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A Multinational Journal

Volume 81, 2008 - Issue 5

102 Views | 15 CrossRef citations to date | 0 Altmetric

Original Articles

Soft mode dispersion and 'waterfall' phenomenon in relaxors revisited

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Pages 491-508 | Received 03 Dec 2007, Accepted 04 Feb 2008, Published online: 07 May 2008

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Abstract

Results of recent inelastic neutron scattering studies of lead-based relaxor ferroelectrics by Gvasaliya et al. [J. Phys.: Condens. Matter 17, 4343 (2005); J. Phys.: Condens. Matter 19, 016219 (2007)] have put in question the existence of the "waterfall" anomaly—an apparent vertical dispersion segment joining the TA and TO branches—observed earlier in low-energy $[\xi 00]$ phonon dispersion curves of these materials. In the present article,

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Acknowledgements

The work is partly based on experiments performed at the Swiss spallation neutron source SINQ, Paul Scherrer Institute, Villigen, Switzerland. This research project has been supported by the European Commission under the 6th Framework Programme through the Key Action: Strengthening the European Research Area, Research Infrastructures. Contract No.: RII3-CT-2003-505925. Additional financial support was obtained from the Czech grant agencies (projects GACR 202/06/0403 and GACR 202/06/0411 and AVOZ 10100520). Authors thank to Dr S. Gvasaliya from Laboratory for Neutron Scattering of ETH Zurich and Paul Scherrer Institut in Villigen for useful discussions and the help with set-up of the experiment at TASP instrument, to Dr J. Petzelt from the Institute of Physics of Czech Academy of Science in Prague for careful reading of the manuscript and to Dr J. Kulda from the Institute Laue-Langevin for his long-term interest, encouragement, valuable suggestions and numerous critical discussions.

Notes

Notes

1. In the rest of this article, we use reduced (dimensionless) phonon wave vectors expressed in reciprocal lattice units (r.l.u.) given by $c^* = 2\pi/c$, (e.g. for PMN, $c = 4.04 \text{ \AA}$, i.e. $c^* = 2\pi/c = 1.555 \text{ \AA}^{-1}$).
2. First two hypotheses are close to those invoked in Ref. [17](#).

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6. In principle, PMN is known to grow also, for example in pyrochlore structure, but in this case both the lattice parameters and the TO mode frequency are completely different.

7. It was argued in [9](#) that the TO mode cannot couple noticeably to the TA branch because the independent mode intensities do not change with temperature. However, this not a valid argument since the measurements shown in figure of Ref. [9](#) were done in (20q) zone, where both TA and TO modes have similar structure factors so that eventual eigenvector change has no chance to produce such drastic intensity changes as those observed in the quoted [9](#) case of SrTiO₃.

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