입자 구조의 대변형 거동에 대한 FFT 해석

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Fourier transformation analysis of LAOS behavior of particle systems

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Introduction

The rheology of particle systems, concentrated colloidal dispersions, flocs and gels, is of considerable practical importance in many industrial systems. But there is still much uncertainty as to the factors that influence the rheological behavior of these systems. The main points of interest depend somewhat on the microstructure of particle systems. The tools to analyze the structures are fractal dimension and radial distribution function (rdf) in equilibrium state. But in non-equilibrium state, that is shear flow, the microstructure is different from the microstructure in equilibrium state. As according to many experimental data, the microstructure is closely related to rheological data in particle systems. Recently there are many experimental data with FT analysis for rheological data. Some papers show that the intensity of higher harmonics is closely related to the microstructures of particle systems as FT analysis. So we analyzed rheological data of particle systems applied FT analysis used Brownian dynamics simulation. BD simulation is widely used to study the structure for particle systems. We calculated the stress response under large amplitude oscillatory shear (LAOS) for particle systems. We choose two particle systems. One is particle gel, which is formed from a model of soft spherical particles incorporating a combination of flexible, irreversible bond formation and non-bonded interparticle interactions. The other is particle aggregation system, which is formed from a model of spherical particles incorporating Lennard-Jones potential.

Theory

Brownian Dynamics

Translational motion by Langevin equation

$$m(dv_i / dt) = -\varsigma v_i(t) + F_i(t) + F_i^R(t) \quad (1)$$

$$\varsigma = 3\pi\eta_s\sigma = k_B T / D_0 \quad (2)$$

$$r_i(t+\Delta t) = r_i(t) + F_i(t) \times (\Delta t / \varsigma) + S_i(D_0, \Delta t) \quad (3)$$

Translational motion for shear flow

$$r_i(t+\Delta t) = r_i(t) + F_i(t) \times (\Delta t / \varsigma) + S_i(D_0, \Delta t) + z_i(t)\dot{\gamma}_{xz}(t)\Delta t \quad (4)$$

I. Particle gel

Core potential

$$\phi_C(r_{ij}) = \varepsilon(\tfrac{\sigma}{r_{ij}})^n \quad \text{(n=36)} \quad (5)$$

Bond potential

$$\begin{aligned} \phi_B(b_{ij}) &= \varepsilon_b(\tfrac{b_{ij}-b_1}{b_0})^2 \quad && b_{\max} > |b_{ij}| > b_1 \\ \phi_B(b_{ij}) &= 0 && |b_{ij}| < b_1, |b_{ij}| > b_{\max} \end{aligned} \quad (6)$$

Long range potential

$$\begin{aligned} \phi_{LR}(r_{ij}) &= \varepsilon_{LR}(\tfrac{r_c - r_{ij}}{r_c - \sigma}) \quad && r_{ij} < r_c \\ \phi_{LR}(\tfrac{r_{ij}}{\sigma}) &= 0 && r_{ij} > r_c \end{aligned} \quad (8)$$

II. Particle aggregation

Lennard-Jones potential

$$u^{LJ}(r) = 4\varepsilon((\tfrac{\sigma}{r})^m - (\tfrac{\sigma}{r})^n), \quad \varepsilon = 1.0, m = 12, n = 6 \quad (9)$$

Results

Some data of FT analysis and rheology for particle systems are given below

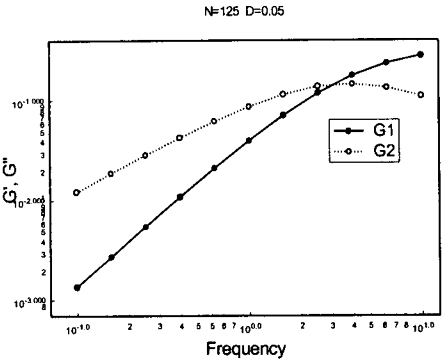

Fig 1. Frequency sweep (Particle aggregation)

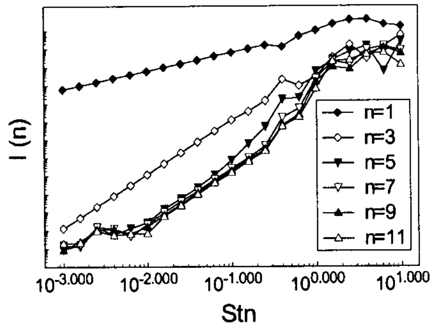

Fig 2. Intensity of higher harmonics

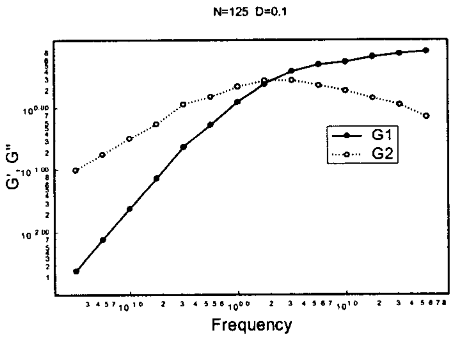

Fig 3. Frequency sweep (Particle gel)

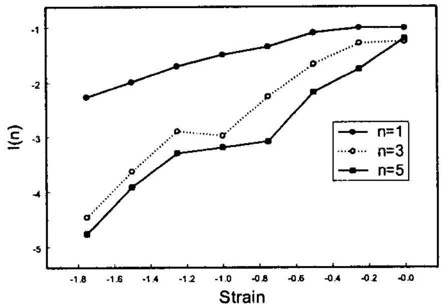

Fig 4. Intensity of higher harmonics

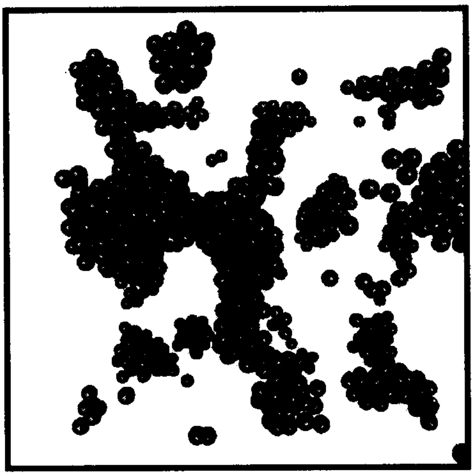

Fig 5. Particle gel structure

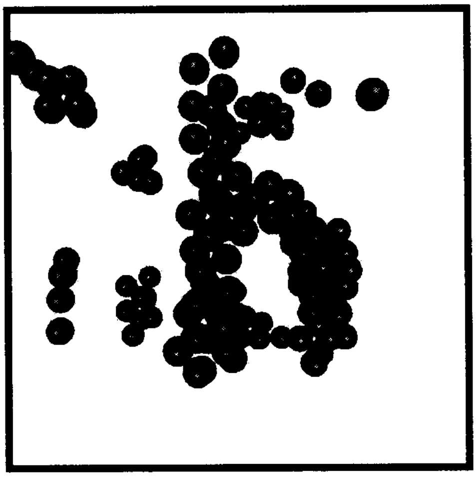

Fig 6. Particle aggregation structure

Conclusions

Particle systems have too complex structures to analyze data. But FT analysis helps to analyze data for particle systems such as colloidal and biological systems. In the FT analysis the intensity of higher harmonics is closely related to the microstructure of particle systems and the higher harmonics have a similar pattern to the properties in the nonlinear region. In the particle systems, the intensity of higher harmonics is in proportion to the square of strain like network models.

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