

Abstract Submitted
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Structural and Dynamical Properties of Barium Stannate D. PHELAN, Argonne National Laboratory, M. J. KROGSTAD, Northern Illinois University / Argonne National Laboratory, A. LOPEZ-BEZANILLA, Argonne National Laboratory, D. PARSHALL, NIST Center for Neutron Research, Y. GIM, S. L. COOPER, University of Illinois, H. ZHENG, Argonne National Laboratory — Barium stannate based perovskites have recently drawn attention due to their potential as transparent conducting oxides and reports of high carrier mobility in La-doped single crystals. Published DFT calculations and experimental results have suggested phonon instabilities at high symmetry zone boundary positions and local octahedral rotations, respectively, for BaSnO_3 . Here, we discuss recent structural measurements of BaSnO_3 , in which we have searched for such distortions by employing a combination of single crystal neutron diffraction and total scattering analysis of powder neutron diffraction. Moreover, we discuss lattice dynamical measurements, comparing phonon dispersion measurements to DFT calculations.

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