Abstract Submitted
for the SHOCK15 Meeting of
The American Physical Society

Modeling of the pressure induced formation of a random network of a mixture of N2 and CO crystals I.G. BATYREV, US Army Research Laboratory, Aberdeen Proving Ground, MD 21005 — First principles calculations were performed to understand the pressure induced transition to an extended solid of substitutional mixtures of N2 and CO in the crystalline delta phase. The transition occurs at $\sim$ 7-9 GPa and has a hysteresis allowing for the stabilization of a covalently bonded random network to much lower pressures. Only two N atoms out of 24 were found to be incorporated into the random network formed mainly by C and O atoms in a 128 atom unit cell.[1] Here, in searching for a new route for the synthesis of polynitrogen materials, higher concentrations of N atoms (50%, 90.625, % and 93.75%) in delta molecular crystal phases under compression up to 50 GPa were calculated using density functional theory. The presence of CO is found to facilitate formation of the random network. In order to understand the importance of the initial molecular crystalline structure, calculations were performed for mixtures of N2 and CO in the delta and epsilon phases and at different sites with spherical and disk-shaped disorder. Calculated IR and Raman spectra are compared with recent experimental results.

[1]I.G. Batyrev and W.D. Mattson, Journal of Physics: Conference Series 500 (2014) 022006.

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Date submitted: 22 Jan 2015 Electronic form version 1.4