ABSTRACT ICTP-2014-SMR-2614

2014 Joint ICTP-IAEA Conference on Models and Data for Plasma-Material Interaction in Fusion Devices, 3–7 November 2014, International Centre for Theoretical Physics (ICTP), Trieste, Italy.

## Hydrogen isotope retention and release in beryllium: The full picture from experiment and ab initio calculations

Ch. Linsmeier<sup>a</sup>, A. Allouche<sup>b</sup>, M. Oberkofler<sup>c</sup>, M. Reinelt<sup>c</sup>, K. Schmid<sup>c</sup>, R. Piechoczek<sup>c</sup>

Beryllium is the material chosen for the first wall in the main chamber of ITER, covering more than 80% of the surfaces directly exposed to the fusion plasma. The interaction of hydrogen isotopes deuterium and tritium with this material is therefore of crucial importance. Both safety (inventory of radioactive tritium) and operational reasons (density control) require a detailed understanding of the interaction physics of kinetic hydrogen isotopes with beryllium. The mechanisms for implantation, retention, diffusion and release are the fundamental steps in this description.

From well-defined laboratory experiments data on these physical processes is collected. In combination with first principles density functional theory calculations, the experimental observations can be modelled in a rate equation-based approach and a full description of the retention and release mechanisms is achieved.

This presentation offers an overview on the experimental observations in the interaction of deuterium ions with well-defined single and polycrystalline beryllium materials. The fundamental physical mechanisms governing retention and release are described and a rate equation model is successfully applied. The combination of both well-defined experiments and density functional theory results allows this complete description. In addition, it is demonstrated how such a detailed understanding of processes at an atomistic level can be combined in the integrated modelling of the interaction of a tokamak plasma with the first wall structures.

<sup>&</sup>lt;sup>a</sup> Forschungszentrum Jülich GmbH, Institut für Energie- und Klimaforschung – Plasmaphysik, 52425 Jülich, Germany

<sup>&</sup>lt;sup>b</sup> Physique des Interactions Ioniques et Moléculaires, CNRS and Université de Provence, Campus de Saint Jérôme, Service 242, 13397 Marseille Cedex 20, France

<sup>&</sup>lt;sup>c</sup> Max-Planck-Institut für Plasmaphysik, Boltzmannstr. 2, 85748 Garching b. München, Germany *Email address of corresponding author: ch.linsmeier@fz-juelich.de*