Study of the hyperfine parameters in Si and Fe doped HfO2 nanoparticles by perturbed angular correlation spectroscopy

T.S.N. Sales[1,2], R.N. Saxena[1] and A.W. Carbonari[1]

[1] *Instituto de Pesquisas Energéticas e Nucleares, IPEN, Universidade de São Paulo, São Paulo, Brazil*
[2] *Universidade Paulista, UNIP, São Paulo, Brazil*

rnsaxena@ipen.br

Nanoparticles (NPs) have attracted a great deal of interest due to their desirable properties suited for technological and medical applications. Hafnium dioxide (HfO_2) can be used in both areas. HfO_2 NPs were synthesized through sol-gel method, which allows an efficient and controlled doping of HfO_2. In this work, we have investigated the effect of (5% at.) doping of HfO_2 NPs with Si and Fe by measuring hyperfine interactions at ^{181}Ta probe nuclei on Hf sites using the perturbed γ–γ angular correlations (PAC) spectroscopy. The structural and morphological analysis was carried out by X-ray diffraction (XRD) and transmission microscopy (TEM) techniques. For both samples, XRD results showed a single phase with the expected monoclinic structure and TEM results indicated NPs with an average diameter of approximately 30 nm. The hyperfine parameters were measured in the temperature range of 200-900 ºC. The radioactive ^{181}Hf was produced by irradiating the samples with neutrons in the IEA-R1 reactor at IPEN. The samples were enclosed in the alumina tube instead of usual silica tube to avoid the formation of hafnon. Results of both samples showed that probe nuclei occupy three sites with different electric quadrupolar interactions. The major fractions (~65%), in both cases however, showed the well-known monoclinic structure of pure HfO_2 [1]. The characterization of one of the minor fractions in Si doped HfO_2 showing a tetragonal structure between 400-600 ºC is discussed.

[1] M. Forker, P. de la Presa, W. Hoffbauer, S. Schlabach, M. Bruns, and D. V. Szabó, Phys. Rev. B 77, 054108, 2008.