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Phonon dispersion relation in cubic $BaTiO_3$[1] IZUMI TOMENO, Akita University, JAIME FERNANDEZ-BACA, RIKI KOBAYASHI, SONGXUE CHI, Oak Ridge National Laboratory, KUNIHIKO OKA, National Institute of Advanced Industrial Science and Technology, YORIHIKO TSUNODA, Waseda University — The lattice dynamics of cubic $BaTiO_3$ (T_c = 405 K) has been investigated along the [100], [110], and [111] directions at T =453, 700 and 890 K using inelastic neutron scattering. The transverse acoustic (TA) phonon dispersion is relatively isotropic. This indicates that all the measured TA branches are mainly governed by the Ba atom motion against the O atoms. The zone-boundary TA phonon energies for $BaTiO_3$ are approximately twice as large as those for cubic $PbTiO_3$. These differences cannot be explained by the A-site atomic mass alone. The large Ba-O force-constant reflects the ionic nature of Ba atom in $BaTiO_3$. The softening of the transverse optical (TO) Δ_5 and Σ_4 branches in a wide q range at T = 453 K is in contrast to the steep softening of the TO Λ_3 branch toward the zone center. The TO Σ_4 mode is heavily damped in the range $q \leq$0.25 at 453 K, whereas the well-defined TO Σ_4 peak for q =0.25 is observed at 890 K. The low-lying TO Δ_5 and Σ_4 branches are primary due to the low-frequency Ti-O-Ti chain-like motion along [001]. The soft mode behavior in $BaTiO_3$ is discussed in comparison with the previous study on $PbTiO_3$.

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

Izumi Tomeno
Akita Univ

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