ABSTRACT
Aerogels have been of interest to the aerospace community primarily for their thermal properties, notably their low thermal conductivities. While each gel is typically fragile, recent advances in the application of conformal polymer layers have led to promising results. In this study, we investigated the role of computational simulations of aerogel thermal conductivity and tensile failure, as well as the effect of secondary particles to the simulation of the strain before breaking. We then conclude on the small-strain energy dependence. Energy versus slab displacement is shown in figures 7(a) to (d). As with the fractal dimension, the density (a) is the dominant variable. Although the energy curves are quite noisy (additional runs, for the purpose of generating smoother curves via averaging, are under way), a simple cubic fit to the lower portion of each curve provides qualitative information. The highest-density cluster is the stiffest, with the other three showing only small differences. There is no meaningful variation in energy with stepsize (b), alpha (c), and gamma (d).

INTRODUCTION
Silica aerogels are low-density materials whose thermal properties have made them of ongoing interest for a wide variety of applications [1-3]. While pristine gels are fragile, polymer coating gels can greatly improve their strength while minimally impacting their insulating properties [4].

AEROGEL STRUCTURE
Aerogels exhibit a row, low-density morphology that displays three levels of structure. X-ray and neutron probes suggest that gels consist of disordered aggregates of connected fractal clusters, with fractal behavior evident over a limited range of length scales [4-6]. Fractal dimensions of 1.7 to 1.9 at small length scales have been observed in low-density colloidal materials [10].

STRUCTURAL MODEL RESULTS—FRAC TAL DIMENSION
DLCA simulations were performed for a range of densities (0.0377, 0.0651, 0.127, and 0.302 g/cm³), and the fractal dimension and coordination were calculated using the DLCA parameters for each density (Figures 3, 4, and 5). The fractal dimension is the same for all densities, while the coordination number decreases with increasing density.

ATOMIC SIMULATION OF BRIDGE STRAIN
Interparticle bridges are typically smaller in diameter than the particles they connect; therefore, we assume that failure occurs only through the straining and breaking of smaller substructures. We examine the strain energetics of the bridges via atomistic simulation and use the results to construct a simplified potential that describes interactions among the secondary particles.

BRIDGE STRAIN RESULTS
A sequence of images from the bridge strain simulation are shown in Figures 4 and 5, and bridge strain energy is shown in Figure 6. While strong evidence for the existence of interparticle bridges is shown in Figures 5(a) to (d), in (e) it can be seen that the bridges are strained only by a small amount, with the atoms in the host-gel matrix remaining nearly rigid. The remainder of the atoms are allowed to relax locally, while the total energy versus strain is recorded.

REFERENCES