Solid State Physics with Nuclear Techniques

EFFECT OF SILICON DOPING IN HfO_2 NANOPARTICLES FROM AN ATOMIC VIEW

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Nanoparticles 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. Simple and low-cost synthesis of HfO_2 as thin films or nanoparticles are, therefore, very important for applicability of these materials. The sol-gel method of synthesis besides fulfilling these characteristics also allows an efficient controlled doping of HfO_2 with different elements to improve its properties. In this work, we investigated the effects of the doping with 5 at.% of silicon in HfO_2 nanoparticles prepared by the sol-gel method by measuring hyperfine interactions at ^{181}Ta probe nuclei on Hf sites using the $\gamma - \gamma$ perturbed angular correlations (PAC) spectroscopy.

The HfO_2 powder was obtained by sol-gel method from high purity Hf (99.99%) and Si (99.99%) elements. Initial colloid includes Hf and Si dissolved in appropriated acids, citric acid and ethylene glycol all in stoichiometric proportion. The solution (sol) was heated to 100°C until gel aggregation. After that, the solution was calcined in air at 550°C for 14 hours in order to evaporate organic materials present in the gel.

Part of the resulting powder had their structure investigated by X-ray diffraction (XRD). Another part was irradiated with neutrons in the IEA-R1 research reactor of IPEN to produce radioactive ^{181}Hf(^{181}Ta) to carry out hyperfine interactions measurements by PAC. This methodology has the advantage to assure an extremely low concentration and highly homogenous distribution of probe nuclei along with a very well defined location of them. These features enable the investigation of different regions inside the nanoparticles, within an atomic resolution, concerning point defects and formation of other phases. Hyperfine paramenters were measured within the range from 200°C to 900°C. XRD results showed a single phase with the expected monoclinic structure for the as-prepared samples indicating that Si atoms are at substitutional Hf sites. However, PAC results for the electric field gradient and asymmetry parameter measured with ^{181}Ta probe at 600°C indicate that Si dopants can induce dislocation of Hf atoms from their native location in HfO_2 throughout the lattice.

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NUCLEAR BASED TECHNIQUES IN MULTIFUNCTIONAL MATERIALS CHARACTERIZATION

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The Nuclear Science and its technologies have provided fundamental tools for the understanding of new chemical and physical properties that help the development of the new age of multifunctional materials such as the Perovskites for photovoltaics and fuel cells, the luminescent oxides for lighting and biomarkers and the thin films in semiconductors. One of the most important parameters that defines key properties of the Perovskites to be applied as the cathode in fuel cells is their crystal structure and its point defects (e.g. oxygen vacancies), which can be determined by neutron diffraction (Fig. 1a).

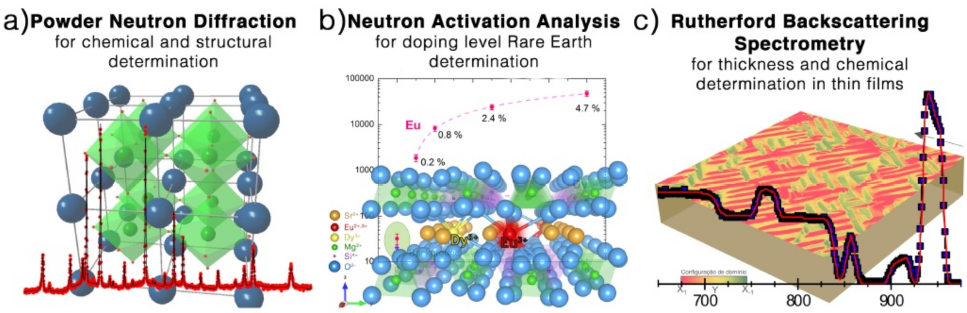

Figure 1: Nuclear based techniques applied on the characterization of multifunctional materials such as Perovskites for Fuel Cells (a), Rare earth doped luminescent oxides for lighting and biomarkers (b) and ferroelectric thin films for logic devices (c)

Photonic materials like luminescent nanoparticles, once doped with Rare Earth ions, they can emit light when excited with UV/IR, being used in probing bioassays. In this case, the precise determination of Rare Earth concentration by Instrumental Neutron Activation Analysis (INAA) leads to ensure the desired spectroscopy properties to prepare efficient probing nanoparticles (Fig.1b). Furthermore, nuclear based techniques such as Rutherford Backscattering Spectrometry (RBS) help us in determining the thickness and the elemental composition of thin films (Fig. 1c), which is not usually easy through other conventional techniques. In other words, the nuclear based techniques applied on materials characterization play a key role in providing a