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Molecular Dynamics Simulation of TATB-like Explosive FILIPP SAPOZHNIKOV, VLADIMIR DREMOV, ILYA DERBENEV, ALEXEY KARAVAEV, RFNC-VNIITF, LAURENT SOULARD, CEA/DAM — A modification of REBO potential has been proposed for the molecular dynamics simulation of a TATB-like condensed explosive whose molecule initially consists of four different atoms. TATB-like means bulk properties of initial state and parameters at CJ point similar to those of real TATB. Parameters of the potential are subdivided into two groups that are responsible for CJ parameters and reaction zone width. The possibility of formation of intermediate detonation products allows variation of reaction zone characteristics without changing CJ parameters. Provided are a number of test MD calculations on the thermodynamic properties of both the original explosive and detonation products, parameters at CJ point, reactions rates and reaction zone width as dependent upon the potential parameters as well as the evaluation of critical diameter. Mechanism of the detonation initiation proper to heterogeneous explosives has been investigated.

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