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Title:On the terahertz dielectric response of cubic $BaTiO_3$: Coexistence of displacive and order-disorder dynamics

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Abstract:Two distinct modes with frequencies below 150 cm^{-1} were recently observed in cubic $BaTiO_3$ (Ponomareva I. et al. , Phys. Rev. B , 77 (2008) 012102). One of these modes perfectly softens to zero while the other saturates at about 60 cm^{-1} as the ferroelectric transition is approached. In the present work, we interpret these modes employing two widely recognized elements: nano-size tetragonal precursors forming in the cubic phase and an eight-well potential model for Ti ions due to Comes, Lambert and Guinier (Solid State Commun., 6 (1968) 715). We show that the frequency squared of the saturating mode (SM), which exists in the cubic phase, and that of an E-symmetry mode (EM), which exists in the tetragonal phase, fall on a single curve, ~33 cm^{-2} K^{-1} (T-T*), thereby suggesting connections between the lattice dynamics across the ferroelectric transition. T* is predicted and confirmed to coincide with the tetragonal-orthorhombic transition temperature of 290 K. The perfectly softening mode (PSM) is argued to be associated with the re-orientational motions of tetragonal precursors. The complex dielectric function is calculated without free inputs and the result agrees satisfactorily with measurements. The SM is characterized as a resonant mode, whereas the PSM as a relaxational mode, confirming that both order-disorder and displacive dynamics coexist in cubic $BaTiO_3$.

Number of references:41

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Uncontrolled terms:terahertz dielectric property - order-disorder dynamics - distinct modes - ferroelectric transition - nanosize tetragonal precursors - cubic phase - eight-well potential model - E-symmetry mode - cubic phase - tetragonal phase - tetragonal-orthorhombic transition - dielectric function - displacive dynamics - $BaTiO_3$

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