§57. Behavior of Hydrogen Atoms in Boron Films

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Hydrogen behavior in boron films has been investigated using SUT(SUrface modification Test-stand) for the study of H recycling control.

The boron films are deposited on whole inner surface of the liner, which has relatively large surface area of 7000 cm^2. It is exposed to H_2 and/or He discharges, or heated up to 500 °C to investigate hydrogen absorption and desorption behavior with monitoring pressure change measured by a diaphragm gauge and quadrupole mass spectrometer.

It has been found that (1) after H evacuation by heating, hydrogen atoms are strongly absorbed for a few tens of minutes, (2) after the strong absorption, hydrogen atoms are slowly but continuously absorbed without saturation up to 10 hours, (3) fifteen percents of the absorbed H atoms are desorbed by He ion bombardment, (4) the helium ion bombardment induces migration of H atoms deeper into the film, and thus, H atoms are accumulated in the film when H_2 and He discharges are repeated alternately, and (5) the hydrogen atoms in the boron films can be desorbed by heating up to 400 °C.

To understand H behavior, a calculation based on a simple model was discussed with the experimental results. An existence of trapped and solute (mobile) hydrogen atoms are assumed as in the models reported for graphite and amorphous carbon. The effects of de-trapping, trapping, implantation, and desorption are considered.

First, the transient release of the H atoms after the termination of the H_2 discharge is modeled. Time evolution of the H re-emission is calculated for two extreme cases, that is, the recombination occurs only through the process of (i) "solute - solute" or (ii) "trapped - solute". The result agrees with the experimental results with assumption (i). On the other hand, the calculation does not give agreement with the experimental result based on assumption (ii). It is concluded that the recombination of two solute H atoms is dominant. The product of $k_{ss} R_i$ is estimated from the best fitting value, where R_i is the implantation depth. The R_i is estimated to be 6.5 nm based on TRIM code calculation, and then, the k_{ss} is estimated as 7.8×10^{-24} cm^3/s.

Based on the findings about the recombination, the transient behavior just after turning on and off of the discharge is investigated, where the slow migration of H atoms is negligible. The differential equation can be written as follows;

$$\frac{\partial c_s}{\partial t} = S_r - 2k_{ss}c_s^2 - k_{st}c_s(c_T - c_t) + \sigma_d \Phi_i c_t$$

$$\frac{\partial c_t}{\partial t} = k_{st}c_s(c_T - c_t) - \sigma_d \Phi_i c_t$$

where c_s and c_t are the density of solute and trapped H atoms respectively, S_r the source term due to hydrogen implantation, c_T the density of the trap site, k_{st} trapping rate coefficient, Φ_i the ion flux, and σ_d the ion impact de-trapping cross-section. The S_r is estimated from the experimental value of the maximum absorption flux assuming that all of the injected hydrogen atoms are absorbed at initial phase. The Φ_i is estimated from the ion current

The transient release of H atoms at initial phase of He discharge can be reproduced fairly well as shown in Fig. 1 if we assume the trapping and detrapping rate are much higher than the desorption rate. The transient release after termination of H_2 discharge can be described with similar assumption. It is found through the calculation that in the presence of the ion flux, the hydrogen atoms of around 20% of the saturation density are in solute state, which is maintained with a balance between trapping and detrapping.

More accurate model including the effects of the depth profile of H implantation and the diffusion of H atoms is required to represent slow absorption effects and strong absorption at initial phase of the hydrogen discharge.

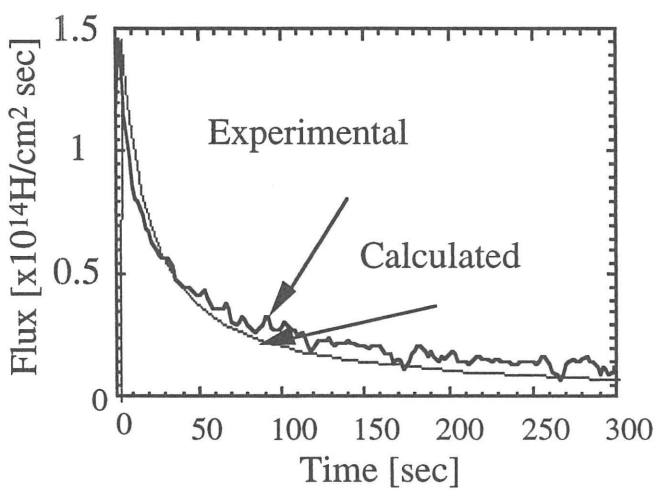

Fig.1 Time evolution of hydrogen desorption flux at initial phase of He discharge.