Higher-order structure and Statistical Properties of Dipolar Nano-Particles

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ダイポール相互作用は，異方性の持つr^{-3}の長距離相互作用であるため自己組織化により特殊な相構造をとる．今回，前回発表した OCTA システムを用いた計算により確認された多様な多階層相構造と熱力学的な性質との比較を行った．計算に用いた系は，ダイポール相互作用と Van der Waals 球を含む粒子系であるが，比熱にダブルピークを持つ．Van der Waals 球に引力項がある場合，このピークは比較的高温で出現するが，斥力項のみの場合ではより低温に出現し生成構造も異なる．

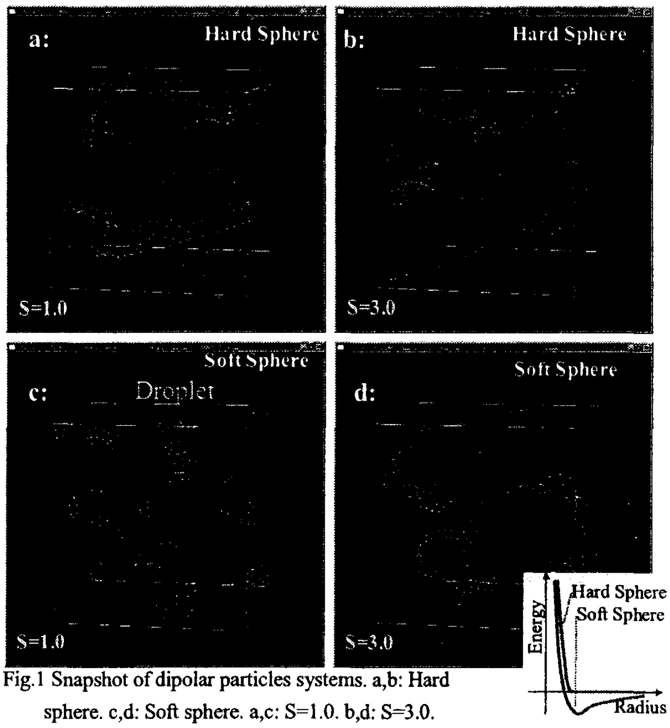

Fig.1 Snapshot of dipolar particles systems. a,b: Hard sphere. c,d: Soft sphere. a,c: S=1.0. b,d: S=3.0.

Dipolar particles system has r^{-3} long-range interaction including the direction dependences. For example, dipolar spin system has some different ordered state depended on the lattice structure and the boundary condition, and ER/MR fluid indicates some specific rheorogical phenomena. We calculated these systems using MD simulations at the viewpoint of self-organized nano-structure. We use COGNAC simulator in OCTA system as coarse-grained MD simulation for nano-particle systems, which have dipolar Hamiltonian and Lennard-Jones Potential,

$$H = J\sum_{i,j}\left(\frac{\vec{S}_i\cdot\vec{S}_j}{r_{ij}^3} - 3\frac{(\vec{S}_i\cdot\vec{r}_{ij})(\vec{S}_j\cdot\vec{r}_{ij})}{r_{ij}^5}\right) + 4\varepsilon\left\{\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^{6}\right\} \qquad \textbf{(1)}$$

As approximation of long-range interaction, we use reaction field method including cutoff for center dipolar particles. Firstly, we calculated the some strength of dipole for two type potentials. One is normal Lennard-Jones potential (Soft Sphere), and the other has only repulsive force by cutoff (Hard Sphere). We can see various structures [Fig.1]. As first order structure, we can see chain type structures [1,2]. And as higher-order structure, we can see two type condensed structures by long calculations, bundle and droplet structures. If we use hard sphere potential, bundle structure is dominant not depending on strength of dipole. If we use soft sphere potential,

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we can see droplet structure for small dipolar system (S=1), and bundle structure for large dipolar system (S=3).

We can estimate the chain interaction by simple model. Fig.2 is the energy surface for two parallel chains, we can see the attractive force between two chains with antiphase, and antiparallel chains also have attractive force under same phase. This estimation agrees with lattice dipolar system, its grand state is ferromagnetic for triangular lattice, and antiferro -magnetic for square lattice. For its chain attractive force is competing with Lennard-Jones attractive force, we can see some type higher-order structures.

Next we calculated the specific heat by annealing simulation for dipolar particles system on soft spheres and on hard spheres [Fig.3]. We can see double peak for both systems. Soft sphere system has peaks at higher temperature than hard sphere system. It means that soft sphere system has stronger attractive interaction than hard sphere system. At the peak of higher temperature, the chain structures grow as first order structure. And at the peak of lower temperature, the condensed structures (bundle and droplet) grow as higher-order structure. In this annealing simulation, we can get droplet and lattice structure with ferromagnetic vortex, that structure is different from bundle structure of Fig.1. However, we can start from this lattice structure for S=10.0, this lattice breaks and become troidal structure like semi flexible polymer. It means that the bundle structure on soft sphere system is one of troidal phase, and the peak of lower temperature will be regard as solid-liquid phase transition.

References

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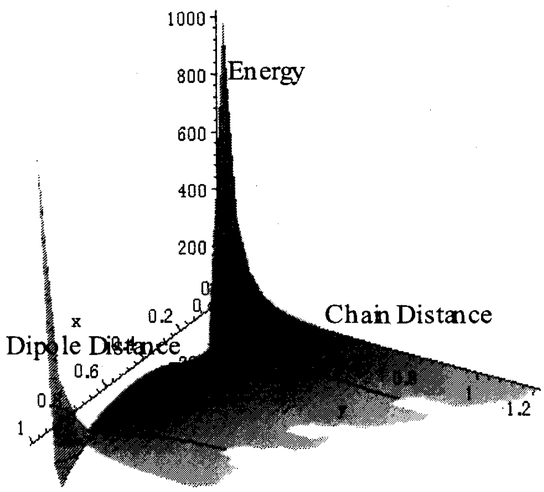

Fig.2 The energy surface for two parallel chains.

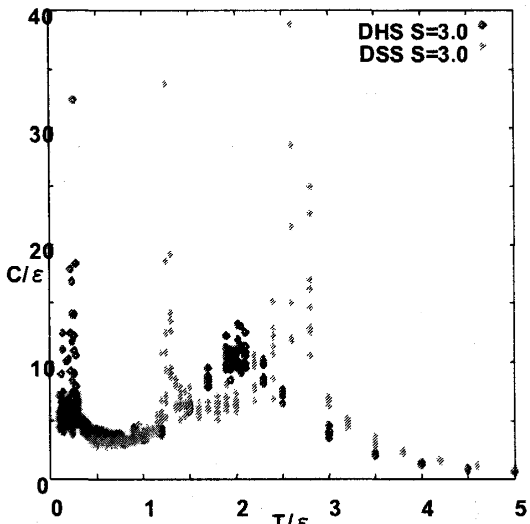

Fig.3 The heat capacity of dipolar systems. ○: Hard sphere system. †: Soft sphere system.