ADVANCED PHASE TRANSITION

Methods development: Improved Molecular Dynamics (MD) and Monte Carlo (MC)
Application : Magnetofluidic separators, sealing and damping devices, etc.

The relationship between the nature of the molecular interactions and the resulting **phase diagram** is the central theme of equilibrium statistical mechanics. Recent computations have provided new insight into the structural and orientating behavior of strongly interacting dipolar hard and soft spheres. The interactions are an isotropic Lennard-Jones (LJ) potential, which favors the condensation when the temperature decreases and an anisotropic dipole-dipole interaction potential, which tends to have a chain formation, i.e.

$$v(\mathbf{r}_{ij}, \mu_i, \mu_j)=4\varepsilon\{(\sigma/r_{ij})^{12}-(\sigma/r_{ij})^{6}] -3(\mu_i\cdot\mathbf{r}_{ij})\ (\mu_j\cdot\mathbf{r}_{ij})/r_{ij}^{5}+\mu_i\cdot\mu_j/\mathbf{r}_{ij}^{3}$$

where ε is the LJ well depth, σ is the LJ diameter, μ_i is the dipole moment of particle i, and $\mathbf{r}_{ij}$ is the vector joining particles I and j. The first term on the right hand of the equation is the isotropic LJ potential and the second term is the anisotropic dipole-dipole interaction potential. The main conclusions of the numerical investigation can be summarized as the follows.

(1) At sufficiently low temperatures a dense system of dipolar hard spheres (or soft spheres) can spontaneously break its symmetry and order into a ferroelectric state. Polarized domains (Fig.1) form in the presence of a depolarizing field.

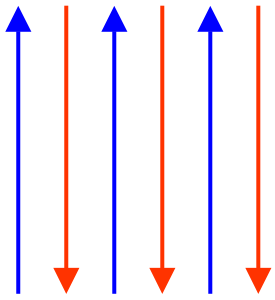

Fig1 Polarized domains. The arrows show the direction of the polarization.

(2) No evidence is observed for the existence of a gas-liquid transition (Fig.2) in a broad density-temperature range in contrast with general belief and a variety of theoretical predictions

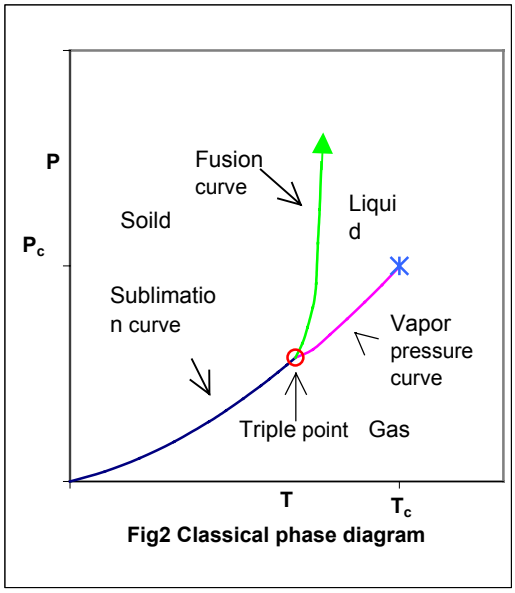

Fig2 Classical phase diagram

(3) Instead, the particles are found to be associated with the chainlike structures (Fig3) at its near contact of the hard spheres and head-to-tail alignment of the dipole moments.

Fig.3 Polymer like chain structures

However, it has been argued that the Gibbs ensemble Monte Carlo (GEMC) method used in some of these simulations is unreliable in the relevant regime of temperature and density. Thus, it is still a problem whether a condensation or a formation of polymer like chain structure is dominant at the low temperatures and densities.