Investigation of (non) polar Crystallographic Structures of (un) doped HfO_2 Bulk Ceramics and Nanoparticles

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Ferroelectric properties were discovered in HfO_2 thin films, which enabled HfO_2 to be considered for lead free ferroelectric capacitors or transistors for non-volatile memories. At ambient conditions HfO_2 is monoclinic and nonpolar, but the ferroelectricity discovered in thin films has been attributed to the formation of an orthorhombic polar phase due to chemical doping and stresses induced by the substrate and capping layer.[1-2] Although the ferroelectric properties of doped HfO_2 films have been rigorously investigated, fundamentals of the relationship between the observed ferroelectric properties and underlying structure are still not fully understood.

To elucidate fundamentals associated with the phase stability and crystallography of these systems, we present here results on powder and bulk compositions of HfO_2-based materials. Specifically, we investigated Y-, Gd-, and Sc-doped HfO_2 nanoparticles and bulk ceramics at various dopant concentrations and as a function of synthesis conditions. These dopants can induce the formation of the cubic or tetragonal phases in the bulk and nanoparticle forms of HfO_2, [3-5] a pathway toward the formation of the orthorhombic phase at lower temperatures. X-ray diffraction patterns were measured for each of the doped HfO_2 powders to determine the structures changes that occurred due to doping and heat treatment. It is observed in the Y and Gd-doped HfO_2 XRD patterns, that the cubic phase can be formed and sustained at ambient conditions. Further analysis of the diffraction patterns was performed using Rietveld Refinement. These results were used to determine the change in phase fractions and lattice parameters of the HfO_2 crystal structure. Based on these results, we consider Y and Gd-doping to be pathways to realizing ferroelectric properties in HfO_2 bulk ceramics.

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