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Molecular dynamics simulation of the burning front propagation in PETN ALEXEY YANILKIN, OLEG SERGEEV, All-Russia Research Institute of Automatics, COMPUTATIONAL MATERIALS SCIENCE TEAM — One of the models of detonation development in condensed explosives under shock loading is the concept of "hot spots." According to this model, the reaction initially starts at various defects and inhomogeneities, where energy is localized during shock wave propagation. In such a region the exothermic reaction may start with heat yield sufficient for the ignition of the adjacent layers of matter. If the reaction propagates fast enough, the merging of the burning fronts from several hot spots may lead to detonation. So there is an interest in determining the burning propagation rate from the hot spot in various conditions. In this work we investigate the propagation of plane burning front from initially heated layer in PETN single crystal using molecular dynamics method with reaction force field (ReaxFF). It is shown that the burning rate depends on the direction in crystal. The kinetics of chemical transformations is considered, main reaction paths are determined. The dependence of the burning front propagation rate on the external pressure in the pressure range of normal to 30 GPa is calculated, it is shown that it grows linearly in the considered range from 50 m/s to 320 m/s. The results are compared with the data from experiments and quantum chemical calculations.

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