

Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

High-pressure synthesis of predicted oxynitride perovskite: Yttrium Silicon Oxynitride (YSiO₂N)¹ MUHTAR AHART, M. SOMAYAZULU, RAJASEKARAKUMAR VADAPOO, Extreme Materials Initiative, Geophysical laboratory, Carnegie institution for Science, R. E. COHEN, Extreme Materials Initiative, Carnegie institution for Science; Department fur Geo und Umweltwissenschaften, Ludwig-Maximilians-Universitaet, Germany — We synthesized the previously predicted [1] polar oxynitride perovskite in a diamond anvil cell with laser heating. YSiO₂N was predicted to have the polar *P4mm* structure with an effective spontaneous polarization of 130 $\mu\text{C}/\text{cm}^2$. A mixture of Yttrium nitride (YN) and amorphous Silicon dioxide (SiO₂) were loaded into a diamond anvil cell and laser heated at or above 1200 C at 12 GPa. The run products were investigated by x-ray diffraction, Raman spectroscopy, and second harmonic generation, for their phase and structural properties. The x-ray diffraction pattern ($a = 3.235 \text{ \AA}$, $c = 4.485 \text{ \AA}$) shows the phase formation of YSiO₂N and matches with the diffraction pattern derived from the first-principle predicted lattice parameters. However, minor unknown peaks are on the diffraction pattern indicating of the co-existence of other unknown phases. Further study of Raman spectroscopy observes the theoretically predicted modes, and second harmonic generation shows strong non-linear optical signal, which confirms the polar properties of YSiO₂N. [1] R. Caracas and R. E. Cohen, Appl. Phys. Lett. 91, 092902 (2007).

¹This work is supported by ONR grants N00014-12-1-1038 and N00014-14-1-0561, by the ERC Advanced grant ToMCA_T.

Muhetaer Aihaiti
Extreme Materials Initiative, Geophysical laboratory, Carnegie institution for Science

Date submitted: 06 Nov 2015

Electronic form version 1.4