Lattice dynamics and dielectric response of Mg-doped SrTiO3 ceramics in a wide frequency range

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Abstract
SrTiO3 - based oxides are attractive materials for a wide range of applications in microelectronics, namely for microwave frequency tunable resonators and filters operating in GHz range [1]. It was recently reported by some of the authors that the solid solubility of Mg in ST is limited and depends on the substitution site of perovskite lattice [2]. Incorporation of Mg into B-site was thermodynamically favourable and a higher solid solubility limit was observed. Dielectric characterization at low frequencies showed that Mg either in A or B-site of the perovskite lattice does not induce any ferroelectric or relaxor-like anomaly. Moreover, Mg B-site doping drives the system away from the ferroelectric instability, decreasing maximum permittivity values significantly. In the present study the dielectric properties of Sr1-xMgxTiO3 (SMT) and SrTi1-yMgyO3-δ (STM) ceramics were investigated in rf, microwave, terahertz and infrared (IR) range. MicroRaman spectroscopy measurements were also conducted. The MicroRaman spectra and the high frequency dielectric properties of SMT do not differ considerably from the properties of undoped ST, confirming the small if any incorporation of Mg into A-site of ST lattice. At the same time, B-site Mg doping results in significant hardening of ST crystal lattice, observed in IR reflectivity spectra. Dielectric permittivity and loss decreasing both in rf and terahertz range corresponds to the hardening of the ferroelectric soft mode. The appearance and enhancing of forbidden polar modes TO4 at 546 cm⁻¹ and TO2 at 171 cm⁻¹ at room temperature in Raman spectra demonstrates the local loss of the inversion centre and the breaking of the ST cubic symmetry by the substitution of Ti⁴⁺ with Mg²⁺ ions. These results confirm more favourable occupation by Mg of B-site of ST lattice [2]. 1. R. Ott and R. Wordenweber: Appl. Phys. Lett. 80, 2150 (2002) 2. A. Tkach, P.M. Vilarinho, A.L. Kholkin: accepted to Appl. Phys. A