Ph.D. defense

Institut de Chimie Séparative de Marcoule / CEA Marcoule
(UMR 5257, CEA, CNRS, Université Montpellier, ENSCM)

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will present his Ph.D. dissertation

Mesoporous silicas behaviour under ion irradiation

The defense will take place on **Friday, December 9, 2016** at **2.00 pm**
in the ICSM Auditorium

In the search of new solutions to treat radioactive effluent, the so-called “separation-conditioning” strategy, which consists in implementing a functionalized porous matrix for the radionuclide adsorption, is an interesting alternative way. Such porous matrix could even act as a long term conditioning matrix in a second step. For this purpose, mesoporous silica presents several advantages like enormous fonctionalisable surface area, low temperature synthesis and possible pore closure through chemical, mechanic or thermal processes, favoring hence long term conditioning. With the presence of radionuclide, the mesoporous structure will be exposed to self-irradiation. This is why it’s important to evaluate the structure evolution under such conditions.

The objective of this thesis is to compare different mesoporous structures under various irradiation conditions which induce two major effects, the ballistic (nuclear) effect and the inelastic (electronic) effect. In order to achieve these objectives, external irradiations with heavy ions were applied to simulate self-irradiation processes. Adapted post-irradiation characterizations, like X-ray reflectivity and gas adsorption, were carried out. In the ballistic regime, a total compaction due to mesopores’ collapse is observed at a dose of about ~10^{22} keV/cm^3 (~1.4 dpa). In the electronic regime, ions of stopping power inferior to 1 keV/nm do not induce obvious effect on the mesoporous structure evolution. Only the Ni-638 MeV with stopping power ~5 keV/nm above track formation threshold induces a significant collapse effect but no total compaction was observed until the maximum studied dose about $E_{elec.}$=10^{21} keV/cm^3. These results indicate a good resistance of these structures against irradiation damage.

The origins of these structural behaviors are still not clearly understood. A comparative study between irradiation and thermal effects showed that the latter, act as a minor effect because it implies completely different densification process. Additionally, a study using classical molecular dynamics modelling for purely ballistic effects was undertaken. Although with the presence of some parametrical incoherence, it allows to successfully reproduce mesopores collapse and to propose preliminary mechanisms explanation in case of ballistic regime. In the electronic regime, the results are compatible with literatures.

Keywords: Ionic irradiation; Mesoporous silica; Separation-Conditioning; Irradiation damage; Molecular Dynamics