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**Molecular dynamics simulations of nanoscale Al structures for energetic formulations** N. SCOTT WEINGARTEN, U. S. Army Research Laboratory, MICHAEL ZACHARIAH, University of Maryland — The addition of metal microparticles, such as aluminum, to molecular explosives results in an increase in the heat of explosion, as well as higher temperatures. It is expected that the use of Al nanoparticles would further enhance these effects, but this has never been realized due to sintering of the nano-Al just prior to the energy release step. Recently, a capability emerged to produce macroscopic quantities of aluminum-based nanoclusters comprising near metallic state Al cores, passivated with an energetic gas generator. We are pursuing the possibility that these nanoclusters can be embedded in a mesoscopic spherical architecture which, upon heating, will lead to the decomposition of the gas generator. This would drive a volumetric expansion that liberates the aluminum nanoclusters which can subsequently undergo exothermic reaction. Atomistic simulations are used to explore the feasibility of this process, and determine the dynamics driving the ejection of the nano-Al particles.

N. Scott Weingarten
U. S. Army Research Laboratory

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