

Abstract Submitted
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Lattice dynamics of cubic PbTiO₃¹ IZUMI TOMENO, Akita University, JAIME A. FERNANDEZ-BACA, KAROL J. MARTY, ORNL, YORIIHIKO TSUNODA, Waseda University, KUNIIHIKO OKA, AIST — The lattice dynamics of cubic PbTiO₃ has been investigated using inelastic neutron scattering. We found four kinds of soft modes in cubic PbTiO₃: (1) the TO modes toward the Γ point, (2) the TA Λ_3 mode toward the R point, (3) the TA Λ_3 mode around the midpoint (1/4,1/4,1/4), and (4) the TA branches in the entire range. Moreover, the TO Σ_4 branch becomes flat away from the zone center. The steep dispersion of the TO modes toward Γ is isotropic and confined to the region $\xi < 0.2$. The temperature dependence of the Γ_{15} mode up to 1173 K is explained by a combination of the Lydanne-Sachs-Teller relation and the Curie-Weiss law. In contrast, the TA Λ_3 modes at the midpoint and R point are weakly temperature dependent. The coexistence of the soft Γ_{15} and R_{25} modes is in agreement with the predicted phonon instability. The midpoint softening suggests the tendency toward forming a fourfold periodicity along the [1,1,1] direction. The energy of the TO Δ_5 branch for cubic PbTiO₃ is considerably higher than that for Pb(Zn_{1/3}Nb_{2/3})O₃. This indicates that the TO modes are dominated by the B-site atom motion.

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