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Molecular-dynamics simulation of hot spots in energetic materials ILYA DERBENEV, VLADIMIR DRYOMOV, YURY NIKITENKO, RFNC-VNIITF — To define the role of a microporosity on critical conditions of initiation, numerical simulation was performed by a MD-method with the simlified REBO potential including two types of atoms. The potential includes also long-range van der Waals term providing for stability of a molecular crystal (AB – are located in lattice points). Obtained results on MD simulation of thermal decomposition are in qualitative agrement with the macroscopic theory. Experiments with planar shock initiation have been simulated for a model set-up containing a gap in HE. The effects of the gap width and the flyer width and velocity have been investigated. The analysis of results has shown for a velocity and width of flyer it is possible to select the range of values alternating the cases of an intensive chemistry and a minor molecular dissociation. For a weak shock wave (without chemistry) the origin of a hot spot on a gap has been researched. The curve subdividing the area with and without reactions after a collaps of a gap has been defined as flyer velocity vs gap width function. The width of flyer was fixed at that.

Ilya Derbenev
RFNC-VNIITF

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