MOLECULAR-DYNAMIC MODELING OF CHEMICAL DECOMPOSITION OF ORGANIC SUBSTANCES IN SHOCK WAVES WITH DIFFERENT SPATIO-TEMPORAL SCALES OF COMPRESSION PHASES

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Abstract: Based on the analysis of numerous publications in the scientific literature, a comparison is made between the experimental and calculated values of the critical parameters of shock waves calculated by the method of molecular dynamics for the onset of the chemical decomposition of liquid organic substances with different spatial and temporal scales of the compression phases: millimeters and microseconds — ordinary shock waves; nanometers and pico- and nanoseconds — ultrashort shock waves created by plasma discharges of lasers. The agreement between the results of molecular dynamics simulation and the measured values of the critical parameters of ultrashort shock waves generated by laser discharges is shown. At the same time, the experimental values of the critical parameters of conventional shock waves created by traditional methods of explosion or explosive throwing turn out to be lower than those predicted by molecular dynamics modeling. Explanations are proposed for the differing values of the critical parameters of shock waves obtained in experiments and calculations with different time and space scales.

Keywords: molecular dynamics; shock waves; compression phases; chemical decomposition; spatial and temporal scales; millimeters and microseconds; pico- and nanoseconds; explosive throwing; laser plasma discharges

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Figure Caption

Ultrafast initiation of exothermic chemical reactions in hydrogen peroxide [11] behind a shock wave created by a laser

Table Caption

Experimental data of critical parameters of the onset of chemical decomposition of organic liquids in nanoscale shock waves [5, 17, 18, 20] and in conventional shock waves [12–14, 22–25]

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