Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

A Microscopic Model of Magnetoelectric Interactions in Ni3V2O8 TANER YILDIRIM, NIST Center for Neutron Research, A. B. HARRIS, University of Pennsylvania, A. AHARONY, O. ENTIN-WOHLMAN, Tel Aviv University, Israel — We develop a microscopic magnetoelectric coupling in $Ni_3V_2O_8$ (NVO) which gives rise to the trilinear phenomenological coupling used previously to explain the phase transition in which magnetic and ferroelectric order parameters appear simultaneously. Using combined neutron scattering measurements and first-principles calculations of the phonons in NVO, we determine eleven phonons which can induce the observed spontaneous polarization. Among these eleven phonons, we find that a few of them can actually induce a significant dipole moment. Using the calculated atomic charges, we find that the required distortion to induce the observed dipole moment is very small ($\sim$0.001 Å) and therefore it would be very difficult to observe the distortion by neutron-powder diffraction. Finally, we identify the derivatives of the exchange tensor with respect to atomic displacements which are needed for a microscopic model of a spin-phonon coupling in NVO and which we hope to obtain from a fundamental quantum calculation such as LDA+U.

Taner Yildirim
NIST

Date submitted: 01 Dec 2006 Electronic form version 1.4