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Thermal Conductivity of Silica Aerogels from Computer Simulations BRIAN GOOD, NASA Glenn Research Center — Aerogels are of current interest to the aerospace community; their light weight and low thermal conductivity make them suitable for use in lightweight thermal insulation. The gels typically exhibit a complex structure; the smallest observed feature is a 2-5nm "primary" particle of amorphous silica. The primary particles aggregate to form "secondary" particles an order of magnitude larger, and these, in turn, form pearl-necklace structures whose details depend on the density. The gels appear to exhibit fractal dimensionality, at least over a small range of length scales. In this work, we investigate the relationship between the structure of the gels, their dimensionality and density, and their thermal conductivity. We model the secondary-particle aggregate structure using a modified diffusion limited cluster aggregation (DLCA) scheme, which produces qualitatively different structures at low and high densities that are consistent with experimental observation. At lower densities, we find evidence for a transition from fractal behavior at small length scales to compact mass scaling at larger lengths. We model the thermal conductivity by assigning a size-dependent thermal conductance to each secondary particle, and an effective thermal conductivity to the gas assumed to be present in the pores between the particles. The conductivity of the gel-gas network is obtained using standard numerical techniques. The scaling of the thermal conductivity with density, fractal dimension, and the ratio of silica to gas conductivities is discussed.

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