

Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Phonon dispersion relation in PbTiO_3 ¹ IZUMI TOMENO, Akita University, JAIME FERNANDEZ-BACA, KAROL MARTY, ORNL, KUNIHICO OKA, AIST, YORIHICO TSUNODA, Waseda University — The phonon dispersion relations for cubic PbTiO_3 ($T_c = 763$ K) have been determined along the high symmetry directions at $T = 793$ K using inelastic neutron scattering. A set of the TO branches drops significantly toward the zone center. This is quite different from the soft mode anomaly in the Pb-based relaxors, named as the waterfall phenomenon. The zone-center TO mode energy softens with decreasing temperature from 1173 to 793 K. The TA branch along $[\xi, \xi, \xi]$ shows significant softening around $\xi = 0.25$ and 0.5. These two anomalies persist up to 1173 K and are weakly temperature dependent. Moreover, the TA branches along $[1,0,0]$ and $[1,1,0]$ soften in the entire q range as the temperature approaches T_c . Although the phonon softening occurs simultaneously, the softening of the zone center TO mode plays an important role in the single phase transition. The phonon dispersion relations for cubic and tetragonal PbTiO_3 are discussed in connection with BaTiO_3 , KTaO_3 , $\text{Pb}(\text{Zn}_{1/3}\text{Nb}_{2/3})\text{O}_3$, and $\text{Pb}(\text{Mg}_{1/3}\text{Nb}_{2/3})\text{O}_3$.

¹U.S.-Japan cooperative program on neutron scattering

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Date submitted: 07 Nov 2012

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