Abstract for an Invited Paper
for the SES06 Meeting of
The American Physical Society

Local Structure in PMSN Across the Ferroelectric Phase Transition[1]

ROBERT VOLD, College of William and Mary

Local structure and ^{93}Nb ion displacement play vital roles in the ferroelectric polarization and phase transitions of solid solutions with composition (1-x)$PbMg_{1/3}Nb_{2/3}O_3$– x $PbSc_{1/2}Nb_{1/2}O_3$ (PMSN). Here, we report variable temperature, high field (17.6Tesla) ^{93}Nb MAS and 3QMAS NMR studies of PMSN with compositions between x = 0.6 and 0 (pure PMN). In PMSN, six narrow components and one broad peak were observed. Spectral assignments agree with previous reports [D.H.Zhou, G.L.Hoatson, R.L.Vold, J. Magn. Reson. 167 (2004) 242-252 and references therein]. The broad peak is resolved only at temperatures below the dielectric susceptibility maximum (i.e., T $<T_c$). This peak represents niobium ions in configurations that contain at least one other niobium in the shell of next nearest B-site neighbors. Decreasing temperature results in broadening of all lines, most notably the distribution peak; its line width increases by nearly a factor of two between 320 and 240 K. 3QMAS spectra show that the broadening of the distribution peak is mainly due to an increase in the distribution of quadrupolar parameters, resulting from asymmetric ion displacements and bond length variations. These changes occur continuously across the broad ferroelectric relaxor phase transition, and allow conclusions to be drawn regarding the chemical composition of polar nanoclusters.

In collaboration with Gina Hoatson and Murugesan Vijayakumar, College of William & Mary.

[1]This work was supported by the Office of Naval Research, Grant N000140310661, and the National Science Foundation, Grant CHE0079136.