Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Multi phonon resonance Raman scattering, spin phonon coupling and lattice dynamics of antiferromagnetic $NdFeO_3$ MANOJ K. SINGH, RAM S. KATIYAR, Department of Physics, University of Puerto Rico,San Juan, PR-00931-3343,USA — The Raman-active phonons in the orthorhombic $NdFeO_3$ single crystals were studied by means of polarized Raman scattering and lattice dynamics computations (LDC). The A_g-symmetry zone-center phonons were distinguished from the B_{1g} eigenmodes by performing polarized Raman scattering experiments using two parallel polarization configurations, X′(ZZ)X′ and Z(X′X′)Z. Observed phonon spectra at 100, 300, 347 cm^{-1} showed anomalous temperature dependence in the range of the magnetic spin reorientation temperature (100 –200K) indicating strong spin -phonon coupling. The anomalously shaped observed phonon between 500 to 1500 $cm^{1}_{,}$observed in the A_g-symmetry X′(ZZ)X′ and B_{1g} spectrum was attributed to a multi-phonon scattering caused either by multiple combination of B_{1g} or by A_{1g}phonons. With the help of lattice dynamics calculations, we were able to assign most of the observed Raman-active modes, including B_{2g} and B_{3g}-symmetry phonons. The LDC results indicated that among the sixteen force constants employed, the force constant corresponding to the stretching vibration between the central Fe cation and the axial oxygen atom in a FeO_6 octahedron unit had the largest value.

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Date submitted: 06 Dec 2006 Electronic form version 1.4