Abstract Submitted
for the SHOCK09 Meeting of
The American Physical Society

Oxidation Phase Diagram of Small Aluminum Clusters Based on First-Principles Calculations LIGEN WANG, MAIJA KUKLJA, University of Maryland, College Park, Maryland 20742 — It is important to understand the properties of individual nanometals before we can exploit their efficiency as energetic materials or as enhancement additives to other energetic formulations. In this paper, we construct the (p, T) phase diagram for the O/Al_{13} system based on first-principles atomistic thermodynamics. The temperature and pressure is taken into account via the oxygen chemical potential. The optimized Al_{13} cluster has an icosahedral shape. We find that O adsorption on the Al_{13} surface is site-specific; in particular, O adsorption at the bridge sites is most stable, whereas adsorption at the hollow sites is slightly unfavorable. For various oxygen adsorption layers, we determine the adsorption configurations/patterns by performing Monte Carlo calculations. We assume that the metal cluster becomes completely oxidized and calculate formation enthalpies of various oxidized metal clusters. The obtained phase diagram shows that an intact Al_{13} cluster is stable at the low O chemical potential range and the fully oxidized metal cluster is stable at the high O chemical potential range. However, the O adsorption phases are never thermodynamically stable. This study provides important insights into basic behavior of small aluminum clusters in the presence of oxygen, and may affect reliable predictions of behavior of Al-high explosive composites.

Ligen Wang
University of Maryland, College Park, Maryland 20742

Date submitted: 17 Feb 2009 Electronic form version 1.4