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Time-domain THz spectroscopy of central modes in BaTiO3 and SrTiO3

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The dielectric response to terahertz (THz) waves of many materials exhibiting ferroelectric phase transition provides unique information about its origin and driving mechanisms. We will discuss this issue within the frame of recently obtained results in perovskite BaTiO3 and SrTiO3 single crystals and strained thin films and multilayers.
Crystals in the vicinity of ferroelectric phase transitions are characterized by a delicate compensation of various microscopic forces. Two excitations, a soft phonon mode and a central mode, are often coexisting in the THz spectral range and represent the driving force of the phase transition. Due to their polar character, they can be easily detected in the THz transmission measurements. The THz spectra can be fitted with a term describing a damped oscillator and a coupled Debye relaxation [1]. Close to the ferroelectric phase transition, anharmonic properties of the crystalline lattice potential often play a crucial role and can be experimentally accessed [2] e.g. by investigating the electric-field dependence of the response.
In parallel, molecular dynamics simulations of the soft mode based on an effective Hamiltonian method [1] allow one to attribute microscopic interpretation to the above phenomenological description. By comparing the experimental data to the simulations in BaTiO3 we have shown [1] that the coexistence of two excitations in this compound is an attribute of a single degree of freedom (Ti displacements within the O6 octahedra) with a complex anharmonic potential.

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