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Simulation of Reaction Time in Spherical Aluminum Oxide Nanoparticles During Rapid Oxidation ZAMART RAMAZANOVA, University of Texas at Brownsville, MAXIM ZYSKIN, Rutgers University, KAREN MARTIROSYAN, University of Texas at Brownsville — Kinetics of oxidation of metal nanoparticles acquired practical importance with rapidly developing nanoenergetic systems and materials. Nanoenergetic thermites include mixtures of Al and metal oxides in nanoscale. Our research focuses on modeling aluminum combustion of nano-sized particles, surrounded by rich amount of oxygen stored by oxides. Oxidation kinetic of spherical aluminum nanoparticles was evaluated by using Cabrera-Mott moving boundary mechanism. The self-consistent Cabrera-Mott electrical potential was determined by solving a nonlinear Poisson equation. Motion of the oxide layer boundary was determined from the gradient of the potential on the boundary (appearing as a Gibbs factor), leading to computation of reaction times. We estimated the reaction time for several different Al nanoparticles sizes and oxide thicknesses, with initial outer/inner oxide layer radius of (a) 5-3 nm; (b) 5-4nm; (c)10-7nm; (d)10-9; (e) 25-22nm; (f) 25-24nm. Our results show dramatic increase of oxidation rate at nanoscale. Nonlinear effects, as well as self-heating, play important role in increased oxidation rates.

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