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Synthesis of (Zn + Nb) co-doped TiO₂ rutile nanoparticles and dielectric properties

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Zn^{2+} / Nb^{5+} co-doped TiO_2 (ZNTiO) nanocrystalline powders were prepared by a combustion process. A pure rutile- TiO_2 phase of powders and sintered ceramics with a dense microstructure was achieved. Both co-dopants were homogeneously dispersed in the ceramic microstructure. The presence of oxygen vacancies was confirmed by Raman techniques. The thermally activated giant-dielectric relaxation of ZNTiO ceramics was observed. Removing the outer-surface layer had a slight effect on the dielectric properties of ZNTiO ceramics. The density functional theory (DFT) calculation showed that, in the energy preferable configuration, the 2Zn atoms are located near the oxygen vacancy, forming a triangle-shaped ZnVoTi defect complex. This defect cluster was close to the diamond-shape 2Nb2Ti defect complex. Thus, the electron-pinned defect-dipoles (EPDD) can be formed. The giant-dielectric relaxation process of the ZNTiO ceramics might be attributed to the interfacial polarization associated with electron hopping between Zn^{2+} / Zn^{3+} and Ti^{3+} / Ti^{4+} ions inside the grains, rather than due to the surface barrier layer capacitor (SBLC) or EPDD effect.

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