Phase behavior of liquid-crystal monolayers of rod-like and plate-like particles

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The structural and dynamical properties of 2D and even 1D complex fluids are experimentally accessible due to the recent development of nanofluidics and optical trapping methods. Liquid crystal monolayers can be prepared by confining colloidal particles between parallel walls[1,2] or by spreading colloidal nanoparticles or amphiphilic molecules at the air/liquid interface[3,4]. In the present work the orientational and positional ordering properties of liquid crystal monolayers are examined by means of Fundamental Measure Density Functional theory. The particles are modeled as hard boards, with their centers of mass restricted to move on a flat surface and their uniaxial axes allowed to rotate freely in three dimensions (within the restricted-orientation approximation). We find that the structure of the monolayer depends strongly on the shape of the constituting particles and the density. In the case of rod-like shapes, the particles align along the layer normal since that gives the lowest occupied area per particle, i.e. the phase is uniaxial nematic even at very low densities. In contrast, the lowest occupied area can be achieved by random in-plane ordering in the monolayer of plate-like particles, i.e. planar nematic ordering takes place even at vanishing densities. This random in-plane ordering is not favourable at higher densities and the system undergoes an in-plane ordering transition forming a biaxial nematic phase or a crystal. For certain values of the aspect ratio, the uniaxial-biaxial nematic phase transition is observed for both rod-like and plate-like particle shapes. The stability region of the biaxial nematic phase enhances with decreasing aspect ratios for plate-like particles, while the rod-like particles exhibit a reentrant phenomenon, with a uniaxial-biaxial-uniaxial nematic phase sequence with increasing density if the aspect ratio is larger than 21.34. In addition, packing fraction inversion is observed with increasing surface pressure due to alignment along the layer normal. At very high densities the nematic phase destabilizes to a nonuniform phase (columnar, smectic or crystalline phase) for both shapes.

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