

Hard-mode infrared spectroscopy of perovskites across the CaTiO₃-SrTiO₃ solid solution

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ABSTRACT

Powder infrared spectra of perovskites across the CaTiO₃-SrTiO₃ solid solution have been collected at room temperature for the range 20–700 cm⁻¹. Frequency, intensity, and line broadening parameters vary with a pattern that appears to follow the development of the orthorhombic shear strain for the *Pnma* structure. The data are at least consistent with the *Pm3m* ↔ *I4/mcm* transition at Sr-rich compositions being continuous in character and the tetragonal ↔ orthorhombic transition at ~62% SrTiO₃ content being discontinuous. In spite of the fact that crystals with intermediate composition have recently been shown to have *Pnma* rather than *Cmcm* symmetry, autocorrelation analysis of their IR spectra shows that they have features which distinguish them from crystals with *Pnma* symmetry for CaTiO₃ rich compositions. In particular, crystals of intermediate composition have the highest values of the line broadening parameter, Δ_{corr} , for the solid solution, suggesting that they are characterized by relatively high degrees of local structural heterogeneity.