highly vibrationally excited molecules $H_2(v'')$ (optimum vibrational level $v'' = 7-9$). Therefore, a population in the upper portion of the vibrational spectrum is essential for the generation of a high concentration of H^- ions. The distribution of the H_2 molecules among the many vibrational levels of the electronic ground state has been the subject of both theoretical and experimental investigations. The vibrational distribution has been measured by Stutzin *et al.*⁴ using vacuum-ultraviolet (VUV) absorption spectroscopy up to $v'' = 8$. No evidence for a plateau was found. The population of the vibrational levels appear to be almost Boltzmann. On the other hand, Eenshuistra *et al.*⁵ have also obtained the vibrational distribution using a resonance-enhanced multiphoton ionization technique. The occupation of $v'' = 3-5$ is strongly superthermal. This effect is more pronounced at higher discharge currents. To clarify the differences in the vibrational population between these two experiments, Hiskes^{6,7} has investigated theoretically the vibrational distribution in a hydrogen discharge for different excitation processes.

We have also studied theoretically mechanisms and optimization of volume-produced H^- ions for both a single-chamber system¹ and a tandem two-chamber system² by solving numerically a set of particle balance equations in a steady-state hydrogen plasma. In this paper, we report some results on the dependence of H^- and $H_2(v'')$ production for different energy distributions of fast electrons, and discuss the vibrational distribution for the tandem two-chamber system.⁸ Effects of other processes^{7,9} for vi-

brational excitation, i.e., neutralization of molecular ions and atom-surface recombination, are briefly described.

II. SIMULATION MODEL

In Fig. 1, the tandem two-chamber model² is shown schematically, where the single chamber of volume $L \times L \times L$ is divided 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. We consider four ion species (H^- , H^+ , H_2^+ , H_3^+), two electron species (plasma electrons e and e_f) and three species of neutral particles [H , H_2 , and $H_2(v'')$]. Particles except e and 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 velocity, respectively.

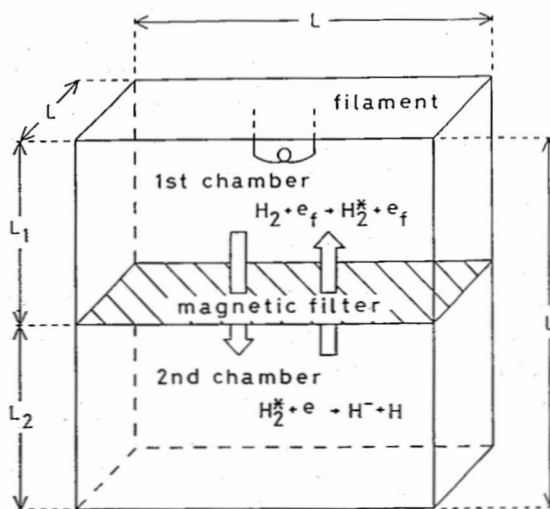
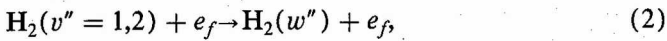
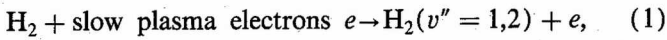


FIG. 1. Simulation model for the tandem two-chamber system.

The present model is an extended version of the previous one,² and is the same model used in studying processes of $H_2(v'')$ production in hydrogen discharges.^{8,9} Characteristic features of the present model are as follows:

(a) Fourteen species of $H_2(v'')$, i.e., $v'' = 1-14$, are considered.

(b) For the production of $H_2(v'')$, the following reactions are included:



Neutralization processes of molecular ions



Wall recombination of atomic hydrogen. (5)

(c) 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 , namely the fast electrons. Then, reaction rates are calculated for these two electron components, respectively. In this paper, the energy distribution function for e_f is assumed to be the two forms, i.e., a plateau distribution and a delta function.

In each chamber, nineteen rate equations for H , $H_2(v'' = 1-14)$, H^- , H^+ , H_2^+ , 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 is solved numerically as a function of plasma parameters.

The calculated vibrational densities $H_2(v'')$, i.e., vibrational distribution, is sensitive to the wall relaxation process.^{1,6} In our model, the term representing loss to the wall surface for $H_2(v'')$ is expressed as $-\gamma_2 N_2(v'')/\tau_2$, where γ_2 is a wall de-excitation collision parameter, $N_2(v'')$ is $H_2(v'')$ density, and τ_2 is a transit time of $H_2(v'')$. Because γ_2 is defined as the ratio of $H_2(v'')$ that strike the surface and are de-excited to $H_2(v'' = 0)$ to the total number colliding with the surface [i.e., $\gamma_2 = 1 - F(\text{out})/F(\text{in})$, where F is the flux of $H_2(v'')$], when $F(\text{out})$ is not equal to zero, γ_2 becomes smaller than unity. Hence the effective lifetime for $H_2(v'')$, τ_2/γ_2 , increases. The value of γ_2 depends not only on wall materials or wall conditions,¹⁰ but also on vibrational level.⁶ After a wall collision, $H_2(v'')$ molecules relax more rapidly with increasing v'' . Previously,^{1,2} we assumed that γ_2 was constant for all $H_2(v'')$. Therefore, $H_2(v'')$ with higher levels might be overestimated. To take into account the effect of v'' -dependent wall relaxation of $H_2(v'')$, in the present calculation, we use the different values of γ_2 for different v'' . Namely, we give the value of $\gamma_2(v'' = 1)$, and the value of $\gamma_2(v'')$ for v'' is estimated with multiplying $\gamma_2(v'' = 1)$ by a factor of average distance between atomic centers $r(v'')/r(v'' = 1)$.^{8,9} So, $\gamma_2(v'')$ increases in its value with increasing v'' ,⁶ although γ_2 is still treated as a numerical parameter.

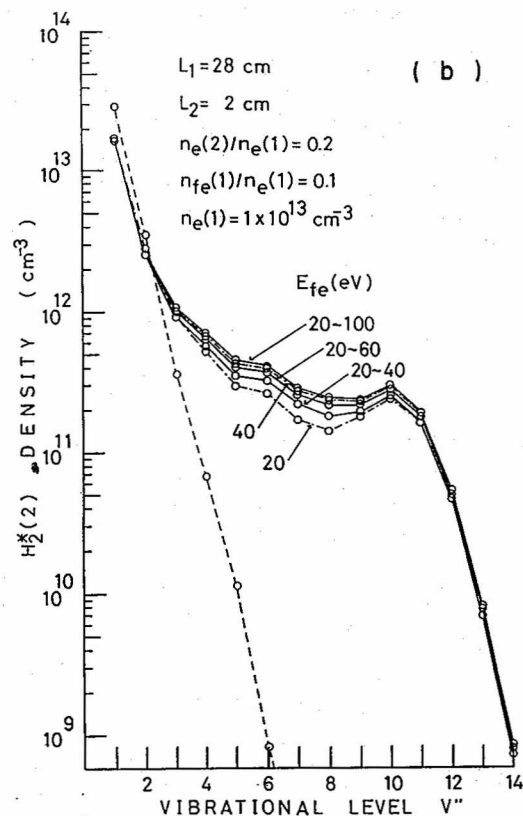
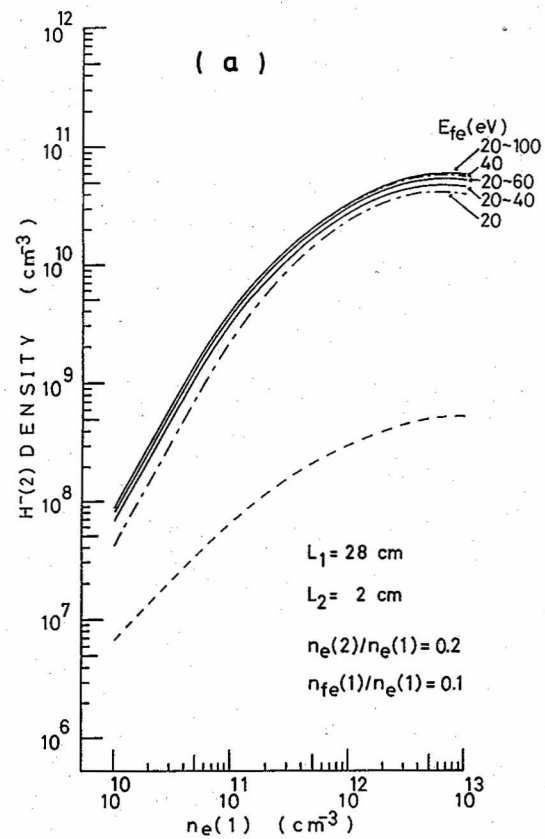


FIG. 2. Effect of fast electron energy distribution for H^- and $H_2(v'')$ productions: (a) H^- density in the 2nd chamber $H^-(2)$ vs n_e in the 1st chamber $n_e(1)$, and (b) $H_2(v'')$ density in the 2nd chamber $H_2^*(2)$ vs vibrational level v'' at $n_e(1) = 10^{13} \text{ cm}^{-3}$, corresponding to H^- density in (a). Full curves are for plateau distributions, chain curves for delta functions, and broken curve for no fast electrons. The wall de-excitation collision parameter γ_2 for $H_2(v'' = 1)$ is 0.1.

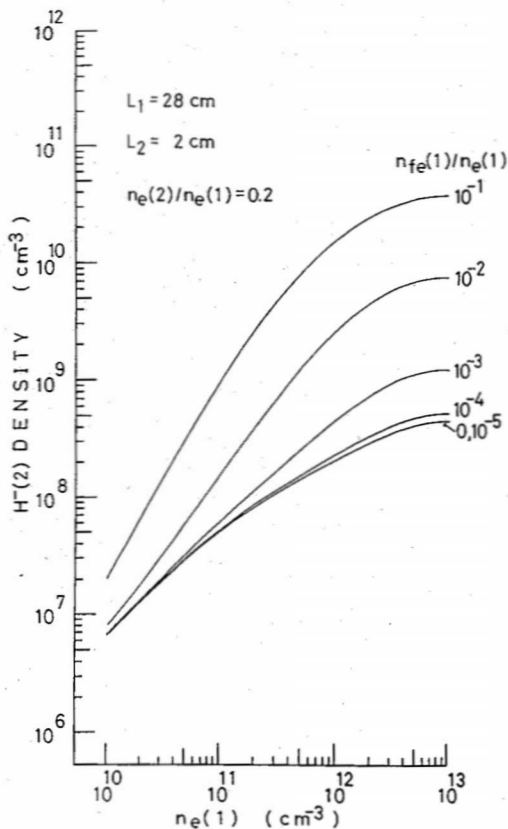


FIG. 3. Effect of fast electrons on H^- production: $H^-(2)$ density vs $n_e(1)$. Parameter is fast electron density in the 1st chamber n_{fe}/n_e . Plasma conditions are the same as the ones in Fig. 2 except that $\gamma_2(v'' = 1)$ is 0.5.

III. NUMERICAL RESULTS AND DISCUSSION

At first, we discuss the effect of the shape of the energy distribution of e_f on the production of $H_2(v'')$ and H^- . To this end, the energy distribution for e_f is assumed to be the two different forms, i.e., a plateau distribution and a delta function. Figure 2 shows the H^- density and the $H_2(v'')$ distribution in the second chamber as a function of the different energy distributions of e_f . In this case, excitation processes (4) and (5) are excluded. Calculations are done by varying $n_e(1)$, electron density in the first chamber, on the assumption that other plasma parameters are kept constant, i.e., the electron density ratio between two chambers $n_e(2)/n_e(1) = 0.2$, the density of e_f in the first chamber $n_{fe}(1)/n_e(1) = 0.1$, hydrogen gas pressure $p = 5 \times 10^{-3}$ Torr, electron temperature in the first chamber $\kappa T_e(1) = 5$ eV and electron temperature in the second chamber $\kappa T_e(2) = 1$ eV, and the filter position $L_1:L_2 = 28:2$ cm. According to the previous results,^{1,2} plasma conditions are chosen to optimize H^- production in the second chamber. At the same time, these values of plasma parameters are reasonable for real ion sources.

Figure 2(a) shows that the H^- yield hardly depends on the shape of the energy distribution of e_f so long as a typical fast electron energy E_{fe} is nearly equal to or higher than 30–40 eV. It is apparent, however, that the presence of e_f is essential to H^- yield.^{1,2} Figure 2(b) shows vibrational distributions at $n_e(1) = 10^{13} \text{ cm}^{-3}$, corresponding

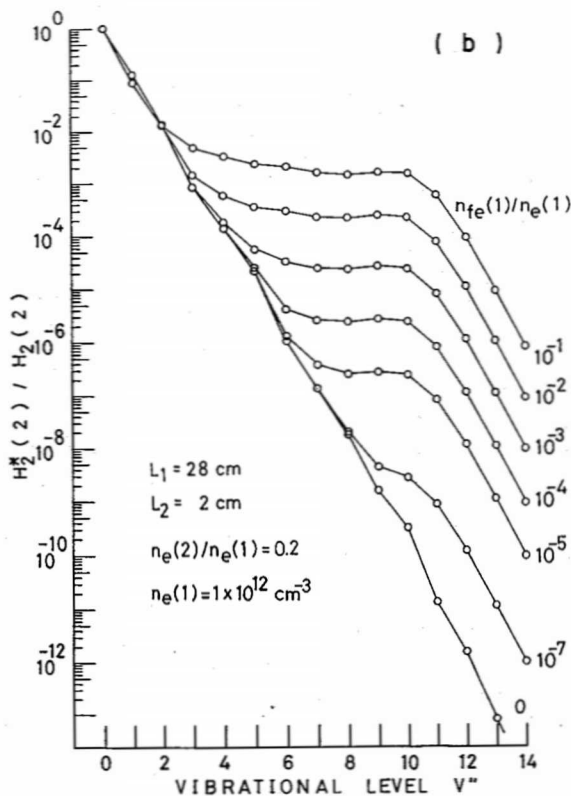
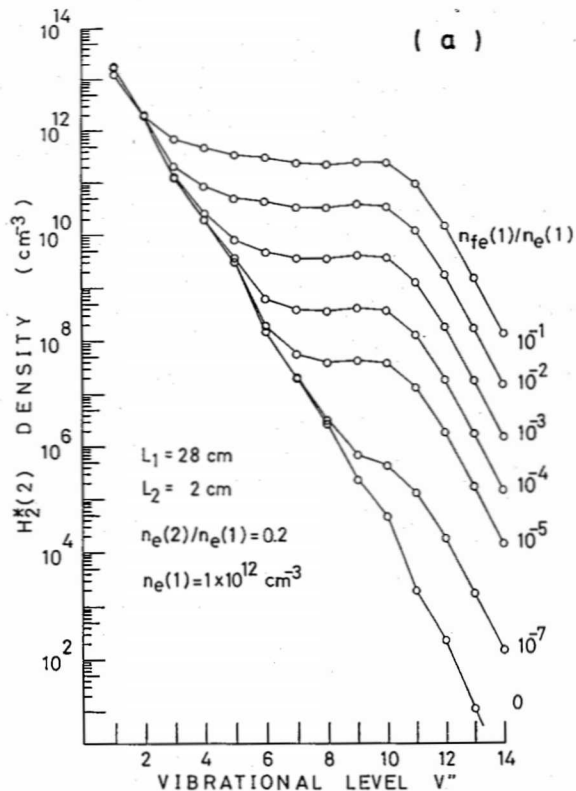


FIG. 4. Effect of fast electrons on $H_2(v'')$ density distribution: (a) $H_2^*(2)$ vs v'' at $n_e(1) = 10^{12} \text{ cm}^{-3}$, corresponding to H^- density in Fig. 3, (b) $H_2(v'')$ density normalized on the $H_2(v'' = 0)$ density.

to the H^- density in Fig. 2(a). In all cases with e_f apparently, vibrational distributions are nearly equal to each other in their densities and forms. This results in the same H^- densities for different e_f distributions. The physical

meaning is as follows: The cross section¹¹ for vibrational excitation by e_f to any level v'' increases steeply for E_{fe} ranging from 15 to 30 eV, reaches a maximum at about 40 eV, and then decreases gradually with E_{fe} . Therefore, the reaction rate for vibrational excitation is approximately constant for E_{fe} ranging from 30 up to 200 eV. Therefore, the production of both $H_2(v'')$ and H^- hardly depends on the shape of the energy distribution of e_f as shown in Fig. 2.

Besides those, it is noted that resultant vibrational distributions are plateau-like. We have also found that vibrational distribution is Boltzmann-like only when e_f is absent (shown by the broken curve).

Next, we consider the relation between e_f collisional excitation of $H_2(v'')$ and its distribution function. Figure 3 shows the effect of e_f collisional excitation of $H_2(v'')$ on H^- production in the second chamber. An important parameter is the density ratio of e_f to e for the first chamber $n_{fe}(1)/n_e(1)$, where the e_f distribution is kept at plateau type (with E_{fe} ranging from 20 to 100 eV). As mentioned above, the presence of e_f is essential to the H^- production. With increasing $n_{fe}(1)/n_e(1)$, the H^- density in the second chamber increases monotonically.

Figure 4(a) shows vibrational density distributions in the second chamber at $n_e(1) = 10^{12} \text{ cm}^{-3}$, corresponding to the H^- yield in Fig. 3. We have reconfirmed that with increasing e_f , vibrational distribution becomes plateau-like distribution. Namely, the upper portion of the vibrational spectrum becomes high with e_f . In Fig. 4(b), the vibrational distribution normalized on the $v'' = 0$ population is also presented. Figure 4 shows that tendencies of the calculated distribution for $n_{fe}/n_e = 10^{-3}$ – 10^{-2} are in qualitative agreement with the experimental results obtained by Eenshuistra *et al.*,⁵ i.e., $v'' = 1$ – 5 . It should also be noted that vibrational distribution is Boltzmann-like only when e_f is absent. In this case, only collisional excitation caused by plasma electrons, i.e., the reaction (1), is included.

We have also discussed the effects of neutralization processes of molecular ions and wall recombination of atomic hydrogen H for the production of $H_2(v'')$ and H^- .⁹ These two processes play an important role only when molecular ions or recombined atoms can be converted into $H_2(v'')$ with high vibrational levels. Besides, their effects also depend strongly on wall conditions, i.e., $\gamma_2(v'')$ for

$H_2(v'')$ and the wall recombination coefficient γ_1 for H. The definition of γ_1 is the same as γ_2 described in Sec. II. Further discussion on the wall effects will be reported elsewhere.

IV. CONCLUSION

The population distribution of $H_2(v'')$ and the H^- yield are investigated theoretically. The collisional excitation of $H_2(v'')$ by e_f is most important to enhance the H^- yield. Besides, the production of $H_2(v'')$ and H^- hardly depends on the shape of the energy distribution of e_f if e_f with energies in excess of 35–40 eV are present. It is also noted that three different excitation processes (i.e., fast electron collisional excitation, neutralization of molecular ions, and wall recombination of atoms) make the vibrational distribution plateau-like. On the other hand, the vibrational distribution results in a Boltzmann-type distribution when only collisional excitation caused by thermal plasma electrons is included.

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