H_2 Formation on the Dust Grain Surface in Divertor Plasma

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Edge plasma of divertor in tokamak is characterized by different values of plasma parameters (plasma density and temperature), plasma composition and overcoming plasma dynamics processes. We survey a model for theoretical study of the interaction of hydrogen with dust surface and apply our results the H_2 formation on dust grain surfaces in the divertor. In this model, considering both physisorbed and chemisorbed sites on the grain surface and then adatoms mobility to go from one site to other site by thermal diffusion, describes the formation of H_2 on grain surfaces. We find H_2 formation rate on the high temperature dust surfaces in divertor for a range of dust and gas temperatures and densities.

Keywords: dust, plasma, divertor, tokamak

1 INTRODUCTION

The knowledge of hydrogen-surfaces interaction mechanism is necessary, since it has various applications in physics and industry. For example, this mechanism has widely been studied in molecular hydrogen formation in space [1], and plasma-surfaces interactions in fusion devices [2].

When hydrogen atoms arrive on the dust surface, they can be weakly adsorbed (physisorbed) or strongly adsorbed (chemisorbed) to the surface. After the sticking of atoms to the surface, their mobility can be governed by quantum mechanical tunneling or thermal hopping, then recombination of H atoms on grain surface leads to H_2 formation [3].

2 H_2 FORMATION IN DIVERTOR PLASMA

We consider plasma conditions for detached divertor plasma with the temperature $T_e \approx 1$ eV [4, 5]. This low temperature, describes a medium with large number of complex atomic collisions in which there are neutral atoms, low-charged ions of impurities and non-detached molecular species. The main part of the neutral gas is formed by hydrogen atoms and molecules. In this area of the edge plasma, ion density is in the range of 10^{13}-10^{15} (cm^{-3}) and the neutral gas densities [H_2], [H] are of the same order of magnitude. Since the lifetime of H^+, H^- and H^* is very short ($<10^{-7}$ s), the relative concentration of these particles is low compared with the electron and neutral gas densities [6]. Therefore, our kinetic model for molecular hydrogen formation on the dust surface is based on the following reaction:

$$\mathrm{H(neutral\ atom) + H(neutral\ atom) \rightarrow H_2}$$

For the adsorption process of hydrogen atoms on the dust surface, depending on the temperature of the incident atoms, two different interactions between the atom and the surface occurs [7, 8]. If the hydrogen atom is weakly bound to the surface by Van der Waals force, the interaction is typically called physisorption, and if the atom is strongly bound to the surface by Covalent force, the interaction is called chemisorption. With the assumption that sticking occurs on every collision with a grain, the accretion rate of H atoms on the dust in units of atoms s^{-1} is given by

$$\psi_H = N_s \phi_H, \qquad (1)$$

which N_s is the number of sites on the surface of dust grain and ϕ_H is the flux of H atoms onto the surface of a dust grain, in units of monolayer per second (ML s^{-1}). The adsorbed hydrogen atom diffuses on the surface by thermal hopping or quantum tunneling mechanism [3, 7 and 8]. In the first mechanism it is necessary to have sufficient thermal energy to overcome the barrier between the sites, this mechanism is dominant in the divertor plasma. We consider a surface which physisorption and chemisorption sites lie at different heights and are also offset horizontally from one another so as to form two offset planar lattices. Diffusion happens horizontally among the sites of the same type (chemisorption or physisorption), while diffusion between the different types of sites has also a vertical component [9, 2]. Mobilities of H atom to pass from

one site to another can be defined as

$$\mu_{ij} = f_i \times P_{ij}, \qquad (2)$$

where i and j represent either physisorption (p) or chemisorption (c) sites, P_{ij} are the transmission probabilities to cross the barrier and f_i is the oscillation factor in the site i where the H atom is bound (E_c or E_p). Hydrogen atoms through two different mechanisms Langmuir-Hinshelwood (LH) and Eley-Rideal (ER) can meet each other on the dust surface [10, 11]. In the LH mechanism, the second incident H atom sticks to the grain surface and then diffuses on the surface until it reaches where the first atom is trapped. Here, two adsorbed atoms that already thermalized by the surface, react with each other. In the ER mechanism, which is a direct interaction between a gas phase atom and an adsorbed atom, a reactive and effective collision occurs when the adsorbed H atom is virtually localized on the surface.

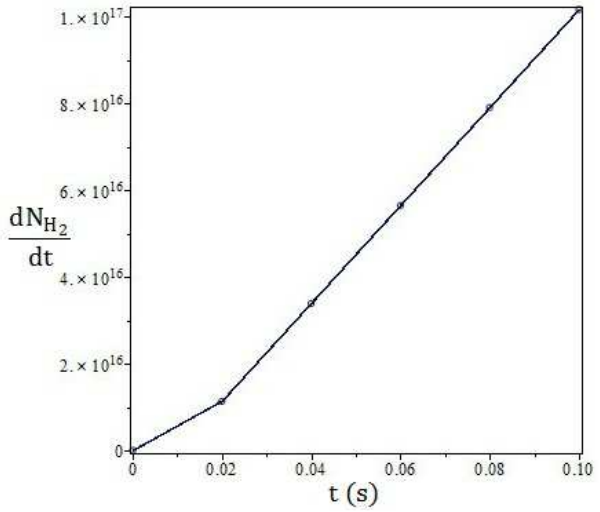

Fig.1: Differentiation of H_2 molecules number on the surface of carbon dust as a function of time

3 H_2 FORMATION EFFICIENCY

We assume the grains with low surface coverage where saturation is not a problem. The formation efficiency of the hydrogen molecules is:

$$\xi = 2N_{H_2} / N_H, \qquad (3)$$

where N_H is the number H deposited on the grain in the time interval before the steady state and N_{H_2} is the number of H_2 formed after the steady state. At high temperatures, the physisorbed atoms instantly evaporate with a rate α_p, and only the chemisorbed atoms remain on the surface, move, recombine and form molecules. As a result the most efficient reaction for H_2 formation at high temperature is due to collision of chemisorbed atoms. It should be noted that mobility on the dust surface occurs by thermal hopping since H atom energy and temperature of dust surface are high enough. At high temperatures, hydrogen atoms coming from the gas phase with a temperature T_{gas} can directly enter a chemisorbed site and form a molecule. For calculating H_2 formation coefficient by directly chemisorbed atoms on high temperature dust surface, we consider two categories of H atoms: A number of these atoms enter some already occupied sites and form molecules by the ER mechanism and the other group of these atoms enter the empty chemisorption sites and then diffuse on the surface to other chemisorption site with a rate $\mu_{cc}(H)$ and form a molecule by the LH mechanism. Moreover, we assume that all of the generated H_2 are immediately desorbed. Therefore, we can write the time evolution at high temperature for chemisorbed hydrogen atoms and produced molecular hydrogen as:

$$\dot{N}_{H_C} = \phi_H - 2\mu_{cc} N_{H_c}^2 - \alpha_c N_{H_c}, \qquad (4)$$

$$\dot{N}_{H_2} = \mu_{cc} N_{H_c}^2, \qquad (5)$$

where ϕ_H is the effective flux of hydrogen atoms on the dust surface and μ_{cc} is the mobility from a chemisorbed site to another nearest-neighbor site. α_c is the desorption rate for H atom or molecule in the chemisorption site, written as $\alpha_c = f_c e^{-E_c/kT}$, where f_c is the frequency factor of chemisorbed H atom. For calculation of the H_2 formation efficiency, we have integrated this time-dependent equation using a Runge-Kutta method with adaptive step size control until steady state was achieved. As analyze from the Fig. 1, the number of hydrogen molecules on the carbon dust surface reaches quickly the steady state, namely the time evolution is very rapid for H_2 formation on the surface of the carbon dust. In other words, the time to reach the steady state (τ_{ss}) is much shorter than the lifetime of the carbon dust ($\tau_{ss} = 10^{-1}$ s) [12]. Therefore, by solving these equations in the steady state conditions, the H_2 formation coefficient obtain

in terms of H flux, temperature of dust surface and the number of sites on the surface.

4 RESULTS AND DISCUSSION

To study the behavior of dust particles of different materials (Li, Be, B, C, Fe, Mo, and W) in fusion plasmas, it has been shown that due to difference in the dynamics of particles made of light and heavy materials, C and Fe dust particles have the longest lifetime in different ranges of plasma temperatures and densities [12].

In the high temperature of divertor plasma, physisorbed atoms on the dust surface rapidly evaporate and chemisorbed H atoms remain. For molecule formation, the residential time (τ_{des}) of H atoms which have sticked to the surface and thermalized with it, should be much longer than the time interval between the successive collisions ($\Delta\tau$) on the grain surface ($\Delta\tau = \tau_{des}$). The $\Delta\tau\left(= n_H v_H \sigma_d\right)^{-1}$ is proportional to the accessible surface of dust grain for colliding with the surrounding gas A, average velocity v_H of H atoms and its density n_H. The thermally desorption or evaporation time for H atoms on the carbon surface is:

$$\tau_{des} = f_i^{-1} \exp\left(E_{des} / kT_d\right), \qquad (6)$$

where E_{des} is desorption energy. In the divertor conditions for chemisorbed H atoms on the carbon surface with temperature T_d = 700 K, $\Delta\tau = 10^{-14}$ s and $\tau_{des} = 10^{-9}$ s. Also in this conditions, the require time for diffusion of H atom after trapping $\tau_{dif}\left(= f_i^{-1} \exp\left(E_{dif} / kT_d\right)\right)$, where $E_{dif} \approx 0.25 E_{des}$, is $\tau_{dif} = 10^{-9}$ s.

By comparing these times, we can see that the chemisorbed hydrogen atoms on the dust surface in the divertor have enough time to recombine. Therefore, the total H_2 formation rate by all of dust grains is written as:

$$\Re_{H_2} = \frac{1}{2} \psi_H n_d \xi, \qquad (7)$$

where n_d is the total number of grains. We plot H_2 formation rate as a function of dust temperature for different atomic hydrogen densities on the carbonaceous grains (Fig. 2), which shows that formation rate increases on the graphitic surface and gradually decreases on the carbonaceous surface by increasing dust temperature.

Considering the above studies, the dust grains from their birth to evaporation have enough time to cause hydrogen atoms to combine and thus a considerable amount of energy and density to depreciate. Hence, the elimination the formation process of hydrogen molecules is subject to removal of dust grains in tokamak plasma.

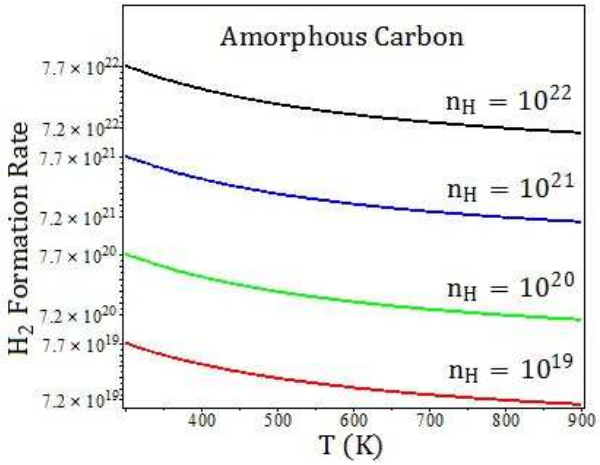

Fig.2: Rate of H_2 formation for carbon surfaces as a function of the grain temperature for different atomic hydrogen densities. The plot is working out the grains of radius 1μm

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