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Modeling of oxidation of aluminum nanoparticles by using Cabrera Mott Model ZAMART RAMAZANOVA, MAXIM ZYSKIN, KAREN MARTIROSYAN, Department of Physics and Astronomy, University of Texas at Brownsville — Our research focuses on modeling new Nanoenergetic Gas-Generator (NGG) formulations that rapidly release a large amount of gaseous products and generates shock and pressure waves. Nanoenergetic thermite reagents include mixtures of Al and metal oxides such as bismuth trioxide and iodine pentoxide. The research problem is considered a spherically symmetric case and used the Cabrera Mott oxidation model to describe the kinetics of oxide growth on spherical Al nanoparticles for evaluating reaction time which a process of the reaction with oxidizer happens on the outer part of oxide layer of aluminum ions are getting in contact with an oxidizing agent and react. We assumed that a ball of Al of radius 20 to 50 nm is covered by a thin oxide layer 2-4 nm and is surrounded by abundant amount of oxygen stored by oxidizers. The ball is rapidly heated up to ignition temperature to initiate self-sustaining oxidation reaction. As a result highly exothermic reaction is generated. In the oxide layer of excess concentrations of electrons and ions are dependent on the electric field potential with the corresponding of the Gibbs factors and that it conducts to the solution of a nonlinear Poisson equation for the electric field potential in a moving boundary domain. Motion of the boundary is determined by the gradient of a solution on the boundary. We investigated oxidation model numerically, using the COMSOL software utilizing finite element analysis. The computing results demonstrate that oxidation rate increases with the decreasing particle radius.

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