

Abstract Submitted
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Carbon solids in oxygen-deficient explosives (LA-UR-13-21151)¹

TRAVIS PEERY, Theoretical Division, Los Alamos National Laboratory — The phase behavior of excess carbon in oxygen-deficient explosives has a significant effect on detonation properties and product equations of state. Mixtures of fuel oil in ammonium nitrate (ANFO) above a stoichiometric ratio demonstrate that even small amounts of graphite, on the order of 5% by mole fraction, can substantially alter the Chapman-Jouget (CJ) state properties, a central ingredient in modeling the products equation of state. Similar effects can be seen for Composition B, which borders the carbon phase boundary between graphite and diamond. Nano-diamond formation adds complexity to the product modeling because of surface adsorption effects. I will discuss these carbon phase issues in our equation of state modeling of detonation products, including our statistical mechanics description of carbon clustering and surface chemistry to properly treat solid carbon formation.

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