Abstract Submitted
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Assembly of hard spheres in a cylinder: a computational and experimental study[1] LIN FU, Duke University, CE BIAN, Shandong University, WYATT SHIELDS, DANIELA CRUZ, GABRIEL LOPEZ, PATRICK CHARBONNEAU, Duke University — Arrangements of hard spheres confined to a hard cylinder have been used to model various experimental systems, such as fullerenes in nanotubes. The study of the densest packings offers a rich set of targets, and the study of their assembly dynamics hints at what may be achievable in experiments. We used enhanced optimization schemes to identify the former, and both simulations and experiments to study the latter. The equilibrium and out-of-equilibrium assembly of hard spheres of diameter σ within cylinders of diameter $\sigma \leq D \leq 2.82\sigma$ reveals that although phase transitions formally do not exist in a quasi-one-dimensional system, marked structural crossovers can nonetheless be observed. The origin of this effect is studied by a transfer matrix approach for small D. We also find that the sequence of equilibrium assemblies echoes the densest packing sequence at equilibrium, but that out-of-equilibrium self-assembly offers a rather rich control over the final morphology. Crossovers for which no continuous line-slip exists, for instance, are found to be dynamically unfavorable. Results from colloidal sedimentation experiments at high Péclet number are found to be consistent with the results of fast compressions, as long as appropriate boundary conditions are used.

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Lin Fu
Duke University

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