Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Vibrational properties of ScN and rare-earth nitrides: theory and and Raman spectra[1] T.R. PAUDEL, W.R.L. LAMBRECHT, Case. Wes. Res. Univ., C. MEYER, H.J. TRODAHL, J. ZHANG, A.R.H. PRESTON, S.E. GRANVILLE, B.J. RUCK, Victoria Univ. of Wellington, New Zealand, G.V.M. WILLAMS, Industrial Research Lab, New Zealand — Frozen phonon calculations are presented for the phonons at Γ, L and X points in the rare-earth nitrides using the FP-LMTO and LSDA+U. The method is found to be in good agreement with linear response pseudopotential calculations for the closely related ScN. Comparison of the calculated phonon DOS in ScN with the Raman spectra (RS) reported in literature, show that the spectum corresponds to disordered induced first order Raman scattering and emphasizes the zone-boundary modes, in particular the LO(L) mode, because the latter correspond to a breathing mode and has the strongest electron-phonon coupling for above band gap Raman excitation. We present the measured RS for SmN, GdN, DyN, ErN, LuN thin films measured with 633 and 514 nm excitation grown by evaporation of the metals in ultrapure N_2 gas. No significant changes were found for GdN below the T_c, indicating that the mechanism is not spin-disorder related but rather to disorder originated in the presence of N vacancies. The main Raman line in the RE-N is found to correspond to the pure N-like LO(L) mode.

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Date submitted: 24 Nov 2008 Electronic form version 1.4