Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Modeling capillary filling of micropores with nanoparticle-filled binary fluid YONGTING MA, AMITABH BHATTACHARYA, OLGA KUKSENOK, University of Pittsburgh, Pittsburgh, PA 15261, DENNIS PERCHAK, Kodak Research Laboratories, Rochester, NY 14650, ANNA C. BALAZS, University of Pittsburgh, Pittsburgh, PA 15261 — We examine the behavior of binary fluids containing nanoparticles that are driven by capillary forces to fill well-defined pores of microchannels. To carry out these studies, we use a hybrid computational approach that combines the lattice Boltzmann model for binary fluids and a Brownian dynamics model for the nanoparticles. The hybrid model allows us to capture the interactions between the binary fluids and the nanoparticles, as well as model the interactions among the fluid, the nanoparticles and the pore walls. We show that the nanoparticles dynamically alter both the interfacial tension between the two fluids and the contact angle on the pore walls; this, in turn, strongly affects the dynamics of the capillary filling. We demonstrate that by tailoring the properties of the nanoparticles, such as their affinity to the fluid components and their interaction with the pore walls, one can effectively control both the filling velocities and the deposition of nanoparticles on the pore walls. Our findings provide fundamental insights into the dynamics of this complex system, as well as potential guidelines for technological processes involving capillary filling with nanoparticles in microchannels with differing geometries.

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Date submitted: 10 Nov 2011 Electronic form version 1.4