

Title: Scale-dependent diffusion anisotropy in nanoporous silicon

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Abstract: Nanoporous silicon produced by electrochemical etching of highly B-doped p-type silicon wafers can be prepared with tubular pores imbedded in a silicon matrix. Such materials have found many technological applications and provide a useful model system for studying phase transitions under confinement. This paper reports a joint experimental and simulation study of diffusion in such materials, covering displacements from molecular dimensions up to tens of micrometers with carefully selected probe molecules. In addition to mass transfer through the channels, diffusion (at much smaller rates) is also found to occur in directions perpendicular to the channels, thus providing clear evidence of connectivity. With increasing displacements, propagation in both axial and transversal directions is progressively retarded, suggesting a scale-dependent, hierarchical distribution of transport resistances (“constrictions” in the channels) and of shortcuts (connecting “bridges”) between adjacent channels. The experimental evidence from these studies is confirmed by molecular dynamics (MD) simulation in the range of atomistic displacements and rationalized with a simple model of statistically distributed “constrictions” and “bridges” for displacements in the micrometer range via dynamic Monte Carlo (DMC) simulation. Both ranges are demonstrated to be mutually transferrable by DMC simulations based on the pore space topology determined by electron tomography.