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The Promise and Challenge of Extended Solids of Nitrogen

JENNIFER CIEZAK-JENKINS, US Army Research Laboratory

The extended solids of nitrogen are of considerable interest as high-energy-density materials, as it has been projected a transformation from a single-bonded polymeric-like material back to the more stable triply-bonded diatomic phase would release over 2.3 eV/atom, which is significantly higher than conventional energetic materials. Although a transformation to the single bonded cubic gauche structure was experimentally confirmed in 2005, efforts to recover this material to ambient conditions have been challenging and unsuccessful to date. In an effort to increase the metastability of the extended solid, recent studies have focused on mixing, or doping, the nitrogen with small amounts of secondary gases, such as hydrogen or carbon monoxide. It was been postulated the secondary gas would passivate the terminal ends thus increasing the stability of the nitrogen extended solid. Our group was the first to demonstrate such an approach could be used successfully to decrease the transition pressure for the formation of the nitrogen extended solid through doping with hydrogen. Although recent studies on nitrogen/hydrogen mixtures by other research groups have also observed several non-molecular nitrogen/hydrogen structures, recovery of these materials to ambient conditions has not yet been demonstrated. In this talk, I will describe our progress in the study of the synthesis, characterization, and recovery of extended solids of nitrogen from high pressure conditions from nitrogen/carbon monoxide mixtures. I will also detail results from our closely coupled modeling and simulation efforts and discuss how these results help guide our experimental efforts. New opportunities and challenges that have arisen in the course of our studies that will be pursued in the future will also be presented.