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Sub-THz Raman response and critical dynamics in BaTiO3

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Sub-THz Raman response and critical dynamics in BaTiO3 (talk)
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BaTiO3 (BTO) is considered as a textbook material for the description of structural phase transitions (SPT) and the appearance of ferroelectricity. On cooling it undergoes successive cubic-tetragonal-orthorhombic-rhombohedral (C-T-O-R) phase transitions [1]. Various concepts such as soft phonon, central peak, relaxational mode, hard phonon are invoked to describe the dynamics of the lattice, the structural changes or the occurrence of ferroelectric state in this material [2,3,4,5]. The displacive or order-disorder (OD) character of the paraelectric-ferroelectric transition is long-standing object of controversies [4,6]. It is now admitted that both mechanisms co-exist [7,8]. It is to be underlined that up to now the simultaneous detection of both processes by the same technique was not so far reported. The possibility of existence of two critical degrees of freedom was only drawn by ab-initio calculations [9], or was indirectly derived from the discrepancy in dielectric permittivity between direct data and calculations via LST relationship [6,7]. Raman spectroscopy was widely used for investigate lattice dynamics and phase transition in BTO, but the very high damping of the soft phonon [3,10] impedes to extract the additional OD feature which should be located at lower frequency. Here we report new Raman spectra recorded as function of temperature in the tetragonal phase, using ultra low-frequency (ULF) set-up. This tool provides the measurement of Raman shift down to 5 cm-1 with respect of the Rayleigh line, providing therefore the detection of vibrational or relaxational modes centered around 200 GHz. Within the contribution we firstly discuss the differences and similarities in the various concepts used to describe lattice dynamics with link with SPT. Then we present new Raman data in BTO and highlight the occurrence of the additional peak lying at frequency lower than the soft phonon. The intensity and shape of this peak are strongly dependent on temperature. This feature is attributed to a local mode, related to Ti-off centering with a characteristic relaxation frequency showing a slowing down on approaching the T-C, and the T-O SPT as well.

[1] F.Jona and G.Shirane, Ferroelectric crystals, (MacMillan, New York), 1962
[2] K.A Muller, Y.Luspin, J.L. Servoin, and F.Gervais, J.Physique 43, L537 (1982)
[3] H. Vogt, J.A. Sanjurjo and G. Rossbroich, Phys. Rev. B 26, 5904 (1982)
[4] J. P. Sokoloff, L. L. Chase and D. Rytz, Phys. Rev. B 38, 597 (1988).
[5] M.D.Fontana, K.Laabidi and B.Jannot, J.Phys. Condens. Matter, 6, 8923 (1994)
[6] K. Laabidi, M. D. Fontana, M. Maglione, B. Jannot and K. A. Muller, Euro. Phys. Lett. 26, 309 (1994).
[7] J. Hlinka, T. Ostapchuk D. Nuzhnyy, J. Petzelt, , P. Kuzel, C. Kadlec, P. Vanek, I. Ponomareva and L. Bellaiche, Phys. Rev. Lett. 101, 167402 (2008).
[8] H.Y.Deng, EPL 100, 270001 (2012).
[9] W. Zhong, D. Vanderbilt and K.M Rabe, Phys Rev B 52, 6301 (1995).
[10] G.Burns and F.H Dacol, Phys. Rev. B 18, 5750 (1978).

Summary

Topic

1. Multiferroics and ferroelectrics

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