

Abstract Submitted
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Detonation initiation in atomistic and mesoscopic simulation of porous explosives SEMEN MURZOV, Dukhov All-Russia Research Institute of Automatics and Moscow Institute of Physics and Technology, VASILY ZHAKHOVSKY, Dukhov All-Russia Research Institute of Automatics — Atomistic simulation of chemical reactions activated by shock compression is feasible at sub-nanosecond timescale, and molecular dynamics simulation indicates that the most energetic reactions accomplish within several tens of picosecond. This is too short time in comparison with microseconds required for experimental shock-to-detonation transition in real solid explosives with pores. Different types of hotspots were found in MD simulation of porous explosive described by AB model. Those types are categorized according to ratios between a characteristic time of reactions, a material motion time and a time of hotspot formation. The characteristic time of reaction is determined in MD simulation of isochoric thermal decomposition at different densities. To transfer such information into macroscopic spatial-time scale a simple model of material decomposition using a local thermodynamic and chemical equilibrium was developed. Consistent MD simulation and hydrodynamics modeling of AB samples by our smoothed particle hydrodynamic code are agreed well. The developed model was utilized in mesoscale modeling of shock-to-detonation transition in real porous explosives.

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