Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Incommensurately modulated sulfur at megabar pressures: experimental and computational study OLGA DEGTYAREVA, RAZVAN CARACAS, EUGENE GREGORYANZ, RONALD COHEN, RUSSELL HEMLEY, Geophysical Laboratory, Carnegie Institution of Washington — Recent discoveries of incommensurate host-guest and/or modulated phases in elemental metals at high pressure suggest that aperiodic structures are a common phenomenon among the elements under pressure. However, the driving force for development of the incommensurability and structural modulations in these elemental systems is poorly understood. Using synchrotron x-ray diffraction, we show that the metallic phase of sulfur, stable above 86 GPa, has an incommensurately modulated (IC) crystal structure similar to those reported for Te and Se [1], with a strong pressure dependence of the modulation vector. The IC phase transforms to a β-Po rhombohedral structure at 140 GPa. Theoretical calculations show a further transition to a bcc phase. We investigate by first-principles calculations the possibility of an electronic instability at the origin of the incommensurability. We analyze the electronic band structure of the average crystal structure and of several commensurate approximants and examine the development of nesting in the Fermi surface. Our calculations also show the development of hybridization between the s and p states of S with increasing pressure. [1] C. Hejny and M.I. McMahon, PRL 91, 215502 (2003). This research is supported by DOE-NNSA (CDAC), DOE-BES, NSF and Carnegie Institution of Washington.

Razvan Caracas
Geophysical Laboratory, Carnegie Institution of Washington

Date submitted: 01 Dec 2004 Electronic form version 1.4