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Clustering in Hard Core/Soft Shoulder Lattice Gas Models

PAUL D. BEALE, University of Colorado at Boulder, CHARLES A. SIEVERS, MATTHEW A. GLASER — Isotropic hard core/soft shoulder interacting particle models have been shown to display a wide variety of thermodynamic phases: structured liquids, micellar solids, layered and columnar liquid crystals, and a variety of modulated solid phases. We have explored the phase diagram of a class of lattice gas models that are designed to approximate continuum models. We use generalizations of Baxter's hard hexagon model on a two-dimensional hexagonal lattice to model the hard core repulsions. The longer-ranged repulsive soft shoulder is included to induce a Klein/Likos clustering instability. The clustering instability creates softly interacting fluidic micelles, as well as several type of modulated solid phases. The lattice gas model allows for efficient Monte Carlo simulation in order to quickly explore the phase diagram. Two dimensional lattice gas models typically only display liquid phases with short-range order and solids with long-range order that is commensurate with the underlying lattice. Preliminary results indicate the model exhibits soft solid phases composed of fluidic micelles that form a quasi-long ranged solid phase characteristic of continuum solid phases in two dimensions. We will also present a mean field theory analysis of the initial clustering instability.

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