Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Development of a Scaling Law for Fractal Aggregate Sintering from Molecular Dynamics Simulation[1] TAKUMI HAWA, MICHAEL ZACHARIAH, Department of Mechanical Engineering, Chemistry and Biochemistry, Unviersity of Maryland and National Institute of Standards and Technology — A simple modification to the Frenkel sintering law is developed for nanoparticle fractal aggregates, based on molecular dynamics (MD) simulations. The fractal aggregates investigated consist of up to 110 primary particles of silicon, with primary particles of 2.5 nm in diameter. Aggregates of Fractal dimension of 1 (wire), 1.9 (complex), and 3 (compact) were considered. Sintering of aggregates consists of three steps, a) reaction between particles to minimize surface defects, (b) sintering of multiple secondary branches to the primary branch, and (c) contraction of the primary branch. The sintering times normalized by the primary particle diameter showed a universal relationship that only depends on the number of particles in an aggregate and its fractal dimension. This result was found to be consistent with a continuum viscous flow mathematical model we developed. Finally the results for the sintering of arbitrary fractal aggregates can be approximated with a power law modification of the Frenkel viscous flow equation, to include a dependence on the number of particles in a fractal aggregate and fractal dimension.

[1]NSF, AHPCRC

Takumi Hawa
Department of Mechanical Engineering, Chemistry and Biochemistry,
University of Maryland and National Institute of Standards and Technology

Date submitted: 13 Dec 2006 Electronic form version 1.4