Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Preparation of nanoporous systems for the study of the mechanical properties of silica aerogels by Molecular Dynamics simulations JOHN S. RIVAS MURILLO, Department of Mechanical and Aerospace Engineering, West Virginia University, MARTINA E. BACHLECHNER, Computer Science, Math and Physics Department, Fairmont State University, EVER J. BARBERO, Department of Mechanical and Aerospace Engineering, West Virginia University — This presentation focuses on the application of the Molecular Dynamics technique to study the mechanical properties of silica aerogels through the simulation of a tension test. It covers multiple areas, including aspects related to the preparation of a well-relaxed nanoporous system from the expansion of an amorphous bulk sample and the influence of the initial configuration of the system on the final results of the simulated tension test. The results presented here will help to develop a more complete procedure to prepare a proper sample for the study of the mechanical properties of a nanoporous system by using Molecular Dynamics. Comparison of the simulation results and previously published experimental data is provided

John S. Rivas Murillo
Dept of Mechanical and Aerospace Engineering, West Virginia University

Date submitted: 11 Dec 2008 Electronic form version 1.4