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Self consistent field theory for smectic ordering of semiflexible homo-polymers.

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We develop a model of liquid crystalline homopolymers using self-consistent field theory (SCFT) for semiflexible spherocylinder-shaped particles that can form the isotropic (I) phase, the nematic (N) phase and the smectic-A phase (SmA). As in previous work by Chen [Macromolecules 26, 3419 (1993)] and Duchs and Sullivan [J. Phys. Cond. Mat. 14 12189 (2002)] we employ the excluded volume interaction based on a second virial approximation (SVA) due to Onsager, which is able to stabilize the N phase for wormlike chains. To stabilize the SmA phase, we also include the excluded volume interaction between cylindrical segments and the terminal end segments as in Hidalgo *et al.* [PRE 71, 041804 (2005)]. However, the work by Hidalgo contains two limitations, which we address in this study: Their numerical algorithm cannot obtain solutions for strongly ordered states, which occur for molecular length to diameter ratio, $L/D > 10$. Also, the phase boundaries occur for packing fractions that are unphysically too high, due to their use of SVA. We develop a Crank-Nicolson type method applied to the orientations having better convergence for strongly ordered states which obtains solutions for L/D as high as ~ 55 for the N-SmA transition. We also implement a technique based on the method of Parsons and Lee which goes beyond the SVA, successfully predicting the N-SmA boundary very close to Monte Carlo simulations. N ordering and SmA ordering is looked at some detail and comparison to Monte Carlo simulations and measurements on virus particles are made. We predict that the stability of rigid rods in the SmA phase increases with increasing L/D, however the stability is lost for only a small amount of flexibility.

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