

## Investigation of HfO<sub>2</sub> and ZrO<sub>2</sub>, Separately and Also in the Form of Mixtures, Pure and Doped with Si

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The HfO<sub>2</sub> has been used in several technological applications, one of which is the replacement of silicon oxide as the material for the door in the manufacture of CMOS-FET devices [1]. ZrO<sub>2</sub> also has several applications, being more used in the form of solid electrolytes and oxygen sensors and also in electrochemical pumps. Due to the similarity of the size and properties, that is found in the proportion of 1 to 2 % in the ore of this one. Since the ions of these elements are nearly identical in size, the separation is difficult, and is in most cases unnecessary due to the similarity of its properties [2]. Doping with other elements improves the specific characteristics of HfO<sub>2</sub> and ZrO<sub>2</sub>, making them useful for different applications and extending their uses in CMOS-FET devices. It also reduces the ZrO<sub>2</sub> defects, such as its low resistance to high temperatures, causing in the formation of polycrystalline films and decreasing the dielectric constant that can occur due to leakage current in the grain boundaries, making it necessary to use an amorphous interface to reduce losses. In addition, grain size and orientation change throughout a polycrystalline film, which can cause variations in the value of producing irreproducible properties [3]. In this project the atomic scale investigation of HfO<sub>2</sub> and ZrO<sub>2</sub> was carried out separately and also in the form of pure, doped mixtures with Si [4]. They were used (RBS), X-ray Diffraction [5] and SEM for characterization. The PAC technique was used to measure the hyperfine parameters, such as the electric field gradient (V<sub>zz</sub>), the asymmetric parameter of the electric field gradient (η) and the possible magnetic hyperfine field over a wide temperature range (from 10 to 1300 K). The measurements were performed in order to correlate the results with the behavior of the characteristic properties of each compound to understand the microscopic mechanisms that give rise to these phenomena [6].

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