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The Jahn-Teller effect in Cr5+-doped PbTiO3: A multi-frequency electron paramagnetic resonance study

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Abstract

Electron paramagnetic resonance (EPR) spectra of Cr5+ defects incorporated on Ti4+ sites in powdered ceramics of PbTiO3 were investigated in the temperature range 50-400K at 9GHz (X), 34GHz (Q) and 94GHz (W band). The Jahn-Teller effect stabilizes the vibronic ground state of the 3d1 electron of the Cr5+ ion and leads to a tetragonally distorted defect- O6 octahedron with the point symmetry D4h. The spontaneous electrical polarization present in the ferroelectric phase of PbTiO3 appears as a further perturbation producing an additional g-tensor contribution by the quadratic field effect. Its symmetry is dependent on the orientation of the electrical polarization with respect to the Jahn-Teller distortion axis, the tetragonal axis of the defect- O6 octahedron. If the polarization of a domain is anti-or parallel to this axis, the local tetragonal symmetry of the Cr5+ ion persists whereas it is reduced by a perpendicular orientation. Anisotropic EPR spectra of tetragonally and orthorhombic distorted Cr5+O6 12- are detected at low temperatures. Increasing the temperature, the peaks of the two spectra are broadened and a motionally averaged isotropic spectrum appears at 200K. © 2010 IOP Publishing Ltd.

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