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Zone Boundary Soft Modes in Relaxor PMN PETER GEHRING, NIST Center for Neutron Research, IAN SWAINSON, NRC, Chalk River Laboratories, CHRIS STOCK, ISIS, Rutherford Appleton Laboratory, GUANGYONG XU, Brookhaven National Laboratory, HAOSU LUO, Shanghai Institute of Ceramics — The lattice dynamics of $\text{PbMg}_{1/3}\text{Nb}_{2/3}\text{O}_3$, a prototypical relaxor, have been studied using neutron TOF techniques at the NIST Center for Neutron Research. Unusual “columns” of inelastic scattering are seen at the M and R-point zone boundaries at 300 K that extend from 5 meV to the elastic line. The columns weaken substantially upon heating to 600 K, suggesting the existence of soft, zone boundary modes. This would imply a dynamical origin to the superlattice peaks previously observed via TEM and x-ray diffraction techniques. Preliminary neutron structure factor calculations indicate that the corresponding ionic displacements involve the Mg/Nb and Pb atoms. This picture is consistent with x-ray studies according to which the superlattice peaks result from $\langle 110 \rangle$ correlated, anti-parallel Pb displacements [1]. The potential relationship between the columns and superlattice peaks is intriguing because the temperature dependence of the M-point superlattice peak tracks that of the soft, zone center mode [2], which is associated with the development of short-range ferroelectric correlations. [1] A. Tkachuk and H. Chen, AIP Conf. Proc., 677, p. 55 (2003); [2] P. M. Gehring, S. Wakimoto, Z.-G. Ye, and G. Shirane, Phys. Rev. Lett. 87, 277601 (2001).

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