Abstract Submitted for the SHOCK11 Meeting of The American Physical Society

MD simulation of condense phase detonation using a Moving Window technique MIKALAI BUDZEVICH, VASILY ZHAKHOVSKY, University of South Florida, CARTER WHITE, Naval Research Laboratory, IVAN OLEYNIK, University of South Florida — The structure of steady detonation waves in solid energetic material (EM) was investigated using a newly developed Moving Window molecular dynamics (MW-MD) technique. The unique feature of this method is its decoupling of simulation time from the propagation distance, which allows us to simulate the steady regime of detonation. The MW-MD technique is applied to the modified AB model of a detonating EM. The standard AB model involves very fast chemical reactions, which lead to a very narrow reaction zone. Therefore, the parameters of the AB model were modified to produce a reaction zone width comparable with the transverse dimension of the sample. The structure of the detonation front and associated atomic-scale processes are discussed.

Vasily Zhakhovsky University of South Florida

Date submitted: 23 Feb 2011 Electronic form version 1.4