Poster Presentation

MS49.P03

Nitrogen-Rich Carbon Nitrides as Novel High Energy Density Materials

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Nitrogen-rich carbon nitride materials hold the promise of constituting novel high density energetic materials if recoverable as metastable polymeric networks of single-bonded atoms at ambient conditions. Upon transition to a lowest-energy configuration, this high pressure synthesized nitrogen-heavy material would release a large amount of energy. In this work, two nitrogen-rich molecular precursors, namely, 5'-bis(1H-tetrazolyl)amine (BTA) and cyanuric triazide (CTA), were studied in their condensed states at elevated pressures and room temperature. Powder x-ray diffraction using synchrotron radiation and micro-Raman spectroscopy were carried out to pressures as high as 12.9 and 59.6 GPa, for BTA and CTA, respectively. In our study, dense BTA is shown to conserve its room condition crystalline structure, an orthorhombic unit cell (Pbca), up to the highest pressure. In the case of CTA, results of Raman spectroscopy and x-ray diffraction indicate structural changes between 29.6 and 33.4 GPa. From numerical simulations of dense CTA [1], a phase transition into either tritetrazole (hexagonal lattice, P-6) or the sought-after polymeric CTA (monoclinic lattice, P21) is expected to take place at a pressure close to 30 GPa. Preliminary results of x-ray diffraction data indicate a transition from a hexagonal to a monoclinic unit cell with parameters similar to those predicted. Moreover, theoretically calculated polymeric nitrogen Raman peaks [2] are well matched to those observed for the high-density phase of CTA [1]. Studies of BTA and CTA under extreme conditions provide a deeper understanding of the behaviour of dense nitrogen-rich materials and guidance for further developments of high energy density compounds.

[1] *A. Hu, F. Zhang, J. Phys.: Condens. Matter, 2010, 22, 505402,* ***[2]*** *T. W. Barbee III, Phys. Rev. B, 1993, 48, 9327-9330.*

Keywords: High energy density materials, Phase transition, High pressure