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Anharmonic Behavior in BaTiO3: Investigation by Raman Spectroscopy

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Abstract : BaTiO3 (BT) is a well known ferroelectric material which has been thoroughly studied during several decades since it undergoes successive cubic-tetragonal-orthorhombic-rhombohedral phase transitions on cooling. It has several ferroelectric properties that allow it to be a good material for electronic applications such as the design of ferroelectric memories and pyroelectric elements. In the present work, we report the analysis of temperature dependence of Raman frequency and damping of the A1 modes polarized along the FE c axis as well as the optical phonons E corresponding to the ionic motions in the plane normal to c. Measurements were carried out at different temperatures ranging from 298 to 408 K (tetragonal phase) within different scattering configurations. Spectroscopic parameters of BT have determined using a high resolution Raman spectrometer and a fitting program. All the first order frequency modes exhibit a quasi linear decrease as function of the temperature, except for the A1[TO1], E[TO2] and E[TO4] lines which reveal a parabolic dependence illustrating an anharmonic process. The phonon frequency downshifts and damping evolutions are interpreted in terms of normal volume expansion and third- and fourth-order anharmonic potentials.

Keywords : BaTiO3, Raman spectroscopy, frequency, damping, anharmonic potential
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