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Numerical study on the dynamics of colloidal particles immersed in nematic liquid crystal

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近年，ネマティック液晶中にコロイド粒子が分散した系において，粒子が数珠状に配列するなど興味深い現象が発見され，多くの研究者達によって活発な研究がなされてきた．しかしながら，粒子に働く力は粒子表面のアンカリング効果によって変形を受けた液晶弾性場に起因するものであるため，本質的に多体効果であり，多粒子系において正しく求めることは難しい．また，液晶の特徴である流動性を取り入れて理論的・数値的研究を行うことも極めて困難である．我々は，コロイド分散系を扱うべく開発した流体粒子ダイナミクス法の分散媒に液晶配向場に関する秩序変数を与えたモデルを考案し，この系の数値シミュレーションを行った．Figure 1 は，多数の粒子を含む液晶・コロイド混合系を温度クエンチし等方相からネマティック相へ転移させた後の時間発展の様子である．液晶配向場は粒子表面に対し垂直にアンカリングする．転移後，液晶場は多くの配向欠陥を形成するが，それは液晶の弾性エネルギーを減らすよう時間とともに減少し，それに従い粒子は複雑な配向欠陥を伴いながら凝集していく．

Understanding of the colloidal science is quite important from both scientific and industrial viewpoints. When we study the dynamic properties of colloidal dispersions either theoretically or numerically, the most difficult problem arises from hydrodynamic interactions among particles. In order to simulate the dynamic behavior of colloidal suspensions efficiently, we have developed a new numerical method, which we named "fluid particle dynamics" (FPD) [1]. The key idea of our method is to treat colloidal particles as fluid ones (not as solid ones), whose viscosity is much higher than that of the surrounding medium.

Applicability to the colloidal dispersions in various soft matters is one of the remarkable merits of this method. Since we solve the flow field with a continuous manner in FPD, we can easily incorporate the various order parameters to the host fluid. In this study, we perform numerical simulations of the colloidal dispersions in nematic liquid crystal [2, 3] by introducing the orientational order parameter [4].

If the director field of nematic phase is anchored normal to the particle surface, Saturn ring-like line defect is formed around a small particle. When a particle is dragged by an external field, the resistance force depends on the direction of its motion toward the orientational order of nematic phase. In the parallel case, if the applied force is weak, the defect can catch up with a particle although it is slightly deformed. As the applied force is stronger, on the other hand,

the separation between the particle and defect increases and the defect cannot catch up with particle eventually. The escape of the defect from a particle is observed at the first time. In the perpendicular case, the defect does not escape from the particle. The front part of the defect enters the inside of the particle virtually and the back part of it cannot follow the particle. Thus, the length of the defect increases with time when we apply the strong perpendicular force on the particle. The defect behaves as an obstacle to a particle motion so that it cannot move straightly along the applied force.

We also simulated the multi-particle systems. Since each particle accompanies a Saturn-ring like defect having a quadruple symmetry, particles are interacting to each other essentially with the quadruple symmetry. However, we found a new type of defect structure around the particle pair, which cannot be described by the quadruple argument. It has an eight-figured shape and binds the two particles strongly. Figure 1 shows the simulated dynamics of the dispersion including many particles. After the quench, the isotropic phase transforms to nematic phase and a lot of defects emerge. The amount of defects decreases with time to reduce the elastic energy, which leads to the aggregation of colloidal particles. The structures of the aggregates and defects are very complex and we could not see apparent ordered structures such as a chain and a crystal in our simulations . Some defects are not Saturn-ring like shaped and shared by a number of particles. The particles are interacting to each other via not only Saturn-ring defect but also the new type ones, which are essentially the same as the eight-figured defect.

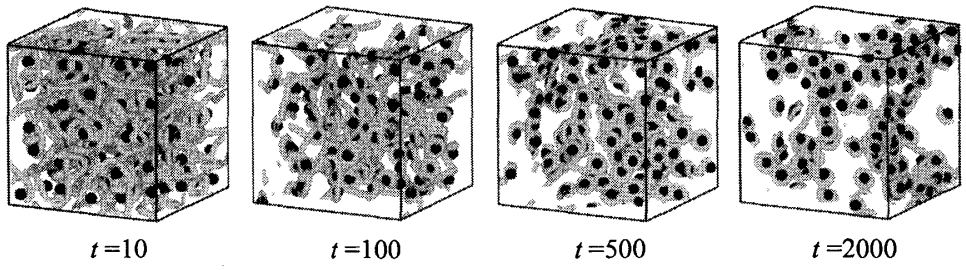

Figure 1: Simulated aggregation process of the colloidal dispersion in nematic liquid crystal. Director field of the nematic phase favors to be normal to the particle surface. At $t = 0$, the isotropic phase is quenched to the nematic phase.

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