Abstract Submitted
for the SHOCK15 Meeting of
The American Physical Society

Kinetic model for thermal decomposition of energetic materials from ReaxFF molecular dynamics OLEG SERGEEV[1], ALEXEY YANILKIN, All-Russia Research Institute of Automatics — In the present work we perform molecular dynamics simulations of the thermal decomposition of isolated molecules and single crystals of PETN, RDX and HMX. For isolated molecules we use multi-replica approach with different preconditioned atomic velocities to obtain statistics of the decomposition. In this model we only consider the initial stage of the reactions, that shows first order kinetics. In the model of single crystal, we directly observe reaction pathways that result in product formation, as well as the dependences of concentrations of main chemical species on time after heating. Initial temperatures are in the range of 1000 to 2800 K. On the basis of the obtained dependences of concentrations we propose a kinetic model that describes thermal decomposition process. Reaction rate constants are well described by the Arrhenius law. Activation energies for the initial stage appear to be lowered by 30-60 kJ/mole in condensed phase compared to the isolated molecule. We compare these results between different ReaxFF parametrizations and DFT calculations.

[1]Please refer the correspondence to this author

Vasily Zhakhovsky
All-Russia Research Institute of Automatics

Date submitted: 30 Jan 2015 Electronic form version 1.4