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Title

Polar lattice vibrations and phase transition dynamics in Pb(Zr(1-x)Ti(x))O(3)

Source

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Abstract

Infrared (IR) reflectivity spectra of nominally pure Pb(Zr(1-x)Ti(x))O(3) ceramics with different Ti/Zr concentration (x = 0.42-0.58) were measured and evaluated, along with the time-domain terahertz transmittance spectra in the temperature range 10 K-900 K. The temperature dependence of the low-frequency vibrations, related to Pb atoms, was analyzed in terms of two overdamped modes-a soft mode and an anharmonic hopping central mode-in the cubic and high-temperature ferroelectric phase and three main vibrations in the low-temperature ferroelectric phase with the doubled unit cell: two E-symmetry modes (the soft mode and a mode corresponding to antiphase vibrations of neighboring Pb atoms in the terahertz range) and the antiferrodistortive mode producing the antiphase tilts of the oxygen octahedra. The last bare mode is not IR active, but it becomes activated by coupling with the soft mode. As predicted by theory, the intrinsic permittivity of Pb(Zr(1-x)Ti(x))O(3) has a maximum at the morphotropic phase boundary, although this represents just a small percentage of the total permittivity at lower frequencies. Its maximum is linked to the softening of the anharmonic vibrations of Pb ions, perpendicular to the polarization, and shifts from x = 0.48 at room temperature to x = 0.52 at 10 K..