The Structure and Properties of Nanoporous Materials

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Our goal is to quantify the microstructure of highly porous materials, and to determine how processing of the porous material relates to the structure and ultimately to the mechanical behavior. We will quantify structural changes with a combination of small angle x-ray scattering (SAXS) and high-resolution x-ray tomography. Finite element modeling, using the structures determined above, will be used to study how a change in pore structure effects mechanical properties.

Project Goals

We plan to make SAXS measurements to understand the effect of synthesis conditions on the change in structure. In particular we are interested in how synthesis may affect the amount of mass at the nodal points in the aerogel and then provide feedback for improved processing to control strength (network morphology), uniformity, and density.

We will characterize the pore structure of metal oxide foams immersed in a cryogenic fluid. Knowledge of how the aerogel wets in a cryogenic fluid is unknown but it is needed information if these foams are to be used in laser targets.

We will use finite element modeling to study the effects of mechanical loading on the cell structures, and to map out relationships among processing, density, and strength.

We will determine the extent of any anisotropy in lattice architecture, and improve spatial resolution to examine and characterize graded density structures.

Relevance to LLNL Mission

This project develops critical experimental technologies for many LLNL applications. A key deliverable will be the ability to predict the mechanical properties of nanoporous materials and characterize gradient density foam microstructures for future laser targets.

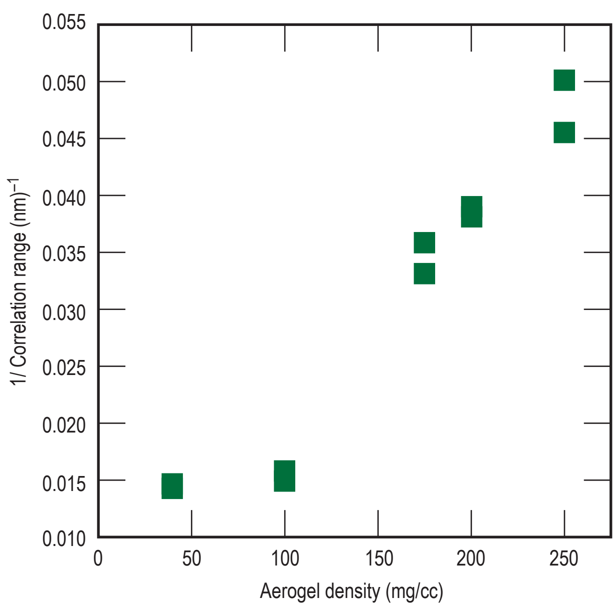

Figure 1. Change in the correlation range (pore diameter) measured by SAXS as a function of Ta_2O_5 aerogel density.

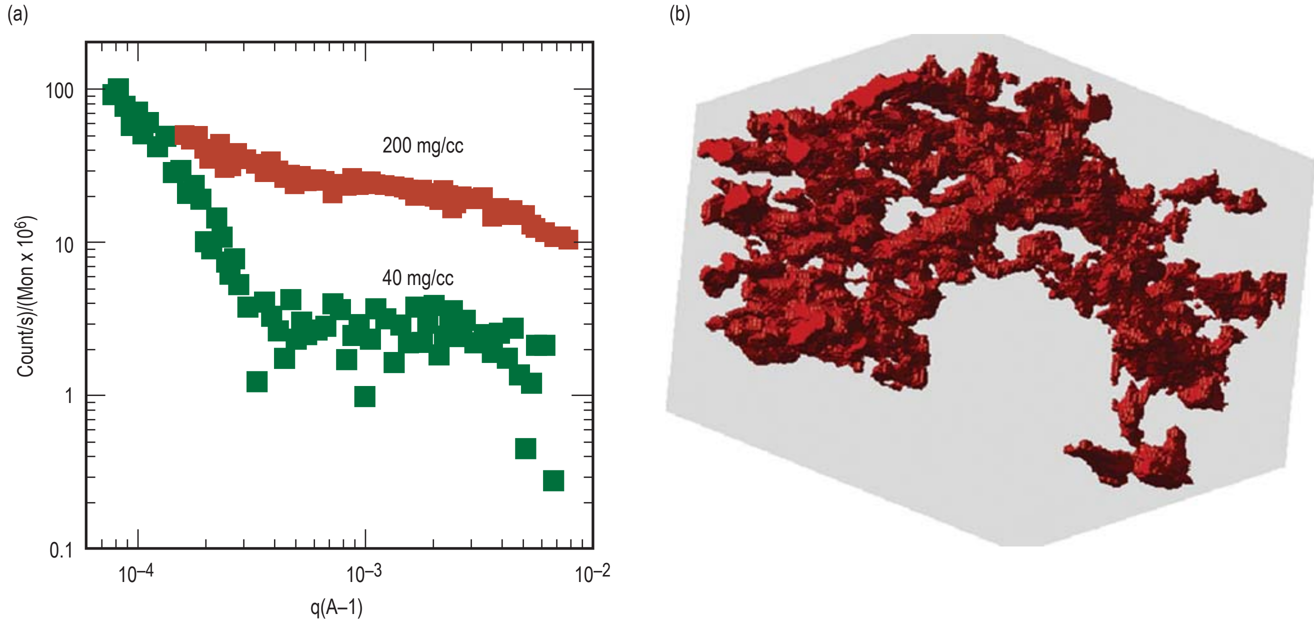

Figure 2. (a) SANS spectra measured on a 40- and 200-mg/cc Ta_2O_5 aerogel; (b) high-resolution rendering of 500-nm cube of Ta_2O_5 aerogel.

FY2007 Accomplishments and Results

One of the main objectives of this project was to quantify the pore structure as measured from the SAXS experiments due to changes in the metal oxide foam preparation condition. In Fig. 1, the correlation range or the distance between two ligaments in the aerogel measured in the SAXS experiment is related to the density of the aerogel. We see that the inverse of the correlation range scales linearly with density until a density of 100 mg/cc. Below this, the density decreases with no corresponding change in correlation range.

An explanation of this surprising result was given by measuring the scattering at smaller q not possible with SAXS, using small angle neutron scattering (SANS). SANS results for 40- and 200-mg/cc are shown in Fig. 2a. The scattering curves show that in the 40- mg/cc sample there is scattering from spherical like objects that are approximately 1 µm in diameter. No such features are observed in the aerogels above 100 mg/cc. The scattering on the µm-length scale comes from large voids or holes in the aerogel. This result is in agreement with our lensless image result (Fig. 2b) that shows large voids in the low-density aerogel. As aerogel density is decreased bellow 100 mg/cc, the nanoporous structure remains constant and the decreased density is obtained by the formation of ~ 1000-nm voids. This may be a fundamental limit on the density of the materials.

We have also been successful in our second goal, to measure the pore structure of the metal oxide foam immersed in a cyrofluids. We have been able to measure the SAXS of a porous material immersed in liquid nitrogen and measure the deformation of the foam.

X-ray tomography was used to measure density fluctuation in the metal oxide foams at better than 1 µm.

The small angle scattering capability developed in this project has successfully lead to a number of follow up projects in support of various programs at LLNL. A number of examples are the measurement of void structure in highly energetic materials, the study of pore structure and volume in Be capsules, and the *in-situ* SAXS study of carbon aerogels immersed in liquid hydrogen.