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The Dielectric Properties of Complex Oxides: $CaCu_3Ti_4O_{12}$ and Other Perovskites¹ GEORGE SAMARA, Sandia National Labs

Detailed studies of the properties of ceramic CaCu₃Ti₄O₁₂ (CCTO) have clarified the physics of this interesting material. The unusual dielectric relaxational properties of CCTO are explained in terms of a capacitive-layer model, as for an inhomogeneous semiconductor consisting of semiconducting grains and insulating grain boundaries. The kinetics of the main (low T) relaxation reveal that two different thermally- activated processes in the CCTO grains control the dynamics. A higher T relaxation is determined by grain boundary conduction. Both Nb and Fe doping lower both the dielectric constant, ε' , and loss, but Fe doping leads to the more dramatic effects; 3 at.% Fe removes the anomalous ε' (T) response making CCTO an intrinsic dielectric. The intrinsic ε' (\simeq 75) and its T dependence are shown to be largely determined by a low-lying soft TO phonon. At low T, cubic CCTO transforms into an antiferromagnetic phase at $T_N = 25$ K. T_N decreases significantly with Fe doping. Analysis of the high T dependence of the magnetic susceptibility provides insight into the role of Fe. Finally, an ε' (T) anomaly associated with the onset of antiferromagnetic order has been discovered providing evidence for coupling between the polarization and sublattice magnetization. Possible origin of this coupling is discussed. We have also observed large dielectric constants and relaxations similar to those in CCTO in doped single crystals of KTaO₃.

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