§3. Modeling of Deuterium Retention in Carbon Fiber Composite NB31

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Understanding the dynamics of in-depth migration and retention of hydrogen isotopes in Carbon Fiber Composites (CFCs) used as plasma facing material has for long time been complicated by the lack on in situ analyzing tools. A dedicated experimental setup coupling an ECR ion source to the Saclay nuclear microprobe (CEA, France) was developed to expose CFC NB31 samples to deuterium implantation at $200 - 300$ eV and fluences from 10^{22} to 10^{24} D/m^2, and then to perform in situ $\mu-$NRA analysis for 3D deuterium profiles.

Main result was that when deuterium concentration at the surface is homogeneous and fluence-independent, the in-bulk deuterium is concentrated in the porosities and increases in quantity with the incident fluence, up to very large depth (500 μm). Moreover, these two distinct mechanisms are simultaneous to the implantation and D profiles evolve very little with in-vacuum storage time [1].

These measurements were complemented by TDS and micro-porosimetry experiments, for characterizing the energy distribution of the deuterium traps and the size distributions and effective surface of the porous network. It was shown that the energy distribution of traps is different in the near surface and porous network, the former been characterized by a much larger ratio of bounds associated to sp3 carbons with respect to those associated to sp2 carbons, and that matrix ($1 >$ diameter (μm) > 0.1) and interfacial fiber/matrix pores ($0.1 >$ diameter (μm) > 0.01) dominate the porous network, both with an effective surface of ~ 0.1 m^2/g.

This ensemble of results suggests a picture where the deuterium concentration saturates in the near surface - partly amorphized due to ion bombardment, when the retention in the porous network increases on a longer timescale, the deuterium atoms penetrating along the pores up to a depth ≥ 100 μm.

For interpreting the measurements, a model was built according to the picture described above. It is based on a Monte Carlo method and calculates the propagation of D atoms in a network of pores assumed to be rectilinear. At each impact, the reflection/absorption coefficient and direction/energy of the reflected particle (atom or molecule) are estimated through TRIM simulations [2]. Input parameters are the diameter, volume, effective surface and average inclination of the pores with respect to the sample macroscopic surface. The three former are deduced of porosimetry measurements, the latter is partly constrained by SEM images.

Preliminary results are displayed in Fig. $1 - 3$, showing the variation of the deuterium concentration profile with incident fluence (Fig. 1), implantation temperature (Fig. 2) and the increase of the retained fluence as a function of the incident fluence (Fig. 3). Corresponding measurements are displayed in Figs. 1 and 2 of Ref. [3]. It is found that the simulations reproduce satisfactorily the main trends of the measurements, but that the porous network contribution to deuterium retention is underestimated. This has been identified to be due to the fact that D-rich deposits form in the pores, increasing their retention capability. Work for including this effect in the code is ongoing.

[1] E. Bernard et al., *J. Nucl. Mat.* **438** (2013) S975
[2] J. F. Ziegler, *Nucl. Instr. Meth.* **B. 219-220** (2004) 1027
[3] J. Roth et al., *J. Nucl. Mat.* **363-365** (2007) 822

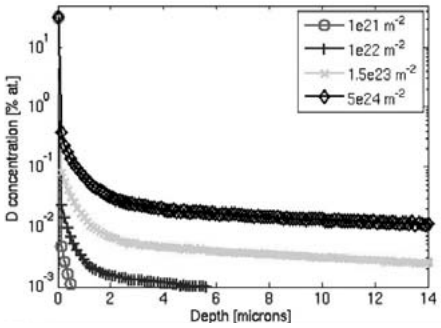

Fig. 1 Simulated deuterium concentration profile of CFC NB31 irradiated by 200 eV D^+ ions as a function of incident fluence. Samples are at a temperature of 50 °C.

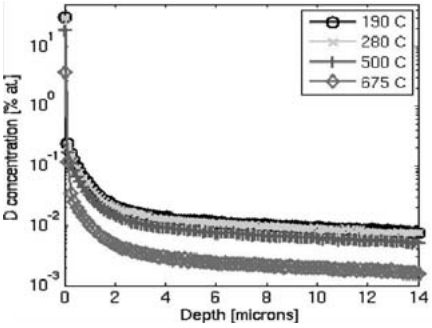

Fig. 2 Simulated deuterium concentration profile of CFC NB31 irradiated by 200 eV D^+ ions as a function of sample temperature (middle), for a fluence of 2×10^{24} D/m^2.

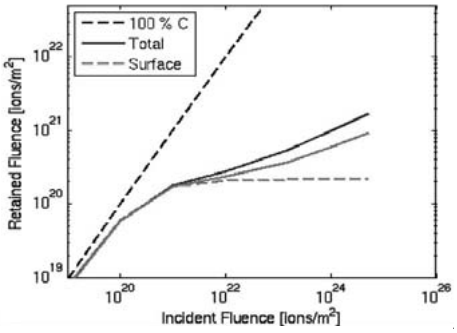

Fig. 3 Retained fluence as a function of the incident fluence: the dashed black line corresponds to 100 % retention, the dashed pink curve to a massive sample, the full lines to porous CFC NB31 (the pink curve is the near surface retention; the blue curve is the total retention, including the porous network).