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Formation of 2D Graphene-like Structures in Reacting Carbon-Rich Energetic Materials RIAD MANAA, LAURENCE FRIED, Lawrence Livermore National Laboratory — The late stages of extreme reactivity in carbon-rich energetic materials such as 1,3,5-triamino-2,4,6-trinitrobenzene (TATB) are characterized by the slow evolution of carbon to different phases. Slow growth from clusters to graphite and even nano-diamonds have been noted experimentally in detonating TATB. We conducted long-time scale, constant volume-temperature molecular dynamics simulations on pre-shocked TATB crystals for over 3 nanoseconds. Using the reactive force-field Reaxff, and at conditions of temperatures of 2500 and 3000 K, and a pressure of 16 $\sim$ 20 GPa, we discover the formation of 2D graphene-like structures of predominantly carbon, with very low heterogeneity of oxygen and nitrogen at the edges. While these simulations have enabled us to track the reactivity of TATB well into the formation of several stable gas products, such as H_2O, N_2, and CO_2, the formation of graphene-like structures and its slow evolution into final graphite and diamond like structures may finally explain the very low reactivity of TATB, as evidenced in its large reaction zone.

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