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Effects of Loading Mode, Pore Morphology, and Thermal Treatment on the Mechanical Behavior of Ultra-Low-Dielectric-Constant Mesoporous Amorphous Silica Films M. RAUF GUNGOR, JAMES WATKINS, DIMITRIOS MAROUDAS, University of Massachusetts, Amherst —
We present a systematic molecular-dynamics analysis of the mechanical behavior of regular mesoporous amorphous silica structures with ultra-low dielectric constants under various modes of applied straining within the elastic limit near room temperature. We examine structures with spherical and cylindrical pores of nanometer-scale diameters. We compute the elastic moduli of the mesoporous structures and analyze their structural stability under tensile and compressive straining as a function of density and pore diameter. We find that the elastic moduli decrease with decreasing pore size and derive modulus-density relationships. The mesoporous films are generally stronger under tensile than compressive straining. The strength of films with cylindrical pores depends on the mechanical loading direction with respect to the pore axes. Thermal treatment of the mesoporous structures below the glassy transition temperature leads to a mild increase of their elastic moduli.

M. Rauf Gungor
University of Massachusetts, Amherst

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