Interface-Controlled Phase Transitions in Nanosystems: Phenomenological Theory and Monte Carlo Simulations

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Fluids and fluid mixtures confined to finite geometries such as bipyramids or pores of square cross section are studied at temperatures where phase separation (between liquid and gas, or an A-rich phase and a B-rich phase in an AB mixture, respectively) occurs in the bulk. Assuming suitable surface forces such that part of the walls prefer the liquid (or A-rich phase) and part of the walls prefer the gas (or B-rich phase), two-phase coexistence in the system is stabilized. However, at a temperature distinctly lower than the critical temperature, a transition may occur where the interface between the two coexisting phases disappears, and the system remains in a pure one-phase state. This transition is rounded by a finite size in nanoscopic geometry, but becomes a sharp transition (with anomalous critical properties) in the thermodynamic limit. These transitions can be understood in terms of relations to cone and wedge filling transitions, respectively. Monte Carlo results will be presented in order to exemplify these considerations.