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Computer simulation of nanoparticle aggregate fracture¹ BRIAN HENZ, U.S. Army Research Laboratory, TAKUMI HAWA, MICHAEL ZACHARIAH, University of Maryland and National Institute of Standards and Technology — Nanoparticle aggregates have been found to possess unique mechanical properties. Aggregates of metal nanoparticles can be strained up to 100% before failure, and even typically brittle materials are observed to have a ductile failure mode. In this effort two materials; namely silver and silicon, were chosen to represent ductile and brittle materials, respectively. Aggregates with 2 to 10 particles were simulated using the molecular dynamics (MD) algorithm to determine the stress-strain behavior of the aggregate. By comparing MD results with the AFM experiments of two sintered nanoparticles we have reaffirmed the observation that even brittle materials may behave as ductile materials at the nanoscale.

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- Prefer Oral Session
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