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Calculation of Hydrogen Outgassing Rate of LHD by Recombination Limited Model

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Abstract

To simulate hydrogen outgassing in the plasma vacuum vessel of LHD, the recombination limited model is presented, where the time evolution of hydrogen concentration in the wall of the plasma vacuum vessel is described by a one-dimensional diffusion equation. The hydrogen outgassing rates when the plasma vacuum vessel is pumped down at room temperature and baked at 100 ℃ are calculated as a function of pumping time. The calculation shows that the hydrogen outgassing rate of the plasma vacuum vessel can be reduced at least by one order of magnitude due to pumping and baking. This prediction is consistent with the recent result of outgassing reduction observed in the pumping-down and baking of the plasma vacuum vessel in LHD.

Keywords: stainless steel chamber, hydrogen outgassing rate, bakeout, recombination limited model

1. Introduction

Recently it has been proposed by Moore [1] that hydrogen outgassing in stainless steel vacuum chamber should be described by the recombination limited model (RLM) rather than the diffusion limited model (DLM). However, it has not been reported so far how to calculate concretely the recombination limited outgassing rate in a vacuum chamber. Then we have developed a model to calculate the hydrogen outgassing rate of a stainless steel chamber with RLM [2]. The calculation model is applied to simulate hydrogen outgassing rates of the plasma vacuum vessel of LHD fabricated of 316 stainless steel in the procedures of pumping-down at room temperature and subsequent baking at 100 ℃.

2. Recombination limited model

The hydrogen desorption from the wall of a stainless steel chamber can be described with a one-dimensional diffusion equation. The equation is

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2}, \qquad (1)$$

where $u(x,t)$ and D are the hydrogen concentration and bulk diffusion coefficient for hydrogen in the wall of the stainless steel chamber, respectively. Equation (1) is solved for the vacuum chamber wall of unit cross section and thickness d. The initial concentration in the vacuum chamber wall is u_0 and is constant throughout the wall. At time $t = 0$ vacuum is applied to one surface of the wall (where $x = 0$) and atmosphere to the other surface of the wall (where $x = d$). The initial condition is

$$u(x,t) = u_0 \text{ for } 0 \le x \le d \text{ at } t = 0. \qquad (2)$$

The boundary conditions are

$$2K_r u^2 = D\frac{\partial u}{\partial x} \text{ for } x = 0 \text{ at } t \ge 0 \qquad (3)$$

and

$$\frac{\partial u}{\partial x} = 0 \text{ for } x = d \text{ at } t \ge 0, \qquad (4)$$

where K_r is the molecular recombination rate constant of hydrogen atom at the wall surface of the stainless steel chamber. The condition (4) shows that hydrogen atoms diffusing in the solid wall are reflected inside the wall at the plane of $x = d$. From the condition (3) the hydrogen outgassing rate q ($\mathrm{H_2 molecules \cdot cm^{-2}s^{-1}}$) is given by

$$q(t) = K_r u^2 = \frac{D}{2}\left(\frac{\partial u}{\partial x}\right) \text{ for } x = 0 \text{ at } t \ge 0. \qquad (5)$$

In the condition (3) the readsorption of hydrogen molecules in the gas phase to the wall surface of the vacuum chamber is not considered, since the sticking probability of hydrogen molecule at the wall surface is negligibly small. In the condition (4) the permeation of atmospheric hydrogen through the wall is not taken into account, since the solubility of atmospheric hydrogen to the wall of stainless steel is negligibly small compared to the initial hydrogen concentration in the wall and the hydrogen pressure in the atmosphere is as low as 10^{-4} Torr.

3. Calculation of hydrogen outgassing rate

Since the boundary condition (3) expresses mathematically a non-linear relation, it is difficult to solve analytically the diffusion equation. So we solve numerically the equation (1) using the finite element method. Using the data of diffusion and recombination coefficients of hydrogen measured experimentally for austenitic stainless steels, Langley [3] has expressed these coefficients as a function of temperature with the following empirical formulas; the coefficient in the bulk diffusion D is

$$D = 3.64 \times 10^{-2} e^{-\frac{E_b}{RT}} \text{ cm}^2\text{s}^{-1}, \qquad (6)$$

where E_b is the activation energy of bulk diffusion and $E_b = 60 \text{ kJ} \cdot \text{mol}^{-1}$, R is the gas constant ($R = 8.314 \text{ J} \cdot \text{mol}^{-1}\text{K}^{-1}$) and T is the absolute temperature, and the recombination coefficient K_r is

$$K_r = 3.90 \times 10^{-16} e^{-\frac{E_r}{RT}} \text{ cm}^4\text{s}^{-1}, \quad (7)$$

where E_r is the activation energy for molecular recombination and $E_r = 70 \text{ kJ} \cdot \text{mol}^{-1}$. The hydrogen outgassing rates of the plasma vacuum vessel in LHD are calculated for the following pumping procedures; (1) the plasma vacuum vessel is pumped down at room temperature for 2 days, and (2) subsequently the plasma vacuum vessel is baked at 100 ℃ (373 K) for 5 days, and (3) after the baking the plasma vacuum vessel is again pumped down at room temperature for 2 days. Temperatures of the plasma vacuum vessel in the start and end of baking are changed equally at the rate of 7.3 K/h. Since Nemanic et al., [4] have recently measured the hydrogen content in the 304 stainless steel sample by the thermal extraction method and reported that the hydrogen content is as high as 9×10^{19} H atoms $\cdot$ cm^{-3}, the initial hydrogen concentration in the wall of the plasma vacuum vessel is assumed at $u_0 = 1 \times 10^{20}$ H atoms $\cdot$ cm^{-3}. The wall thickness d is taken as $d = 15$ mm which is the same as that of the plasma vacuum vessel in LHD. Figures 1 shows the surface concentration $u(0,t)$ and the outgassing rate $2q$ $(= D\partial u / \partial x)$ calculated as a function of pumping time for the plasma vacuum vessel. Figure 2 shows the hydrogen concentration $u(x,t)$ calculated as a function of position x in the wall of the plasma vacuum vessel at different pumping times.

4. Discussion and summary

From Fig. 1 we can see that by the pumping-down at room temperature for 2 days without baking, the surface hydrogen concentration of the plasma vacuum vessel is reduced by about one order of magnitude from $u_0 = 10^{20}$ to

$u(0,t) \cong 1.4\times10^{19}\ \mathrm{H}\cdot\mathrm{cm}^{-3}$ and as a result, the outgassing rate is reduced to $q \cong\ 5.0\times10^{10}\,\mathrm{H}_2\cdot\mathrm{cm}^{-2}\mathrm{s}^{-1}$, which value is equivalent to about 1.4×10^{-9} Torr $\ell\cdot\mathrm{cm}^{-2}\mathrm{s}^{-1}$. In the recent operation of LHD, it has been observed that the ultimate pressure of hydrogen in the plasma vacuum vessel after pumping down at room temperature for 5 days reaches about 2×10^{-6} Pa ($\cong 1.5\times10^{-8}$ Torr). The hydrogen outgassing rate measured in the plasma vacuum vessel q_{exp} can be expressed as

$$q_{\mathrm{exp}} = S_{\mathrm{H}_2} P_{\mathrm{H}_2} / A, \qquad (8)$$

where A is the surface area of the plasma vacuum vessel, P_{H_2} is the hydrogen pressure, S_{H_2} is the pumping speed for hydrogen. Since the nominal pumping speed provided with the pumping system in LHD is expressed with the pumping speed for nitrogen S_{N_2}, using the root of mass ratio of hydrogen and nitrogen molecules ($\sqrt{m_{\mathrm{N}_2} / m_{\mathrm{H}_2}} \cong 3.7$) we can estimate the pumping speed for hydrogen as follows;

$$S_{\mathrm{H}_2} = \sqrt{m_{\mathrm{N}_2} / m_{\mathrm{H}_2}}\, S_{\mathrm{N}_2}.$$

Then, by substituting $S_{\mathrm{N}_2} = 1\times10^4\ \ell\cdot\mathrm{s}^{-1}$, $A =\ 5\times10^6\,\mathrm{cm}^2$ and the ultimate pressure of hydrogen $P_{\mathrm{H}_2} = 1.5\times10^{-8}$ Torr into the equation (8), the experimental outgassing rate of hydrogen for the plasma vacuum vessel is estimated at $q_{\mathrm{exp}} \cong 1.2\times10^{-10}$ Torr $\ell\cdot\mathrm{cm}^{-2}\mathrm{s}^{-1}$. If we accept this experimental outgassing rate as a reasonable one for the plasma vacuum vessel, we can conclude that the calculation with RLM estimates the outgassing rate for the plasma vacuum vessel one order of magnitude larger than the experimental one. To improve the accuracy in the calculation of outgassing rate, we need to select properly numerical values for the recombination coefficient and initial hydrogen concentration. Pick and Sonnenberg [5] have discussed that the variation of recombination coefficient varies in orders of magnitude with contamination of the surface of solid wall. It is reported by Nemanic et al,. [4] that the initial concentration of hydrogen in stainless steel as raw material distributes in the range $1.6\times10^{19} \le u_0 \le 10^{20}\,\mathrm{H}\cdot\mathrm{cm}^{-3}$. Therefore we are allowable to select suitably values of K_r and u_0 for fitting the calculated outgassing rate to the experimental one. From the recent study [2] for the dependence of recombination coefficient on outgassing rate, following set of values $K_r \cong 10^{-27}\,\mathrm{cm}^4\mathrm{s}^{-1}$ at 300 K and $u_0 \cong 3\times10^{19}\,\mathrm{H}\cdot\mathrm{cm}^{-3}$ are recommended to simulate the outgassing rate in the plasma vacuum vessel. Fig. 1(b) shows that by the baking at 100 ℃ for 5 days for the plasma vacuum vessel, the hydrogen outgassing rate is reduced by one order of magnitude from $q = 5\times10^{10}$ to 3.5×10^{9} $H_2\cdot cm^{-2}s^{-1}$(at t =200h). On the other hand, when the plasma vacuum vessel in LHD was baked at 100℃ for 6 days, it has been observed that the hydrogen pressure is reduced by about one order of magnitude from 1.5×10^{-6} to 2.5×10^{-7} Pa. Thus one can say that the calculation predicts well the effect of baking at 100℃ for the reduction of outgassing rate. In Fig. 1(a) it is shown that the surface hydrogen concentration $u(0,t)$ at the end of baking starts to increase from pumping time of $t = 180$ h. The increase may be explained as the accumulation of diffusing hydrogen at the wall surface, since the desorption rate of hydrogen from the wall surface is limited to low due to the rapid decrease of recombination coefficient with decrease of wall temperature. Fig. 2 shows that the hydrogen concentration in the range from $x = 0.024$ to 1.5 cm in the wall remains unchanged by the baking at 100 ℃. The vacant range of hydrogen in the near surface of the wall can be considered with the diffusion length x_D, which is given as $x_D \cong \sqrt{\pi Dt}$. For the baking time $t = 5$ days (= 4.32×10^{5}s) and the diffusion coefficient $D =$ $1.44\times10^{-10}\,cm^{2}s^{-1}$ at 373 K, the relation yields $x_D = 0.014$ cm. As shown in Fig. 2, this length is roughly coincident with the range of concentration reduction $x = 0.02$ cm in the wall of the plasma vacuum vessel after the baking for 5 days. Since the wall thickness of the plasma vacuum vessel of LHD is $d = 1.5$ cm, the range of concentration reduction corresponds to 1 % of the total thickness of the wall.

The outgassing model based on RLM is described and is applied to simulate the hydrogen outgassing rate in the plasma vacuum vessel of LHD. It is shown from the simulation that when the plasma vacuum vessel is degassed by the baking at 100℃, the hydrogen content near surface region of the wall of the plasma vacuum vessel is reduced by about one order of magnitude. For the best fitting of outgassing rates between the calculation and the experiment, it is necessary to select suitably numerical values of recombination coefficient K_r and initial hydrogen concentration u_0 which are used in the calculation model.

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Figure captions:

Figure 1: (a) The surface concentration $u(0,t)$ and (b) the outgassing rate $2q$ $(= D\partial u/\partial x)$ of the plasma vacuum vessel as a function of pumping time.

Figure 2: The hydrogen concentration as a function of position x in the wall of the plasma vacuum vessel at different pumping times.

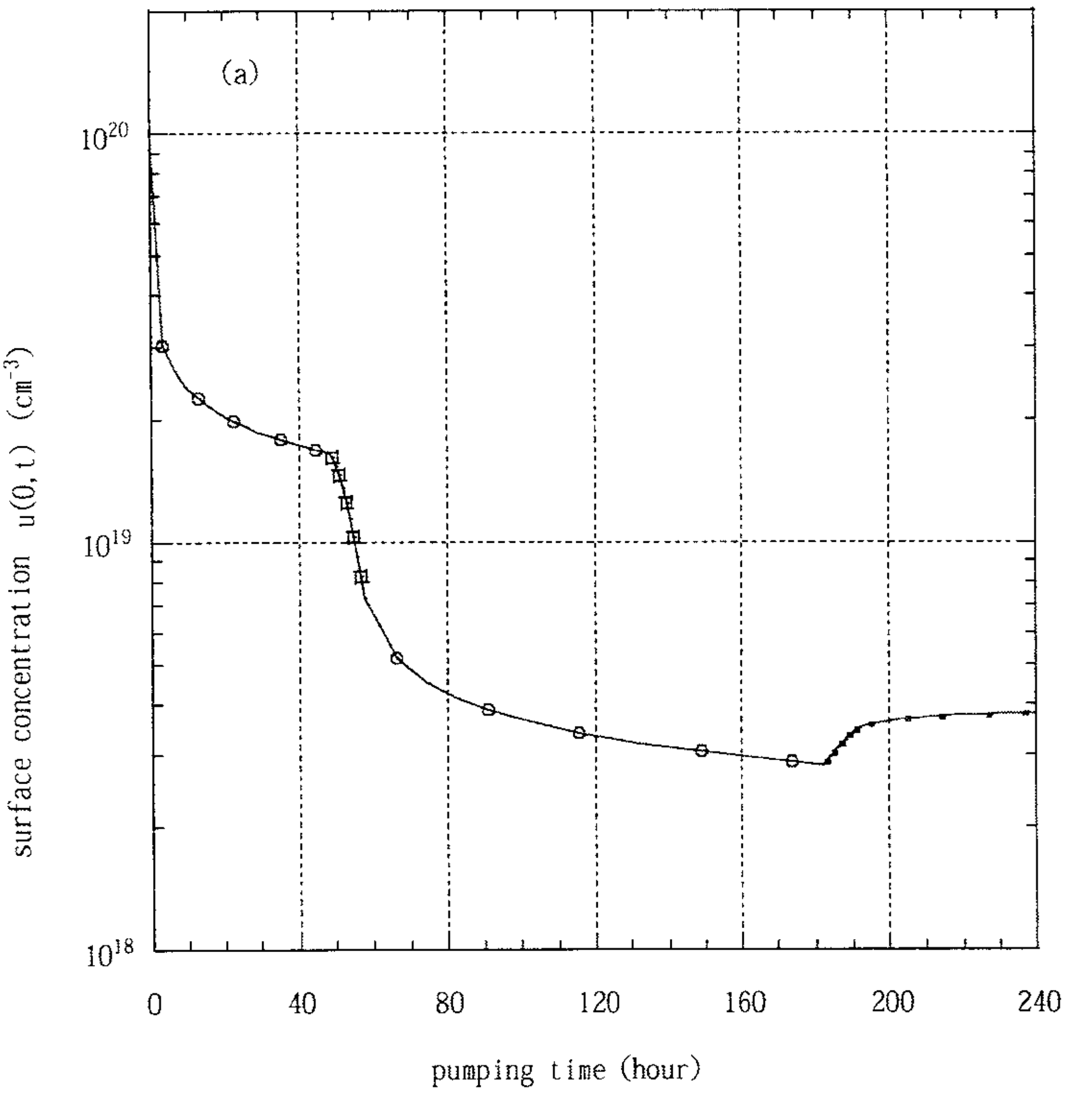

(a)
10^{20}
10^{19}
10^{18}
surface concentration u(0, t) (cm^{-3})
0
40
80
120
160
200
240
pumping time (hour)

Fig. 1(a)

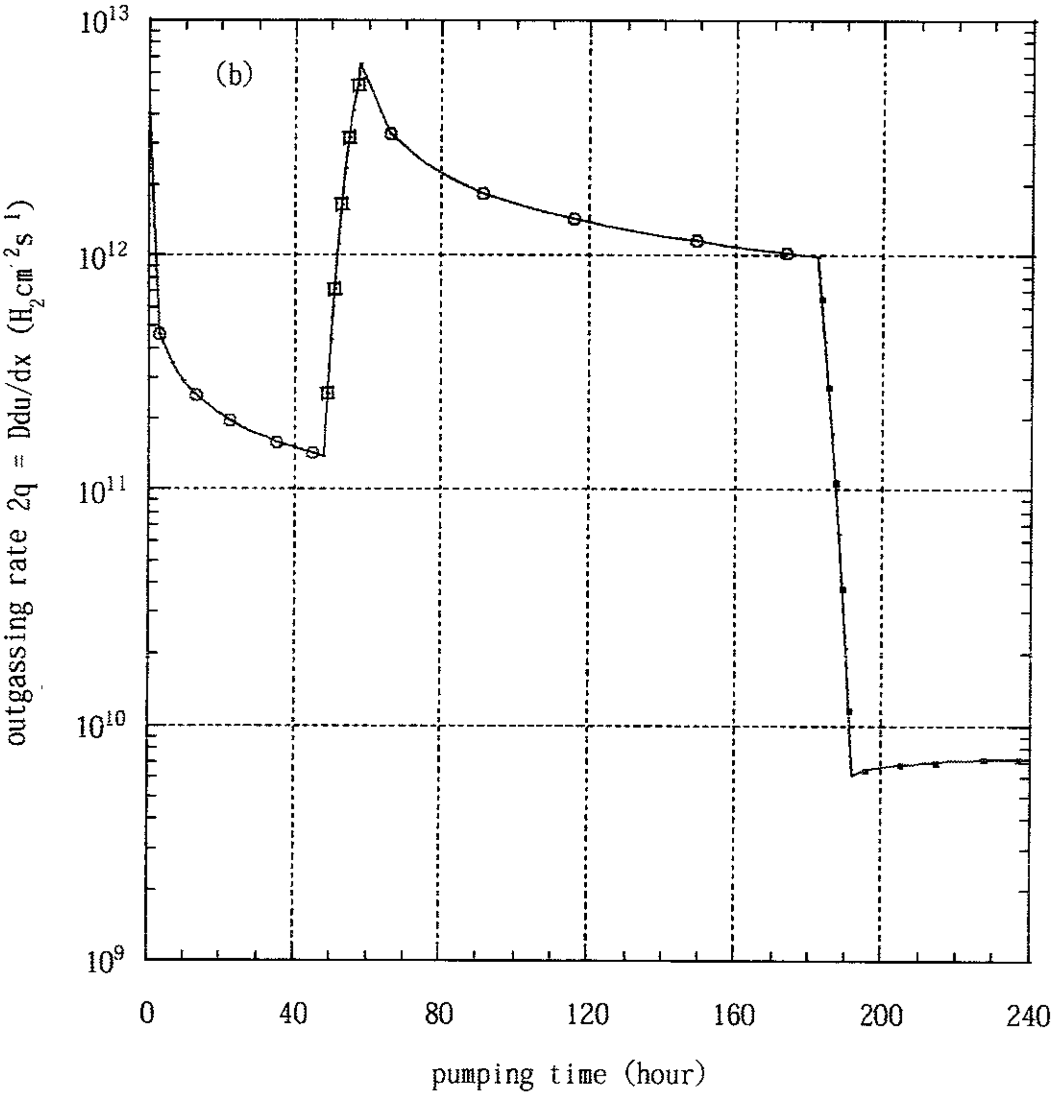
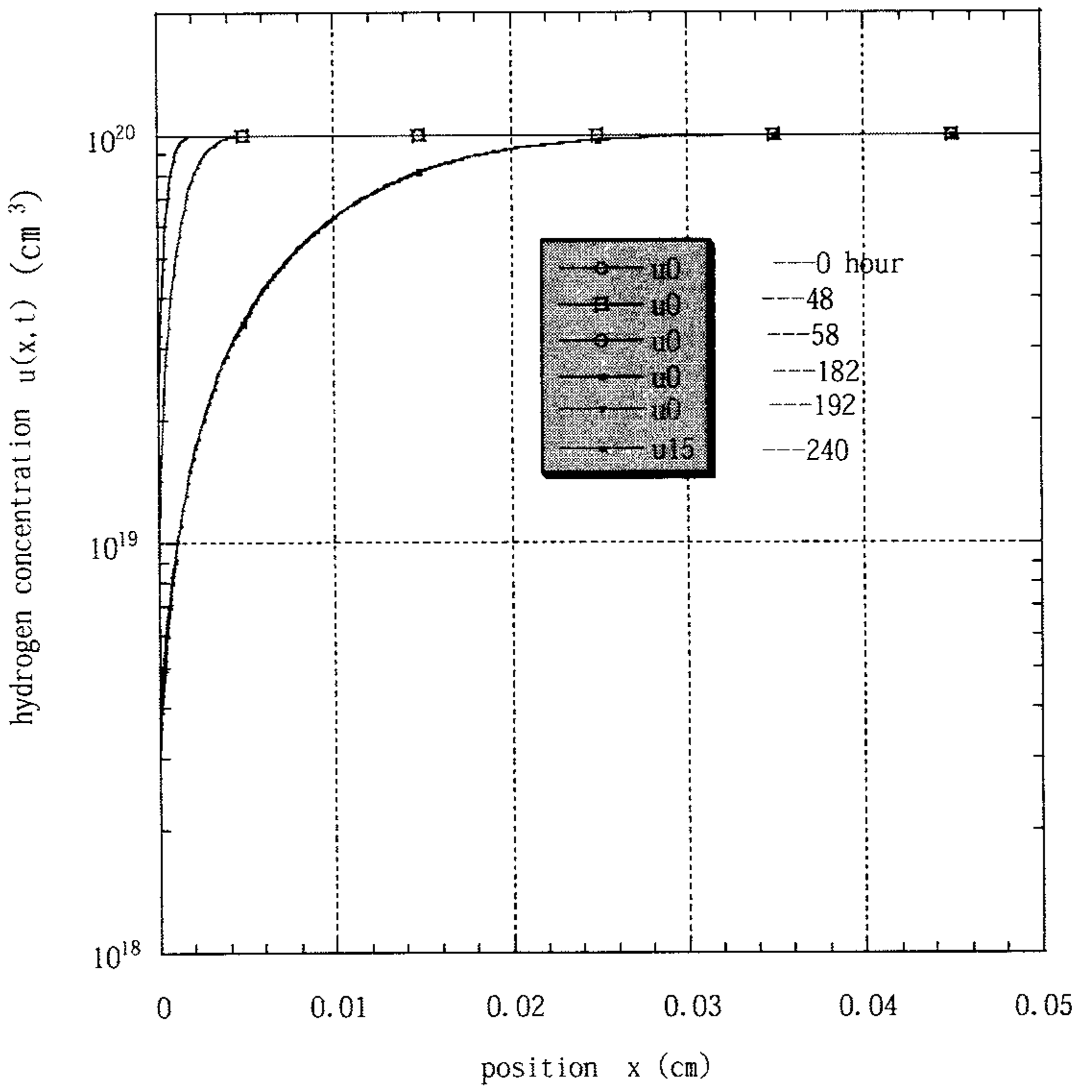

(b)
outgassing rate $2q = Ddu/dx$ ($H_2cm^{-2}s^{-1}$)
10^{13}
10^{12}
10^{11}
10^{10}
10^{9}
0
40
80
120
160
200
240
pumping time (hour)

Fig. 1(b)



10^{20}
10^{19}
10^{18}
hydrogen concentration u(x,t) (cm ^{3})
u0 ---0 hour
u0 ---48
u0 ---58
u0 ---182
u0 ---192
u15 ---240
0
0.01
0.02
0.03
0.04
0.05
position x (cm)

Fig. 2

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