Mesoscopic Behavior of Nanostructured Simple Fluids

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Abstract. Mesoscopic behavior of nanostructured simple fluids will be reported, which was studied by Monte Carlo simulation and renormalizing approaches.

Introduction. Fluids are formed as flows of materials. Especially, we focus on nanostructured fluids. Nano-structured materials [1] consist of grains/clusters and interfaces, on nanometer scales. Every grain/cluster possesses the non-equilibrium properties, depending on the size, the constituent interactions and the symmetry of order parameters, of the referred grain/cluster. It makes phase transitions from solid-like phases to ideal gas phase, through liquid-like and gas-like phases, as a local equilibrium of a finite sized system. The conventional liquid/gas phase in equilibrium [2] is separated into a collection of liquid-like/gas-like phases in different local equilibrium [3]. Near the borders between mesoscopic phases of them, a first order-like phase transition occurs resulting in mesoscopic spinodal-like/glass-like phases. The mesoscopic behavior of nanostructured fluids will be discussed in the form of liquid-like, gas-like, and glass-like phases, together with anisotropic membrane- like interfaces.

Methods. For simulations [1], the fluid systems are divided into small block-cell systems and Monte Carlo methods are used. In renormalizing approaches [3], finite size field theoretic analysis for stochastic Langevin dynamics is adopted for each grain/cluster, by taking into account the local temperature fluctuations inside the respective grain/cluster and the stochastic random forces derived from the thermal reservoir.

Common properties to the mesoscopic phases.

In weak nonlinear regimes, thermal stability of every composite grain/cluster is determined by its size; smaller sizes become unstable at lower temperatures. Hence, at any temperature, the smallest grain/cluster may be regarded as a (reference) "system" and the remaining grains/clusters and interfaces as the "thermal reservoir". The fluid dynamics of the "system" lead to mesoscopic behavior of every necessary local system. This behavior hierarchically arises over the entire temperature regime ranging from the temperature of the smallest grain/cluster to the temperature of the largest grain/cluster disappearing. Summing up over all grains/clusters and interfaces leads to the bulk properties of the respective fluids [2]. Every composite atom/molecule of grains is frustrated until all grains/clusters form a mesoscopic phase. The largest grain/cluster undergo phase transitions to disordered state as a bulk phase transition; liquid-like phase from solid phase, gas-like phase from liquid phase and ideal gas phase from gas phase. The value of mesoscopic phase transition temperature and the roundness, of each peak, e.g. for specific heat, are determined from finite size scaling relations.

Inherent properties to every mesoscopic phase.

*Mesoscopic liquid-like phases***:** We take into account the two kinds of random fields for d-dimensional simple fluids. The characteristics of the mesoscopic critical exponents and universal functions with liquid symmetry are hierarchically obtained, for every grain/cluster, in a form of ε (=6-d) expansion with a few exceptions. Short-range correlations play an essential role on every phase.

Mesoscopic gas-like phases: Every phase is described with Maxwell distributions and Boltzmann equations, and possesses gas symmetry. The constituent atoms/molecules inside a certain grain/cluster are connected with each other with short-range correlations during collisions. In the case of finite atomic/molecular density inside every grain/cluster, even if it is very small, the two-body/three- body interaction in the Boltzmann equations becomes positive finite, and the mesoscopic second/first order-like phase transition may be possible to occur.

Mesoscopic glass-like phases: In the case of systems consisting of same sized grains/clusters, mesoscopic glass-like phases hierarchically appear. The mesoscopic behavior of these systems may be obtained as the non-equilibrium behavior of each local system. The values of the power exponent for the non-equilibrium distribution are obtained by the renormalizing approaches.

*Mesoscopic spinodal-like phases***.** The mesoscopic liquid- like and gas-like phases display the spinodal-like properties at the mesoscopic first order-like phase transition point. The behavior for every mesoscopic transition point was obtained by the renormalizing approaches.

Anisotropic membrane-like interfaces: As an example of surface evolution of interfaces, the system of D-dimensional nanostructured crystalline membrane-like surface with anisotropic interactions was studied, and the characteristics of mesoscopic, flat-like, tubule-like and crumpled-like phases, were obtained.

Concluding remarks. The main characteristic properties of nanostructured fluids were obtained. Using these, the control of material characteristics and fabrications may be possible.

References

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