

276g Computation of the Nonhomogeneous Equilibrium Phase Behavior of a Rigid Rod System

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The nonhomogeneous equilibrium phase behavior of a solution of rigid rods is analyzed for a periodic one-dimensional system. Equilibrium solutions for the distribution function are calculated by minimizing the free energy of the system using the nonhomogeneous generalization of Onsager's theory which models interaction of the rods on the scale of a single rod length. A general method for computing biaxial equilibrium solutions in a periodic system is developed by discretizing the Euler-Lagrange nonlinear integral equation by the finite element method and using Newton's method to solve the resulting nonlinear equations. Stable states for isotropic-nematic coexistence are computed in a periodic system of finite size. The density and order parameter profiles are monotonic; the isotropic side of the interface shows a peak in biaxiality. The method is also used to compute the multiple unstable nonhomogeneous equilibrium states that occur when the concentration of rods exceeds the value for spinodal decomposition. The states are characterized by combinations of bend, twist, and splay distortions in physical space. These nonhomogeneous equilibrium solutions correspond to unstable attractors in the dynamic process of isotropic-nematic spinodal decomposition. Finally, wall-rod interaction calculations show the impact of hard walls on the nonhomogeneous phase behavior of the system.