612d Investigation of the Phase Behavior of a Fluid in the Vicinity of a Nanowire

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Fluids in the presence of one or more surfaces exhibit a rich variety of phase transitions that are absent in bulk fluids. Examples include prewetting, layering, and capillary condensation transitions. Even the simplest of systems display a broad range of phase behavior, with surface phase diagrams depending qualitatively on the relative strengths and ranges of fluid-fluid and fluid-substrate interactions as well as structural characteristics of the substrate. In this presentation, we examine the influence of substrate curvature on the surface phase behavior of a fluid by describing the behavior of a fluid in the presence of a long nanowire. Results were obtained with a model that consists of an infinitely long structureless cylinder and a simple monatomic fluid. Fluid-fluid and surface-fluid interactions were described using the Lennard-Jones potential. Grand canonical transition matrix Monte Carlo simulations [1] were used to determine thermophysical properties of the system.

We began our study by examining the phase behavior of a fluid interacting with a cylinder of intermediate strength. More specifically, we adopted the interaction parameters introduced by Ebner and Saam to describe an Ar-CO_2 system [2]. The surface phase behavior of this system with a planar wall as the substrate has been well characterized [3]. With a planar wall one observes prewetting transitions over a relatively broad range of temperatures. In our study we examined how characteristics of the prewetting transitions evolve with curvature. This was accomplished by performing a series of simulations using nanowires with diameters spanning from 5 to 1000 molecular diameters. We find that substrate curvature has a significant influence on the prewetting phase behavior. For example, the wetting temperature initially increases and eventually vanishes as the cylinder radius decreases. We also find that the thickness of the adsorbed film does not diverge at the wetting temperature as it does with a planar substrate. Many of our finding are in qualitative agreement with those found in a density functional theory study of Bieker and Dietrich [4].

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