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Multiscale Computer Simulation of Failure in Aerogels BRIAN GOOD, NASA GRC — Aerogels have been of interest to the aerospace community primarily for their thermal properties, notably their low thermal conductivities. While such gels are typically fragile, recent advances in the application of conformal polymer layers to these gels has made them potentially useful as lightweight structural materials as well. We have performed computer simulations of aerogel thermal conductivity and tensile and compressive failure, with results that are in qualitative, and sometimes quantitative, agreement with experiment. However, recent experiments in our laboratory suggest that gels having similar densities may exhibit substantially different properties. In this work, we extend our original diffusion limited cluster aggregation (DLCA) model for gel structure to incorporate additional variation in DLCA simulation parameters, with the aim of producing DLCA clusters of similar densities that nevertheless have different fractal dimension and secondary particle coordination. We perform particle statics of gel failure on these clusters, and consider the effects of differing DLCA simulation conditions, and the resultant differences in fractal dimension and coordination, on gel strength and failure mode.

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