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Detonation initiation in solid explosive: MD simulation using AB interatomic potential SEMEN MURZOV, Moscow Institute of Physics and Technology, Russia, VASILY ZHAKHOVSKY, All-Russia Research Institute of Automatics — Molecular dynamics simulation of impact detonation initiation in an AB model of condensed-phase explosive is performed with using a simplified reactive empirical bond order potential. Simulation of ultra-short piston-driven compression of AB explosive for the duration of a few picoseconds represents the indirect initiation of detonation by an ultra-short shock wave (SW) generated in a thin metal foil irradiated by a femtosecond laser pulse. Impact conditions required for transition of SW to detonation wave (DW) are studied. Variation of loading time and piston velocity, which controls piston pressure and input energy, is used to plot 2D regions of transition from SW to DW in pressure-time and energy-time planes. We demonstrate that the input energy required for initiation has a global minimum. Analysis of evolution of calculated pressure profiles gives a critical thickness of such AB explosive film in which transition from SW to DW can be completed. The effect of porosity and roughness of AB sample on impact detonation initiation is discussed.

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