§18. Simulation Studies of Chemical Sputtering on Carbon Material under Hydrogen Bombardment

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We had simulated the incident ion fluence dependence of methane emission rate from carbon under hydrogen bombardment using the ACAT-DIFFUSE code [1], a Monte Carlo code with a binary collision approximation with diffusion effects take into account. The chemical sputtering was studied by Roth [2]. But the Roth's model is only suitable for steady state methane reaction. Then, we have proposed an empirical formula, modifying Roth's formula. In this empirical formula, we assumed the reaction region where chemical sputtering takes place. The reaction region was defined with respect to the implantation range of hydrogen as shown in Fig.1.

Empirical formula for chemical reaction

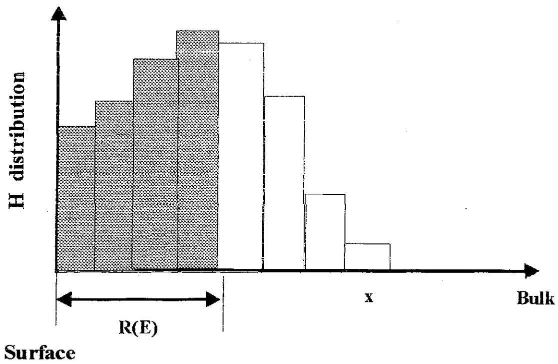

Fig.1 Chemical reaction model

In Fig.1, R (E) is the peak range of hydrogen distribution. E is the incident energy. The empirical formula for methane reaction yield is given by the following equation :

$$Y_{CH_4}(E,t,T)= \frac{A\exp\left(-\frac{Q_1}{k_BT}\right)}{B+C\exp\left(-\frac{Q_2}{k_BT}\right)}\int_0^{R(E)} n_H(x,t,T)dx \quad (1).$$

where Y_{CH4} is the methane reaction yield (CH_4 molecules/ion), n_H is the surface concentration of hydrogen (cm^{-2}), Q_1 is the activation energy (eV) of methane formation, Q_2 is the activation energy (eV) of recombination, T is the temperature, t is the irradiation time. x is the depth from surface, k_B is Bolztmann constant and A, B and C are fitting parameters. Furthermore, we assumed that D/C ratio in graphite is 0.4.

Results and disscusion

The ACAT-DIFFUSE code, which incorporates the above empirical formula on chemical sputtering, was used to fit Yamada's data [3]

Figure 2 shows depth distribution of deuterium in graphite at several fluence. The hydrogen in graphite indicate the saturation concentration at the fluence of 1.0×10^{17} (H /cm^2/s) because we assume the H/C ration is 0.4.

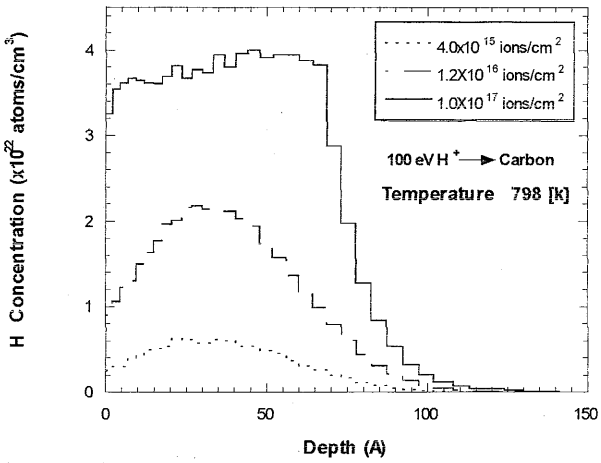

Fig. 2 Depth distribution of hydrogen concentration in graphite

Figure 3 shows the result indicating that generally there is good agreement between the model and data although further adjustment may be necessary.

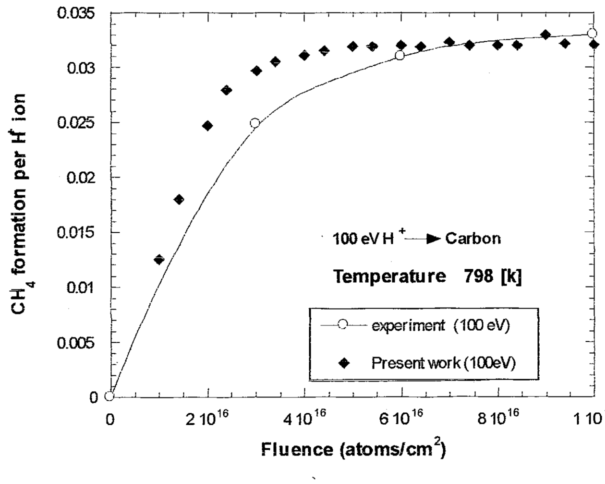

Fig.3 Fluence dependence of methane formation

[1] Y.Yamamura, Nucl. Instrum. Methods **B28** (1987) 17
[2] J. Roth and C. Garcia-Rosales, Nuclear Fusion **vol. 36 no. 12** (1996) 1647
[3] R.Yamada, K. Nakamura, K. Sone and M. Saido, J. Nucl. Mater. **95** (1980) 278