Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

High Pressure Structural Phase Transitions in Lithium Nitride
AMY LAZICKI, Lawrence Livermore National Laboratory, University of California at Davis, CHOONG-SHIK YOO, Lawrence Livermore National Laboratory, WARREN PICKETT, RICHARD SCALETTAR, University of California at Davis, MADDOURY SOMAYAZULU, DANIEL HAUSERMANN, HP-CAT, Advanced Photon Source — High pressure behaviors of Li_3N have been investigated by using synchrotron x-ray diffraction up to 200 GPa in a diamond anvil cell. We found that Li_3N undergoes a structural phase transition from a layered hexagonal to a close-packed cubic phase at 36-45 GPa with a large volume collapse of 8%. The high-pressure cubic phase is stable up to at least 200 GPa, the maximum pressure applied in the present experiments. We have also carried out first principles calculations on the high-pressure phase and found good agreement between the calculated and measured EOS. These calculations further predict a widening of the band gap up to a volume compression of 33% of the initial volume before the eventual collapse and metallization at a pressure of 7.9 TPa. The high-stability of wide-band gap Li_3N is, therefore, analogus to those of NaCl, MgO and Ne. This work has been supported by the LDRD-04-ERD-020 at the LLNL, University of California, under the auspices of the U.S. DOE under Contract No. W-7405-ENG-48 .

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Date submitted: 01 Dec 2004 Electronic form version 1.4