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Nanoindentation in Nanoporous Silica: Multimillion-Atom Molecular Dynamics Simulations ADARSH SHEKHAR, University of Southern California, CAMILLA N. KIRKEMO, ANDERS MALTHE-SØRENSSEN, University of Oslo, RAJIV K. KALIA, AIICHIRO NAKANO, PRIYA VASHISHTA, University of Southern California — Nanoporous silica is widely used in catalysis, chromatography, anticorrosion coatings, desalination membranes, and as drug delivery vehicles because it is easy to tune the size of pores and their morphologies and to functionalize pore surfaces with a variety of molecular moieties. We have performed multimillion-atom molecular dynamics simulations to examine the structural properties and mechanical behavior of nanoporous silica at various densities. The simulations are based on experimentally validated force field for silica. We have examined the pore size distribution, and calculated roughness exponents of pores to characterize pore morphologies. We have determined the scaling of elastic moduli, hardness and fracture toughness with porosity of nanoporous silica through nanoindentation simulations. Our calculated value of hardness (10.6 GPa) for amorphous silica at normal density agrees very well with the experimental value (10 GPa) [1].

[1] K. Nomura, Y. Chen, R. K. Kalia, A. Nakano and P. Vashishta, Appl Phys Lett **99** (11), 111906 (2011).

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