Charge Distribution Model in Cubic Perovskite-type Compounds

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A non-zero electric field gradient tensor, detected by probes that occupy sites with cubic point group symmetry, was observed in many ABO_3 perovskite-type compounds. This breakdown of local cubic symmetry is commonly associated with the presence of oxygen vacancies around the probe. This effect in $BaTi_xHf_{1-x}O_3$ with x = 0.7, 0.5, 0.3, 0.1, 0.05 and 0.01 is studied in this work. The cell parameters were obtained at laboratory temperature using XRD spectroscopy. The hyperfine parameters were measured at a ^{181}Ta probe in the B site using Perturbed Angular Correlations (PAC) spectroscopy as a function of both temperature and composition. As a common trend, a static asymmetric and distributed quadrupolar interaction, strongly dependent on composition has been observed. The results, together with those corresponding to $1 > x \geq 0.75$, are analyzed using the point-charge model in terms of polarized oxygen vacancies, different covalence of the Ti-O and Hf-O bonds with computational simulation for the lattice positions of cations and oxygen vacancies.

Key words: Perovskites; Ferroelectrics Materials; Defects; Polarized Oxygen Vacancies; Electric Field Gardient.