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NMR quadruopole spectra of PZT from first-principles[1] DANDAN MAO, College of William and Mary, ERIC J. WALTER, College of William and Mary, HENRY KRAKAUER, College of William and Mary — High performance piezoelectric materials are disordered alloys, so it can be difficult to determine the local atomic geometry. Recently, high field NMR measurements have shown great promise as a microscopic probe of ABO_3 perovskite-based alloys [2] by their ability to resolve line-splittings due to nuclear quadrupolar coupling with the electric field gradient (EFG) at the nucleus. We report first-principles LDA calculations of the EFG's in monoclinic and tetragonal $Pb(Zr_{0.5}Ti_{0.5})O_3$ systems using the linear augmented planewave (LAPW) method, and we compute NMR static powder spectra for ^{91}Zr, ^{47}Ti, and ^{17}O atoms as a function of applied strain. With decreasing c/a ratio PZT converts from tetragonal to monoclinic symmetry. We observe that the calculated NMR spectra show dramatic deviations with decreasing c/a from that in tetragonal $P4mm$ well before the electric polarization begins to rotate away from the [001] direction. This indicates that NMR measurements can be a very accurate probe of local structural changes in perovskite piezoelectrics.

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[2]G. L. Hoatson, D. H. Zhou, F. Fayon, D. Massiot, and R. L. Vold, Phys. Rev. B, **66**, 224103 (2002).

Dandan Mao
College of William and Mary

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