Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Pressure-induced phase transitions in $PbTiO_3$[1] MUHTAR AHART, P. DERA, R. E. COHEN, RUSSELL J. HEMLEY, Carnegie Institution of Washington — We have investigated $PbTiO_3$ under pressure in a diamond anvil cell for temperatures of 20K to 300K using micro-Raman spectroscopy and x-ray diffraction. The Raman spectra show large changes: three peaks, centered at 200, 240 and 250 cm^{-1} disappeared above 20, 19 and 17 GPa at 20, 47 and 77 K, respectively. Furthermore, a new peak centered at 300 cm^{-1} appears above transition points. The disappearance of peaks and the appearance of new peaks are consistent with theoretical calculations of Z. Wu *et al.*, *Phys. Rev. Lett.* 95, 37601, 2005, and suggest a zone boundary instability at high pressures. The experimental results also indicate that pressure induced phase transitions at low temperature are reversible. At room temperature the first order Raman spectrum disappears above 12 GPa consistent with a transition to the cubic phase, but x-ray diffraction data suggests a rhombohedral or monoclinic phase between the tetragonal and cubic phases, consistent with the predictions of Z. Wu et al. The experimental results provide a new phase diagram for $PbTiO_3$.

[1]This work is supported by the ONR under the contract number N000140210506 and the Carnegie/Department of Energy Alliance Center (DE-FC03N00144)

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Date submitted: 30 Nov 2005 Electronic form version 1.4