Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

CrN electronic structure and vibrational modes: an optical analysis[1] XUNYUAN ZHANG, DANIEL GALL, Department of Materials Science and Engineering, Rensselaer Polytechnic Institute, 110 8th ST, Troy, NY 12180 — The electronic structure of the paramagnetic insulating phase of CrN is investigated using optical spectra from epitaxial CrN(001) layers. The imaginary part of the dielectric function indicates direct interband transitions at $h\omega = 0.64$, 1.5 and 2.9 eV, and suggests a depletion in the density of states at the Fermi level. This is attributed to local magnetic moments that cause splitting of the t_{2g} bands and the formation of an indirect band gap of 0.19±0.46 eV, as estimated by comparing the optical transition energies with reported direct gap energies from calculations with different magnetic ordering and Coulomb interaction terms. The dielectric function shows a strong resonance at $h\omega_0 = 48.7\pm0.2$ meV, and values of dielectric constants $\varepsilon_{dc} = 53\pm5$ and $\varepsilon_\infty = 22\pm2$, respectively, providing values for transverse and longitudinal optical phonon frequencies at the zone center of 11.7 and 18.2 THz, respectively. The vibrational frequencies are confirmed by Raman spectroscopy peaks at 800, 1170, and 1330 cm^{-1} which are attributed to 2TO(X), 2LO(X), and 2LO(L) modes.

X.Y. Zhang and D. Gall, *Phys. Rev. B* **82**, 045116 (2010).

[1]This research was supported by the National Science Foundation, under grant No. 0645312.

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Date submitted: 12 Nov 2010 Electronic form version 1.4