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Initial steps of condensed-phase decomposition of TATB from reactive molecular dynamics¹ HYUNGJUN KIM, SERGEY ZYBIN, ADRI VAN DUIN, WILLIAM GODDARD, California Institute of Technology — The initial steps of condensed-phase decomposition of TATB high explosive have been investigated by molecular dynamics method using ReaxFF reactive force field parameterized from the first-principles calculations. We study the dependence of primary and secondary reaction kinetics on the initial temperature and density both in pure crystal and in presence of various defects such as voids and inclusions. We found that at lower temperature the primary decomposition steps mainly involve intramolecular hydrogen transfer followed by the formation of water molecules while at higher temperatures the homolytic cleavage of N-NO₂ bond can appear, providing a temperature-dependent effect on the decomposition pathway. Besides, we also observe the formation of carbonaceous clusters during thermal and shock induced decomposition in TATB that initially capture large amount of the oxygen and nitrogen atoms delaying secondary reactions of formation of small molecules and further transformation of the cluster into carbon soot. We analyze the primary and secondary reaction mechanisms as well as the evolution of decomposition products in TATB crystals under various thermal and shock conditions.

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Sergey Zybin
California Institute of Technology

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