The Analysis of Self-Organized Structures of Dipolar Nano-Particle Systems

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ダイポール相互作用は，異方性の持つ $1/r^3$ 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 OCTA システムを用い，これらの構造について計算並びに解析を行った．計算によると，一次構造として紐状構造[1,2]が観測されるが，条件により円環を形成するもの．分岐を形成するものなど出現する．又，二時構造として，紐状構造がバンドルを形成するが，条件によりシート状にスタックするもの．糸鞠状に巻き付く物などが現れた．今回これらの構造の特徴付けや出現機構について解析したので紹介する．

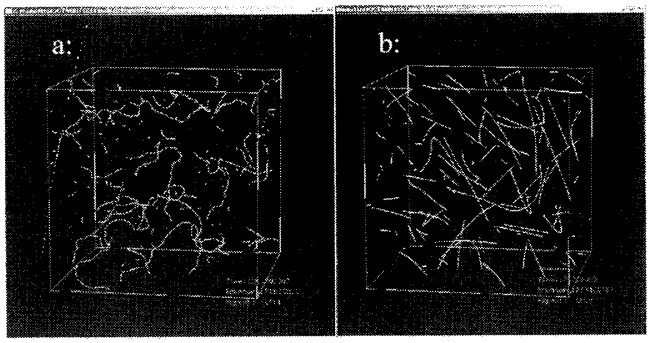

Fig.1 Snapshot of calculation for pair charged particles a: Calculation by Ewald method. b: Calculation by reaction filed method.

Dipolar particles system has r^{-3} long-range interaction including the direction dependence. 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 it have dipolar Hamiltonian

$$\mathcal{H} = J\sum_{i,j}\left(\frac{\vec{S}_i\cdot\vec{S}_j}{r_{ij}^3} - 3\frac{(\vec{S}_i\cdot\vec{r}_{ij})(\vec{S}_j\cdot\vec{r}_{ij})}{r_{ij}^5}\right), \qquad (1)$$

and Leonard-Jones Potential. As approximation of long-range interaction, we use two calculation methods, one is Ewald summation method and the other one is reaction field method. For treatment with dipolar particle, we use two models for dipolar particle, one is putting the dipolar moment on the center of particle and the other one is putting the two opposite charge on the particle. Firstly, we calculated the difference of calculation method to know the influence of cut-off range.

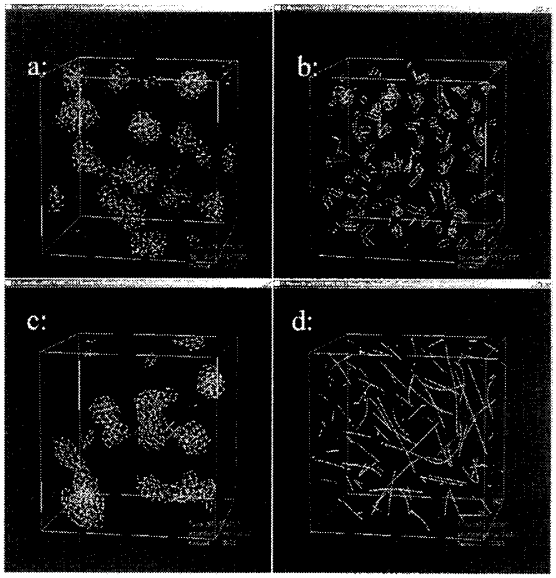

Fig.2 Snapshot of calculation by reaction filed method for dipole particles. a,b: D is small. a,c: J is small.

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We could observe the similar chain shape cluster structure [1,2] under the both calculation method [Fig.1]. Next we calculated the difference of the dipolar particle type for coupling constant J and charged distance D [Fig.2]. If the system had large J compared with van der Waals interaction (ε), straight chain structure was dominant as ordered structure, but if J was enough smaller than ε, these chains shrank. This behavior didn't have large dependency on the charge distance, but curvature became small as D was large, then we could observe cyclic structure. Fig.3 is the plots of these structures energy for the number of particles. The most stable structure is straight chain without edge, and next is cyclic structure and bending structure, and straight structure with edge is most unstable.

We also calculated the long time behavior; these chains stacked as secondary structure. Its bundle structure was generated by competition with Van der Waals interaction and dipolar interaction. If J was enough small than ε, chain shrank like droplet and wound, then it became coil like structure. And opposite side, if ε was enough small than J, straight chain structure was organized and bundled, then it became sheet like structure. Fig.4 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. These dynamics is also interesting in viewpoint of protein folding.

We also report the stability of these chain structures using one chain or bundled chains simulations, and the analysis using order parameter characterized these structures.

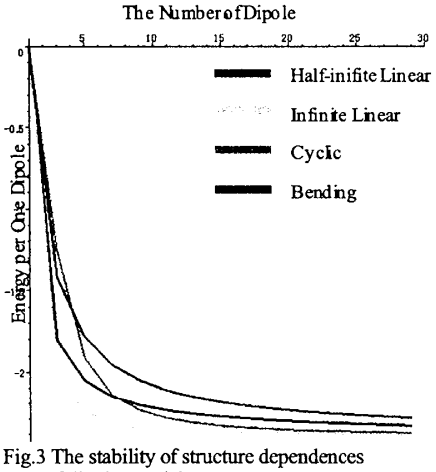

Fig.3 The stability of structure dependences of dipolar particle systems.

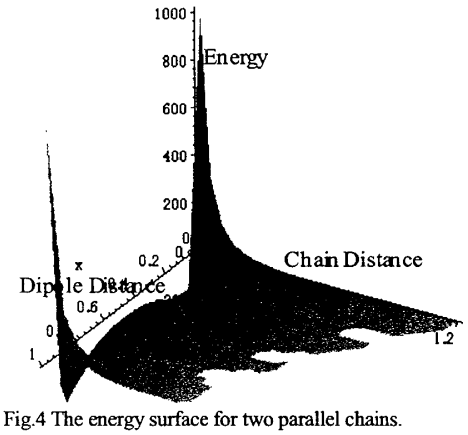

Fig.4 The energy surface for two parallel chains.

References

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[2] S. C. McGrother and G. JacksonPhys. Rev. Lett., **76-22** (1996), 4183-4186.