§3. Dynamics of Hydrogen Isotopes in a Boron Coating

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i) Introduction

In LHD, since the baking temperature for vacuum vessel is limited to be below 100 °C, the alternative method for improving plasma performance is required. Boronization, which is one of the most attractive wall conditioning methods to reduce impurities, such as oxygen, carbon, and iron, is considered as one of key issues to achieve high plasma performance [1]. From the viewpoint of safety for D-D and/or D-T fusion reactors, dynamics of hydrogen isotopes, such as tritium inventory, trapping states, and desorption behaviors implanted into a boron coating must be required to elucidate. In this fiscal year, the chemical behavior of deuterium in pure boron coatings, helium irradiation effect on the deuterium retention in boron coating, tritium desorption behavior from boron coatings were studied by means of X-ray photoelectron spectroscopy (XPS), Thermal desorption spectroscopy (TDS), and β-ray-induced X-ray spectrometry (BIXS).

ii) Experimental

The pure boron coatings were achieved by PCVD with $B_{10}H_{14}$ diluted with helium using a PCVD apparatus fabricated at Shizuoka University. The residual hydrogen retention and implanted deuterium retention in boron coatings were evaluated by TDS. To evaluate the stability of hydrogen in boron coatings and its activation energy, quantum chemical calculation using Gaussian 03 code was applied using HF or B3LYP model chemistry and 6-31+g(d,p) base set..

The stability of boron coating deposited on various substrate, was also studied by heating the sample up to 1300 K. The boron concentration was evaluated by XPS.

For the elucidation of tritium desorption behavior from boron coatings, tritium ion was irradiated to the boron coatings and dynamic behavior of tritium by isochronal and isothermal heating. The retention of residual tritium in boron coatings was measured by BIXS.

iii) Results and discussion

Figure 1 shows the TDS spectra of residual hydrogen and irradiated deuterium in boron coatings. It was found that the hydrogen desorption range was between 300 and 1000 K. However, the deuterium desorption range was limited to 350-800 K. The hydrogen desorption spectrum and desorption temperature range were almost as same as the previous report by A.Annen [1].From these results lower and higher temperature ranges were, respectively, the desorption of hydrogen bound to boron as B-H-B bond and that as B-H bond [2]. The deuterium desorption stages also consisted of two stages. These activation energy was evaluated using P.A.Redhead equation and achieved to be 1.11±0.21 eV (B-D-B bond) and 2.17±0.36 eV (B-D bond), respectively. The stability of hydrogen in boron crystal was studied by quantum chemical calculation as shown in Fig.2. It was found that the total energy of hydrogen in boron was the smallest in the B-H distance of about 1.35 angstrom and its activation energy was estimated to be about 0.1 hartree, which corresponds to about 2.7 eV. These results were almost consistent with the experimental results [3].

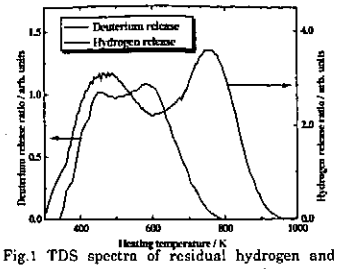

Fig.1 TDS spectra of residual hydrogen and implanted deuterium from boron coatings.

For the stability study of boron coatings, boron was deposited on silicon, IG-430U and SS-316 substrates. Fig.3 shows the boron concentration as a function of heating temperature for various substrates. It was clearly found that the boron coatings deposited on silicon and IG-430U still exist over the temperature of 1000 K. However, boron concentration deposited on SS-316 decreased over 750 K. This temperature region would correspond to the decomposition temperature of oxide layer on the surface of SS-316. Therefore, the boron coatings would not remain on the SS-316 substrate over this temperature range.

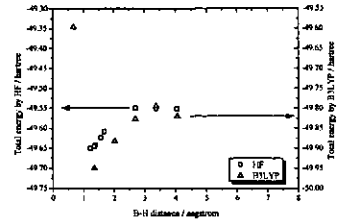

Fig.2 Energy dependence on B-H distance calculated by Gaussian 03.

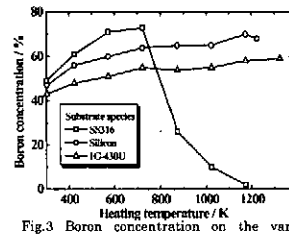

Fig.3 Boron concentration on the various substrates as a function of heating temperature

In the tritium desorption behavior experiment, most of the desorbed tritium at room temperature was an oxidized form and the residual amount decreased by 10-20 % of the initial amount at 773 K. Changes in the residual amount with time was well represented by exponential function (Fig.4), suggesting that the tritium release obeys the first order reaction kinetics and the rate-determining step is a diffusion process. Apparent activation energy of diffusion was determined to be 0.17 eV.

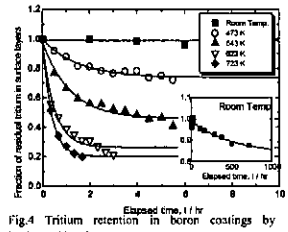

Fig.4 Tritium retention in boron coatings by isothermal heating

iv) Conclusion

To investigate the dynamics of hydrogen isotope in boron coatings, the residual hydrogen retention and implanted deuterium retention in boron coatings were evaluated by XPS and these results were compared with the results of quantum chemical calculation. The stability of boron coatings deposited on various substrates was also evaluated and the boron coatings on SS-316 were not stable over 750 K, which would be governed by the stability of the oxide layer on SS-316. For the tritium experiment, the major chemical form of desorbed tritium was an oxidized form and tritium release obeys the first order reaction kinetics.

References

[1] A.Annen et al.: Thin Solid Films, 300 (1997) 101-106
[2] H.Kodama et al.: J. Nucl. Mater., in press.
[3] Y.Oya et al.: J. Nucl. Mater., in press.