

Abstract Submitted
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Multiscale computer simulation of failure in silica aerogels BRIAN GOOD, NASA Glenn Research Center — Silica aerogels are low-density materials whose low thermal conductivity makes them of interest for applications requiring lightweight thermal insulation. However, the fragility of these gels is problematic; they exhibit brittle failure at low stress levels. In order to better understand the mechanical behavior of these materials, we have performed multiscale computer simulations of failure in aerogels. Gel structure is modeled using Diffusion Limited Cluster Aggregation (DLCA) simulation, resulting in clusters having the stranded “pearl necklace” morphology characteristic of the gels. Such strands consist of so-called “secondary particles” connected by bridges of low-density amorphous silica. We model the mechanical behavior of our model gel clusters by assuming that failure occurs through the breaking of bridges. The energetics of bridge strain are computed by atomistic simulation using a Rappe-Goddard potential for amorphous silica, and the results used to determine an effective secondary particle interaction potential that includes a Morse pair contribution and an angular component. We present strain energetics of a number of model clusters, and discuss the factors which determine the ductility of the cluster failure.

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