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Molecular Dynamics Simulation Of The Energetic Reaction Between Ni And Al Nanoparticle Aggregates JACOB SPARKS, TAKUMI HAWA, The University of Oklahoma — Molecular Dynamics simulations are used to simulate the energetic reaction of Ni and Al particles at the nanometer scale. The effect of particle size and structures on reaction time and temperature for Ni and Al separate nanoparticles has been considered. The differences in melting temperature and phase change behavior between Al and Ni are expected to produce differing results for the nanoparticle aggregates systems. Simulation results show that the sintering time increases with increasing mass of the aggregates and with decreasing the fractal dimension of the aggregate. The final temperature of the systems increases with decreasing the primary particle sizes when mass of the aggregates remains unchanged. The phenomenological model is a power law including a dependence on the number of particles in an aggregates and fractal dimension is also developed.

Takumi Hawa
The University of Oklahoma

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