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COMPARISON BETWEEN THEORETICAL VALUES AND SIMULATION RESULTS OF TRANSPORT COEFFICIENTS FOR THE DISSIPATIVE PARTICLE DYNAMICS METHOD

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ABSTRACT

In the present study, we have derived an expression for transport coefficients such as viscosity, from the equation of motion of dissipative particles. In the concrete, we have shown the Fokker-Planck equation in phase space, and macroscopic conservation equations such as the equation of continuity and the equation of momentum conservation. The basic equations of the single-particle and pair distribution functions have been derived using the Fokker-Planck equation. The solutions of these distribution functions have approximately been solved by the perturbation method under the assumption of molecular chaos. The expression of the viscosity due to dissipative forces has been obtained using the approximate solutions of the distribution functions. Also, we have conducted non-equilibrium dynamics simulations to investigate the influence of the parameters, which have appeared in defining the equation of motion in the dissipative particle dynamics method.

1. INTRODUCTION

The hydrodynamic solution for a three-particle system has to be combined into a simulation method in order to take into account multi-body hydrodynamic interactions among colloidal particles more precisely. However, it is highly difficult even to solve analytically the flow field for a three-particle system [1,2], and, therefore, it seems to be almost hopeless to obtain the analytical solution for a non-spherical particle system such as a system composed of rodlike particles. Thus, we have a choice to take another approach to develop a more precise simulation method for colloidal dispersions. If both colloidal particles and solvent molecules are simulated, we can obtain the particle motion and the solution of the flow field simultaneously. However, if molecules themselves are treated in simulations, we cannot develop an effective simulation method, since the characteristic time for the motion of colloidal panicles is significantly different from that of solvent molecules. In other words, this kind of molecular-dynamics-like method is unrealistic as a simulation technique of a colloidal dispersion from a simulation time point of view. To circumvent this difficulty, the concept of fluid particles seems to be promising. Hoogerbrugge and Koelman [3,4] have developed the dissipative particle dynamics method in terms of fluid particles. In their theory, a fluid is regarded as being composed of such virtual particles, and the flow field is solved by simulating these particles. The fluid particles interact with each other, exchange momentum, and should make random motion like Brownian particles. From now on, such fluid particles are called dissipative particles.

For the simulation of the flow field for a colloidal dispersion, the motion of colloidal particles is dependent on the interaction between colloidal particles themselves, the interaction between colloidal particles

and dissipative particles, and the interaction between colloidal particles and an applied field such as a magnetic field. Hence, in this simulation technique, the solution of pair or three-body hydrodynamic interactions is unnecessary to be combined into, in order to simulate colloidal particles. This is in highly contrast with the ordinary simulation methods such as Stokesian dynamics methods [5-8]. Multi-body hydrodynamic interactions among colloidal particles are automatically taken into account from the interactions of colloidal particles with dissipative ones.

The present study attempts firstly to derive an analytical expression of transport coefficients such as viscosity using the equation of motion, secondly to obtain the numerical data in terms of dissipative particle dynamics simulations, and finally to compare the simulation results with the analytical solutions.

2. DYNAMICS OF DISSIPATIVE PARTICLES

2.1. Kinetic Equation of Dissipative Particles

We concentrate our attention on particle i and consider the forces acting on this particle. The following three kinds of forces may be physically reasonable as forces acting on particle i: a repulsive conservative force $\mathbf{F}_{ij}^{C}$ exerted by the other particles, a dissipative force $\mathbf{F}_{ij}^{D}$ providing a viscous drag to the system, and a random or stochastic force $\mathbf{F}_{ij}^{R}$ inducing the thermal motion of particles. With these forces, the equation of motion of particle i can be written as [9-11]

$$m\frac{d\boldsymbol{v}_i}{dt}=\sum_{j(\neq i)}\boldsymbol{F}_{ij}^{C}+\sum_{j(\neq i)}\boldsymbol{F}_{ij}^{D}+\sum_{j(\neq i)}\boldsymbol{F}_{ij}^{R}, \tag{1}$$

in which m is the mass of particle i, $\mathbf{v}_i$ is the velocity, and, concerning the subscripts, for example, $\mathbf{F}_{ij}^{C}$ is the force acting on particle i by particle j.

Now we have to embody specific forms of the above-mentioned forces. It may be reasonable to assume that the conservative force $\mathbf{F}_{ij}^{C}$ depends only on the relative position $\mathbf{r}_{ij}$ (=$\mathbf{r}_i$-$\mathbf{r}_j$), and not on the particle velocities. An explicit expression for this force will be shown later. Since the Galilean invariance has to be satisfied, the dissipative force $\mathbf{F}_{ij}^{D}$ and the random force $\mathbf{F}_{ij}^{R}$ should not be dependent on the position $\mathbf{r}_i$ and velocity $\mathbf{v}_i$ themselves, but should be functions of the relative position $\mathbf{r}_{ij}$ and relative velocity $\mathbf{v}_{ij}$ (=$\mathbf{v}_i$-$\mathbf{v}_j$), if necessarily. Additionally, it may be reasonable to assume that the random force $\mathbf{F}_{ij}^{R}$ does not depend on the relative velocity but the relative position $\mathbf{r}_{ij}$ alone. Furthermore, we have to take into account the isotropy of the particle motion and the decrease in the magnitude of forces with particle-particle separation. The following expressions for $\mathbf{F}_{ij}^{D}$ and $\mathbf{F}_{ij}^{R}$ satisfy these physical requirements [9-11]:

$$\boldsymbol{F}_{ij}^{D}=-\gamma w_D(r_{ij})(\boldsymbol{e}_{ij}\cdot\boldsymbol{v}_{ij})\boldsymbol{e}_{ij}, \tag{2}$$

$$\boldsymbol{F}_{ij}^{R}=\sigma w_R(r_{ij})\boldsymbol{e}_{ij}\zeta_{ij}, \tag{3}$$

in which r_{ij}=| $\mathbf{r}_{ij}$|, and $\mathbf{e}_{ij}$ is the unit vector denoting the direction of particle i from particle j, expressed as $\mathbf{e}_{ij}$=$\mathbf{r}_{ij}$/r_{ij}. Also ζ_{ij} is a random variable inducing the random motion of particles and has to satisfy the following stochastic properties:

$$\left\langle\zeta_{ij}(t)\right\rangle=0,\quad \left\langle\zeta_{ij}(t)\zeta_{i'j'}(t')\right\rangle=(\delta_{ii'}\delta_{jj'}+\delta_{ij'}\delta_{ji'})\delta(t-t'). \tag{4}$$

This variable satisfies the characteristic of the symmetry ζ_{ij} =ζ_{ji}, which ensures that the total momentum of the system is conserved. The $w_D(r_{ij})$ and $w_R(r_{ij})$ are weight functions to reproduce the decrease in forces with particle-particle separation, and γ and σ are constants specifying the magnitude of forces. These constants can be related to the system temperature and friction coefficient, which will be shown later.

The substitution of Eqs. (2) and (3) into Eq. (1) leads to the following equation:

$$\begin{aligned}m\frac{d\boldsymbol{v}_i}{dt}=&\sum_{j(\neq i)}\boldsymbol{F}_{ij}^{C}(\boldsymbol{r}_{ij})-\sum_{j(\neq i)}\gamma w_D(r_{ij})(\boldsymbol{e}_{ij}\cdot\boldsymbol{v}_{ij})\boldsymbol{e}_{ij}\\&+\sum_{j(\neq i)}\sigma w_R(r_{ij})\boldsymbol{e}_{ij}\zeta_{ij}.\end{aligned} \tag{5}$$

If this equation is integrated with respect to time over a small time interval from t to t+Δt, then the finite difference equations governing the particle motion in simulations can be obtained as

$$\Delta\boldsymbol{r}_i=\boldsymbol{v}_i\Delta t, \tag{6}$$

$$\begin{aligned}\Delta\boldsymbol{v}_i=&\frac{1}{m}\left(\sum_{j(\neq i)}\boldsymbol{F}_{ij}^{C}(\boldsymbol{r}_{ij})-\sum_{j(\neq i)}\gamma w_D(r_{ij})(\boldsymbol{e}_{ij}\cdot\boldsymbol{v}_{ij})\boldsymbol{e}_{ij}\right)\Delta t\\&+\frac{1}{m}\sum_{j(\neq i)}\sigma w_R(r_{ij})\boldsymbol{e}_{ij}\theta_{ij}\sqrt{\Delta t},\end{aligned} \tag{7}$$

in which θ_{ij} has to satisfy the following stochastic properties:

$$\left\langle\theta_{ij}\right\rangle=0,\quad \left\langle\theta_{ij}\theta_{i'j'}\right\rangle=(\delta_{ii'}\delta_{jj'}+\delta_{ij'}\delta_{ji'}). \tag{8}$$

2.2. Fokker-Planck Equation

We use the notation $\mathbf{r}_i$ for the position vector of particle i and $\mathbf{v}_i$ for the velocity vector. Also, for simplicity of expression, the vector $\mathbf{v}^N$ is used for describing the velocity vectors of all the particles and

similarly $\mathbf{r}^N$ is for the position vectors of all the particles. If the probability that a particle position and velocity are found within the range from ($\mathbf{r}^N$,$\mathbf{v}^N$) to ($\mathbf{r}^N$ +$\Delta\mathbf{r}^N$, $\mathbf{v}^N$+$\Delta\mathbf{v}^N$) is denoted by $W(\mathbf{r}^N,\mathbf{v}^N,t)d\mathbf{r}^N d\mathbf{v}^N$, then the probability density function $W(\mathbf{r}^N,\mathbf{v}^N,t)$ satisfies the following Fokker-Planck equation in phase space:

$$\frac{\partial W}{\partial t}+\sum_i \boldsymbol{v}_i\cdot\frac{\partial W}{\partial \boldsymbol{r}_i}+\sum_i\sum_{j\,(i\neq j)}\frac{\boldsymbol{F}_{ij}^C}{m}\cdot\frac{\partial W}{\partial \boldsymbol{v}_i}$$
$$=\sum_i\sum_{j\,(i\neq j)}\boldsymbol{e}_{ij}\cdot\frac{\partial}{\partial \boldsymbol{v}_i}\left\{\frac{1}{m}\gamma w_D(r_{ij})(\boldsymbol{e}_{ij}\cdot\boldsymbol{v}_{ij})W\right\} \tag{9}$$
$$+\frac{1}{2}\sum_i\sum_{j\,(i\neq j)}\frac{1}{m^2}\sigma^2 w_R^2(r_{ij})\boldsymbol{e}_{ij}\cdot\frac{\partial}{\partial \boldsymbol{v}_i}\left(\boldsymbol{e}_{ij}\cdot\frac{\partial}{\partial \boldsymbol{v}_i}-\boldsymbol{e}_{ij}\cdot\frac{\partial}{\partial \boldsymbol{v}_j}\right)W.$$

2.3. Final Expression of Equation of Motion and Its Non-dimensional Form

If a system composed of dissipative particles is in equilibrium, then the equilibrium distribution W_{eq} becomes the canonical distribution for an ensemble which is specified by a given particle number N, volume V, and temperature T. The equilibrium distribution W_{eq} has to satisfy the Fokker-Planck equation in phase space in Eq. (9). Since the left-hand side in Eq. (9) vanishes for the substitution of W_{eq}, the right-hand side also has to become zero. This is accomplished by the following requirements:

$$w_D(r_{ij})=w_R^2(r_{ij}),\quad \sigma^2=2\gamma kT, \tag{10}$$

in which k is Boltzmann's constant.

$\mathbf{F}_{ij}{}^C(r_{ij})$ is a repulsive force for preventing unphysical excessive overlaps between particles, and $w_R(r_{ij})$ has to be set so that inter-particle forces decrease with increasing particle-particle separations. These requirements are satisfied by the following expressions:

$$\boldsymbol{F}_{ij}^C=\alpha w_R(r_{ij})\boldsymbol{e}_{ij}, \tag{11}$$

$$w_R(r_{ij})=\begin{cases}1-\dfrac{r_{ij}}{r_c} & \text{for } r_{ij}\le r_c,\\ 0 & \text{for } r_{ij}>r_c,\end{cases} \tag{12}$$

in which α is a constant representing the magnitude of the repulsive forces. By substituting these equations into Eqs. (6) and (7) with considering Eq. (10), the final non-dimensional expression for the equation of motion of the dissipative particle dynamics can be written as

$$\Delta\boldsymbol{r}_i^*=\boldsymbol{v}_i^*\Delta t^*, \tag{13}$$

$$\Delta\boldsymbol{v}_i^*=\alpha^*\sum_{j(\neq i)}w_R(r_{ij}^*)\boldsymbol{e}_{ij}\Delta t^*-\gamma^*\sum_{j(\neq i)}w_R^2(r_{ij}^*)(\boldsymbol{e}_{ij}\cdot\boldsymbol{v}_{ij}^*)\boldsymbol{e}_{ij}\Delta t^*$$
$$+(2\gamma^*)^{1/2}\sum_{j(\neq i)}w_R(r_{ij}^*)\boldsymbol{e}_{ij}\theta_{ij}\sqrt{\Delta t^*}, \tag{14}$$

in which

$$w_R(r_{ij}^*)=\begin{cases}1-r_{ij}^* & \text{for } r_{ij}^*\le 1,\\ 0 & \text{for } r_{ij}^*>1,\end{cases} \tag{15}$$

$$\alpha^*=\alpha\frac{r_c}{kT},\quad \gamma^*=\gamma\frac{r_c}{(mkT)^{1/2}}. \tag{16}$$

To non-dimensionalize each quantity, the following representative values have been used: (kT/m)$^{1/2}$ for velocities, r_c for distances, $r_c(m/kT)^{1/2}$ for time, $(1/r_c^3)$ for number densities, etc.

3. TRANSPORT EQUATIONS

If an arbitrary physical quantity $A(\mathbf{r}^N,\mathbf{v}^N)$ is not dependent on time explicitly, the time average <A> can be expressed, using the probability density function W which satisfies Eq. (9), as

$$\langle A\rangle=\int\!\!\int AW(\boldsymbol{r}^N,\boldsymbol{v}^N,t)\,d\boldsymbol{r}^N d\boldsymbol{v}^N, \tag{17}$$

in which

$$\int\!\!\int W(\boldsymbol{r}^N,\boldsymbol{v}^N,t)\,d\boldsymbol{r}^N d\boldsymbol{v}^N=1. \tag{18}$$

Hence, the time variation of <A> can be expressed, from Eq. (9), as

$$\frac{\partial}{\partial t}\langle A\rangle=\int\!\!\int A\frac{\partial W}{\partial t}d\boldsymbol{r}^N d\boldsymbol{v}^N=\left\langle\sum_i \boldsymbol{v}_i\cdot\frac{\partial A}{\partial \boldsymbol{r}_i}\right.$$
$$-\sum_i\sum_{j\,(i\neq j)}\frac{\boldsymbol{F}_{ij}^C}{m}\cdot\frac{\partial A}{\partial \boldsymbol{v}_i}-\sum_i\sum_{j\,(i\neq j)}\frac{\gamma}{m}w_D(r_{ij})(\boldsymbol{e}_{ij}\cdot\boldsymbol{v}_{ij})\boldsymbol{e}_{ij}\cdot\frac{\partial A}{\partial \boldsymbol{v}_i} \tag{19}$$
$$\left.+\frac{1}{2}\sum_i\sum_{j\,(i\neq j)}\frac{1}{m^2}\sigma^2 w_R^2(r_{ij})\left(\boldsymbol{e}_{ij}\cdot\frac{\partial}{\partial \boldsymbol{v}_i}\right)\left(\boldsymbol{e}_{ij}\cdot\frac{\partial}{\partial \boldsymbol{v}_i}-\boldsymbol{e}_{ij}\cdot\frac{\partial}{\partial \boldsymbol{v}_j}\right)A\right\rangle.$$

If A is defined by the following equation:

$$A=\sum_{i=1}^N m\delta(\boldsymbol{r}-\boldsymbol{r}_i), \tag{20}$$

then the average <A> which is evaluated from Eq. (17) is equal to a local density $\rho(\mathbf{r})$. That is,

$$\langle A\rangle=\left\langle\sum_{i=1}^N m\delta(\boldsymbol{r}-\boldsymbol{r}_i)\right\rangle=\rho(\boldsymbol{r}). \tag{21}$$

If A is taken as

$$A=\sum_{i=1}^N m\boldsymbol{v}_i\delta(\boldsymbol{r}-\boldsymbol{r}_i), \tag{22}$$

then the average <A> is now

$$\langle A \rangle = \rho(\boldsymbol{r})\boldsymbol{u}(\boldsymbol{r}), \tag{23}$$

in which $\mathbf{u}(\mathbf{r})$ is a macroscopic fluid velocity.

The substitution of Eq. (20) into Eq. (19) leads to the following expression:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial \boldsymbol{r}} \cdot (\rho \boldsymbol{u}) = 0. \tag{24}$$

This is no other than the equation of continuity.

Next the substitution of Eq. (22) into Eq. (19) leads to the following equation:

$$\begin{aligned} \frac{\partial}{\partial t}(\rho \boldsymbol{u}) = & \\ \Bigg\langle \sum_i m\boldsymbol{v}_i \cdot \frac{\partial}{\partial \boldsymbol{r}_i}(\boldsymbol{v}_i \delta(\boldsymbol{r}-\boldsymbol{r}_i)) + \sum_i \sum_{\substack{j \\ (i \neq j)}} \boldsymbol{F}_{ij}^C \cdot \frac{\partial}{\partial \boldsymbol{v}_i}(\boldsymbol{v}_i \delta(\boldsymbol{r}-\boldsymbol{r}_i)) & \\ - \sum_i \sum_{\substack{j \\ (i \neq j)}} \gamma w_D(r_{ij})(\boldsymbol{e}_{ij} \cdot \boldsymbol{v}_{ij}) \left\{ \boldsymbol{e}_{ij} \cdot \frac{\partial}{\partial \boldsymbol{v}_i}(\boldsymbol{v}_i \delta(\boldsymbol{r}-\boldsymbol{r}_i)) \right\} & \\ + \frac{1}{2} \sum_i \sum_{\substack{j \\ (i \neq j)}} \frac{1}{m} \sigma^2 w_R^2(r_{ij}) \left(\boldsymbol{e}_{ij} \cdot \frac{\partial}{\partial \boldsymbol{v}_i} \right) \boldsymbol{e}_{ij} & \\ \cdot \left\{ \frac{\partial}{\partial \boldsymbol{v}_i}(\boldsymbol{v}_i \delta(\boldsymbol{r}-\boldsymbol{r}_i)) - \frac{\partial}{\partial \boldsymbol{v}_j}(\boldsymbol{v}_j \delta(\boldsymbol{r}-\boldsymbol{r}_j)) \right\} \Bigg\rangle. & \end{aligned} \tag{25}$$

Thus, by taking into account Eq. (2), Eq. (25) can be simplified as

$$\begin{aligned} \frac{\partial}{\partial t}(\rho \boldsymbol{u}) = & \Bigg\langle - \frac{\partial}{\partial \boldsymbol{r}} \cdot \left\{ \sum_i m\boldsymbol{v}_i \boldsymbol{v}_i \delta(\boldsymbol{r}-\boldsymbol{r}_i) \right\} \\ & + \sum_i \sum_{\substack{j \\ (i \neq j)}} (\boldsymbol{F}_{ij}^C + \boldsymbol{F}_{ij}^D) \delta(\boldsymbol{r}-\boldsymbol{r}_i) \Bigg\rangle. \end{aligned} \tag{26}$$

By taking account of the relation $\mathbf{F}_{ij}^D = F_{ij}^D \mathbf{e}_{ij}$ (similarly, for $\mathbf{F}_{ij}^C$), Eq. (26) can finally be written as

$$\frac{\partial}{\partial t}(\rho \boldsymbol{u}) = -\frac{\partial}{\partial \boldsymbol{r}} \cdot (\rho \boldsymbol{u}\boldsymbol{u}) + \frac{\partial}{\partial \boldsymbol{r}} \cdot (\boldsymbol{\tau}^K + \boldsymbol{\tau}^U), \tag{27}$$

in which

$$\left. \begin{aligned} \boldsymbol{\tau}^K &= -\left\langle \sum_i m(\boldsymbol{v}_i - \boldsymbol{u})(\boldsymbol{v}_i - \boldsymbol{u}) \delta(\boldsymbol{r}-\boldsymbol{r}_i) \right\rangle, \\ \boldsymbol{\tau}^U &= -\frac{1}{2} \left\langle \sum_i \sum_{\substack{j \\ (i \neq j)}} (F_{ij}^C + F_{ij}^D) \boldsymbol{e}_{ij} \boldsymbol{e}_{ij} \int_0^{r_{ij}} \delta(\boldsymbol{r}-\boldsymbol{r}_i + \xi \boldsymbol{e}_{ij}) d\xi \right\rangle. \end{aligned} \right\} \tag{28}$$

If the equation of continuity in Eq. (24) is taken into consideration, Eq. (27) reduces to the momentum equation of the fluid:

$$\rho \left(\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u} \cdot \frac{\partial \boldsymbol{u}}{\partial \boldsymbol{r}} \right) = \frac{\partial}{\partial \boldsymbol{r}} \cdot (\boldsymbol{\tau}^K + \boldsymbol{\tau}^U), \tag{29}$$

4. EXPRESSIONS FOR TRANSPORT COEFFICIENTS

4.1. Distribution Functions

The local number density $n(\mathbf{r},t)$ at position $\mathbf{r}$ at time t can be expressed using $W(\mathbf{r}^N,\mathbf{v}^N,t)$ as [12]

$$\begin{aligned} n(\boldsymbol{r},t) &= \left\langle \sum_{i=1}^N \delta(\boldsymbol{r}-\boldsymbol{r}_i) \right\rangle = \int \cdots \int \sum_i \delta(\boldsymbol{r}-\boldsymbol{r}_i) W(\boldsymbol{r}^N,\boldsymbol{v}^N,t) d\boldsymbol{r}^N d\boldsymbol{v}^N \\ &= N \int \cdots \int W(\boldsymbol{r},\boldsymbol{r}_2,\cdots,\boldsymbol{r}_N,\boldsymbol{v}^N,t) d\boldsymbol{r}_2 \cdots d\boldsymbol{r}_N d\boldsymbol{v}^N. \end{aligned} \tag{30}$$

Similarly, the pair correlation function $g(\mathbf{r},\mathbf{r}',t)$ can be written as [12]

$$\begin{aligned} g(\boldsymbol{r},\boldsymbol{r}',t) &= \frac{1}{n_0^2} \int \cdots \int \sum_i^N \sum_{\substack{j \\ (i \neq j)}}^N \delta(\boldsymbol{r}-\boldsymbol{r}_i) \delta(\boldsymbol{r}'-\boldsymbol{r}_j) W(\boldsymbol{r}^N,\boldsymbol{v}^N,t) d\boldsymbol{r}^N d\boldsymbol{v}^1 \\ &= \frac{N(N-1)}{n_0^2} \int \cdots \int W(\boldsymbol{r},\boldsymbol{r}',\boldsymbol{r}_3,\cdots,\boldsymbol{r}_N,\boldsymbol{v}^N,t) d\boldsymbol{r}_3 \cdots d\boldsymbol{r}_N d\boldsymbol{v}^N, \end{aligned} \tag{31}$$

in which n_0 is the mean number density, given by $n_0 = N/V$.

If the distribution function $f(\mathbf{r},\mathbf{v},t)$ is defined as [11]

$$f(\boldsymbol{r},\boldsymbol{v},t) = \left\langle \sum_{i=1}^N \delta(\boldsymbol{r}-\boldsymbol{r}_i) \delta(\boldsymbol{v}-\boldsymbol{v}_i) \right\rangle, \tag{32}$$

$f(\mathbf{r},\mathbf{v},t)$ can be written, using $W(\mathbf{r}^N,\mathbf{v}^N,t)$, as

$$f(\boldsymbol{r},\boldsymbol{v},t) = N \int \cdots \int W(\boldsymbol{r},\boldsymbol{r}_2,\cdots,\boldsymbol{r}_N,\boldsymbol{v},\boldsymbol{v}_2,\cdots,\boldsymbol{v}_N,t) d\boldsymbol{r}_2 \cdots d\boldsymbol{r}_N d\boldsymbol{v}_2 \cdots d\boldsymbol{v}_N. \tag{33}$$

By comparing Eq. (33) with Eq. (30), it is seen that there is a relationship between $f(\mathbf{r},\mathbf{v},t)$ and $n(\mathbf{r},t)$:

$$n(\boldsymbol{r},t) = \int f(\boldsymbol{r},\boldsymbol{v},t) d\boldsymbol{v}. \tag{34}$$

Similarly,

$$n(\boldsymbol{r},t)\boldsymbol{u}(\boldsymbol{r},t) = \left\langle \sum_i^N \boldsymbol{v}_i \delta(\boldsymbol{r}-\boldsymbol{r}_i) \right\rangle = \int \boldsymbol{v} f(\boldsymbol{r},\boldsymbol{v},t) d\boldsymbol{v}. \tag{35}$$

Next, if we define the pair distribution $f^{(2)}(\mathbf{r},\mathbf{r}',\mathbf{v},\mathbf{v}',t)$ by the following equation [11]:

$$\begin{aligned} f^{(2)}(\boldsymbol{r},\boldsymbol{r}',\boldsymbol{v},\boldsymbol{v}',t) &= \left\langle \sum_{i=1}^N \sum_{\substack{i=1 \\ (i \neq j)}}^N \delta(\boldsymbol{r}-\boldsymbol{r}_i) \delta(\boldsymbol{r}'-\boldsymbol{r}_j) \delta(\boldsymbol{v}-\boldsymbol{v}_i) \delta(\boldsymbol{v}'-\boldsymbol{v}_j) \right\rangle \\ &= N(N-1) \int \cdots \int W(\boldsymbol{r},\boldsymbol{r}',\boldsymbol{r}_3,\cdots,\boldsymbol{r}_N,\boldsymbol{v},\boldsymbol{v}',\boldsymbol{v}_3,\cdots,\boldsymbol{v}_N,t) d\boldsymbol{r}_3 \cdots d\boldsymbol{r}_N d\boldsymbol{v}_3 \cdots d\boldsymbol{v}_N, \end{aligned} \tag{36}$$

then the pair distribution can be related to the pair correlation function $g(\mathbf{r},\mathbf{r}',t)$ as

$$n_0^2 g(\boldsymbol{r},\boldsymbol{r}',t) = \int \int f^{(2)}(\boldsymbol{r},\boldsymbol{r}',\boldsymbol{v},\boldsymbol{v}',t) d\boldsymbol{v} d\boldsymbol{v}'. \tag{37}$$

It is clear from Eq. (19) that the average of an arbitrary quantity $A(\mathbf{r}^N,\mathbf{v}^N)$ can be evaluated using

$f(\mathbf{r},\mathbf{v},t)$ and $f^{(2)}(\mathbf{r},\mathbf{r}',\mathbf{v},\mathbf{v}',t)$ without obtaining the expression of $W(\mathbf{r}^N,\mathbf{v}^N,t)$. Hence, we here first show the basic equations for f and $f^{(2)}$, and then solve analytically the equations to obtain the approximate solutions.

If we set $A=\sum \delta(\boldsymbol{r}-\boldsymbol{r}_i)\delta(\boldsymbol{v}-\boldsymbol{v}_i)$ in Eq. (19), and reform the equation with the formulae of vector operations, the following equation can be obtained:

$$\begin{aligned}&\frac{\partial}{\partial t}f(\boldsymbol{r},\boldsymbol{v},t)+\boldsymbol{v}\cdot\frac{\partial}{\partial \boldsymbol{r}}f(\boldsymbol{r},\boldsymbol{v},t)\\&=\frac{\gamma}{m}\int\!\!\int w_D(R)\hat{\boldsymbol{R}}\hat{\boldsymbol{R}}:\frac{\partial}{\partial \boldsymbol{v}}\left\{(\boldsymbol{v}-\boldsymbol{v}')\,f^{(2)}(\boldsymbol{r},\boldsymbol{r}+\boldsymbol{R},\boldsymbol{v},\boldsymbol{v}',t)\right\}d\boldsymbol{R}d\boldsymbol{v}'\\&\quad+\frac{\sigma^2}{2m^2}\int\!\!\int w_R^2(R)\hat{\boldsymbol{R}}\hat{\boldsymbol{R}}:\frac{\partial^2}{\partial \boldsymbol{v}\partial \boldsymbol{v}}f^{(2)}(\boldsymbol{r},\boldsymbol{r}+\boldsymbol{R},\boldsymbol{v},\boldsymbol{v}',t)\,d\boldsymbol{R}d\boldsymbol{v}'.\end{aligned}\tag{38}$$

It has been assumed in deriving this equation that there are no conservative forces. In Eq. (38), $\hat{\mathbf{R}}$ is the unit vector, denoted by $\hat{\mathbf{R}}=\mathbf{R}/|\mathbf{R}|$. It is seen from Eq. (38) that the pair distribution function $f^{(2)}(\mathbf{r},\mathbf{r}',\mathbf{v},\mathbf{v}',t)$ is necessary for obtaining the solution of $f(\mathbf{r},\mathbf{v},t)$, and, similarly, the multi-body distribution functions more than the pair distribution is required to get the solution of $f^{(2)}$. This clearly shows that Eq. (38) is not closed, but a hierarchy equation. To close the equation for f, the following assumption of molecular chaos is introduced [11]:

$$f^{(2)}(\boldsymbol{r},\boldsymbol{r}',\boldsymbol{v},\boldsymbol{v}',t)\simeq f(\boldsymbol{r},\boldsymbol{v},t)f(\boldsymbol{r}',\boldsymbol{v}',t).\tag{39}$$

This assumption theoretically enables us to solve the equation of the distribution function. The substitution of Eq. (39) into Eq. (38) leads to the following non-dimensional equation:

$$\begin{aligned}&\frac{\partial}{\partial t^*}f^*(\boldsymbol{r}^*,\boldsymbol{v}^*,t^*)+\boldsymbol{v}^*\cdot\frac{\partial}{\partial \boldsymbol{r}^*}f^*(\boldsymbol{r}^*,\boldsymbol{v}^*,t^*)=\gamma^* n_0^*\int\!\!\int w_D(R^*)\\&\times f^*(\boldsymbol{r}^*+\boldsymbol{R}^*,\boldsymbol{v}'^*,t^*)\hat{\boldsymbol{R}}\hat{\boldsymbol{R}}:\frac{\partial}{\partial \boldsymbol{v}^*}\left\{(\boldsymbol{v}^*-\boldsymbol{v}'^*)f^*(\boldsymbol{r}^*,\boldsymbol{v}^*,t^*)\right\}d\boldsymbol{R}^*d\boldsymbol{v}'^*\\&\quad+\gamma^* n_0^*\int\!\!\int w_D(R^*)f^*(\boldsymbol{r}^*+\boldsymbol{R}^*,\boldsymbol{v}'^*,t^*)\hat{\boldsymbol{R}}\hat{\boldsymbol{R}}\\&\quad:\frac{\partial^2}{\partial \boldsymbol{v}^*\partial \boldsymbol{v}^*}f^*(\boldsymbol{r}^*,\boldsymbol{v}^*,t^*)d\boldsymbol{R}^*d\boldsymbol{v}'^*,\end{aligned}\tag{40}$$

in which the distribution function f has been non-dimensionalized as $f^*=(1/n_0)(kT/m)^{3/2}f$. If we set $\xi=1/\gamma^* n_0^*$ and assume ξ to be much smaller than unity, the perturbation method is applicable. Hence, f^* is expanded, with the perturbation parameter ξ, as

$$f^*(\boldsymbol{r}^*,\boldsymbol{v}^*,t^*)=f_0^*(\boldsymbol{r}^*,\boldsymbol{v}^*,t^*)+\xi f_1^*(\boldsymbol{r}^*,\boldsymbol{v}^*,t^*)+\xi^2 f_2^*(\boldsymbol{r}^*,\boldsymbol{v}^*,t^*)+\cdots\tag{41}$$

By substituting this equation into Eq. (40) and neglecting the higher-order terms, we can obtain the following expression:

$$\begin{aligned}&\xi\left\{\frac{\partial}{\partial t^*}f_0^*+\boldsymbol{v}^*\cdot\frac{\partial}{\partial \boldsymbol{r}^*}f_0^*\right\}+\xi^2\left\{\frac{\partial}{\partial t^*}f_1^*+\boldsymbol{v}^*\cdot\frac{\partial}{\partial \boldsymbol{r}^*}f_1^*\right\}=\int\!\!\int w_D(R^*)\\&\quad\times\left\{f_0^*(\boldsymbol{r}^*+\boldsymbol{R}^*,\boldsymbol{v}'^*,t^*)+\xi f_1^*(\boldsymbol{r}^*+\boldsymbol{R}^*,\boldsymbol{v}'^*,t^*)\right\}\hat{\boldsymbol{R}}\hat{\boldsymbol{R}}\\&\quad:\frac{\partial}{\partial \boldsymbol{v}^*}\left\{(\boldsymbol{v}^*-\boldsymbol{v}'^*)(f_0^*(\boldsymbol{r}^*,\boldsymbol{v}^*,t^*)+\xi f_1^*(\boldsymbol{r}^*,\boldsymbol{v}^*,t^*))\right\}d\boldsymbol{R}^*d\boldsymbol{v}'^*\\&+\int\!\!\int w_D(R^*)\left\{f_0^*(\boldsymbol{r}^*+\boldsymbol{R}^*,\boldsymbol{v}'^*,t^*)+\xi f_1^*(\boldsymbol{r}^*+\boldsymbol{R}^*,\boldsymbol{v}'^*,t^*)\right\}\hat{\boldsymbol{R}}\hat{\boldsymbol{R}}\\&\quad:\frac{\partial^2}{\partial \boldsymbol{v}^*\partial \boldsymbol{v}^*}\left\{f_0^*(\boldsymbol{r}^*,\boldsymbol{v}^*,t^*)+\xi f_1^*(\boldsymbol{r}^*,\boldsymbol{v}^*,t^*)\right\}d\boldsymbol{R}^*d\boldsymbol{v}'^*.\end{aligned}\tag{42}$$

The equation for the zero-th order of ξ can straightforwardly be solved as

$$f_0^*(\boldsymbol{r}^*,\boldsymbol{v}^*,t^*)=n^*\left(\frac{1}{2\pi}\right)^{3/2}\exp\left\{-\frac{1}{2}(\boldsymbol{v}^*-\boldsymbol{u}^*)^2\right\}.\tag{43}$$

The equation for the first-order of ξ can be obtained as

$$\begin{aligned}&\frac{\partial}{\partial t^*}f_0^*+\boldsymbol{v}^*\cdot\frac{\partial}{\partial \boldsymbol{r}^*}f_0^*=\int n^*(\boldsymbol{r}^*+\boldsymbol{R}^*,t^*)w_D(R^*)\hat{\boldsymbol{R}}\hat{\boldsymbol{R}}\\&:\left[\frac{\partial}{\partial \boldsymbol{v}^*}\left\{(\boldsymbol{v}^*-\boldsymbol{u}^*)f_1^*(\boldsymbol{r}^*,\boldsymbol{v}^*,t^*)\right\}+\frac{\partial^2}{\partial \boldsymbol{v}^*\partial \boldsymbol{v}^*}f_1^*(\boldsymbol{r}^*,\boldsymbol{v}^*,t^*)\right]d\boldsymbol{R}^*.\end{aligned}\tag{44}$$

If it is assumed that $n^*(\mathbf{r}^*+\mathbf{R}^*,t^*)$ $(=n/n_0)$ is independent of the position and is constant, and the integration is carried out using the polar axis coordinates of $\hat{\mathbf{R}}$, then Eq. (44) can be simplified as

$$\begin{aligned}&\frac{\partial}{\partial t^*}f_0^*+\boldsymbol{v}^*\cdot\frac{\partial}{\partial \boldsymbol{r}^*}f_0^*=\frac{[w]}{3}\left[\frac{\partial}{\partial \boldsymbol{v}^*}\cdot\left\{(\boldsymbol{v}^*-\boldsymbol{u}^*)f_1^*(\boldsymbol{r}^*,\boldsymbol{v}^*,t^*)\right\}\right.\\&\qquad\left.+\frac{\partial}{\partial \boldsymbol{v}^*}\cdot\frac{\partial}{\partial \boldsymbol{v}^*}f_1^*(\boldsymbol{r}^*,\boldsymbol{v}^*,t^*)\right],\end{aligned}\tag{45}$$

in which $[w]$ is defined as

$$[w]=\int_0^1 w_D d\boldsymbol{R}^*=\int_0^1 w_D 4\pi R^{*2}dR^*.\tag{46}$$

The left-hand side of Eq. (45) can finally be reformed, by taking account of Eq. (43), as

$$\frac{\partial}{\partial t^*}f_0^*+\boldsymbol{v}^*\cdot\frac{\partial}{\partial \boldsymbol{r}^*}f_0^*=\frac{1}{2}f_0^*\boldsymbol{U}^*\boldsymbol{U}^*:\left\{\frac{\partial}{\partial \boldsymbol{r}^*}\boldsymbol{u}^*+\left(\frac{\partial}{\partial \boldsymbol{r}^*}\boldsymbol{u}^*\right)^t\right\},\tag{47}$$

in which the notation $\mathbf{U}^*$, defined by $\mathbf{U}^*=(\mathbf{v}^*-\mathbf{u}^*)$, has been used. Also, the superscript t means a transposed tensor. The solution of Eq. (45) can straightforwardly be seen to be the following expression:

$$f_1^* = -\frac{3}{2}\cdot\frac{1}{n_0^*[w]}\cdot\left\{\boldsymbol{U}^*\boldsymbol{U}^* f_0^* - \frac{1}{3}U^{*2} f_0^* \boldsymbol{I}\right\} : \frac{1}{2}\left\{\frac{\partial}{\partial \boldsymbol{r}^*}\boldsymbol{u}^* + \left(\frac{\partial}{\partial \boldsymbol{r}^*}\boldsymbol{u}^*\right)^t\right\}. \tag{48}$$

We now have obtained the zero-th and first order solutions of f^*:

$$f^* = f_0^* + \xi f_1^*. \tag{49}$$

4.2. Viscosity due to Dissipative Forces

With the following Taylor series expansion of the Dirac delta function:

$$\delta(\boldsymbol{r}-\boldsymbol{r}_i+\xi\boldsymbol{e}_{ij}) = \delta(\boldsymbol{r}-\boldsymbol{r}_i) + \xi\boldsymbol{e}_{ij}\cdot\frac{\partial}{\partial \boldsymbol{r}}\delta(\boldsymbol{r}-\boldsymbol{r}_i) + \frac{1}{2!}\xi^2\boldsymbol{e}_{ij}\boldsymbol{e}_{ij}:\frac{\partial}{\partial \boldsymbol{r}}\frac{\partial}{\partial \boldsymbol{r}}\delta(\boldsymbol{r}-\boldsymbol{r}_i) + \cdots, \tag{50}$$

the stress tensor due to dissipative forces can be written as

$$\boldsymbol{\tau}^D = \frac{1}{2}\left\langle \sum_i \sum_{(i\neq j)} \gamma w_D(r_{ij})(\boldsymbol{e}_{ij}\cdot\boldsymbol{v}_{ij})\boldsymbol{e}_{ij}\boldsymbol{r}_{ij}\delta(\boldsymbol{r}-\boldsymbol{r}_i)\right\rangle + \frac{1}{4}\frac{\partial}{\partial \boldsymbol{r}}\cdot\left\langle \sum_i \sum_{(i\neq j)} \gamma w_D(r_{ij})(\boldsymbol{e}_{ij}\cdot\boldsymbol{v}_{ij})\boldsymbol{e}_{ij}\boldsymbol{r}_{ij}\boldsymbol{r}_{ij}\delta(\boldsymbol{r}-\boldsymbol{r}_i)\right\rangle + \cdots. \tag{51}$$

The second term on the right-hand side in this equation is negligible unless there is a significant non-uniformity of the system. Equation (51) is, therefore, rewritten as

$$\boldsymbol{\tau}^{D*} = -\frac{1}{2}n_0^{*2}\gamma^*\int\cdots\int R^* w_D(R^*)\left\{\hat{\boldsymbol{R}}\cdot(\boldsymbol{v}^*-\boldsymbol{v}'^*)\right\}\hat{\boldsymbol{R}}\hat{\boldsymbol{R}} \times f^{(2)*}(\boldsymbol{r}^*,\boldsymbol{r}^*+\boldsymbol{R}^*,\boldsymbol{v}^*,\boldsymbol{v}'^*,t^*)\,d\boldsymbol{R}^*d\boldsymbol{v}^*d\boldsymbol{v}'^*. \tag{52}$$

By the assumption of molecular chaos, written in Eq. (39), with Eq. (49) for f^*, the expression for $f^{(2)*}$ can be written as

$$f^{(2)*}(\boldsymbol{r}^*,\boldsymbol{r}'^*,\boldsymbol{v}^*,\boldsymbol{v}'^*,t^*) = f_0^*(\boldsymbol{r}^*,\boldsymbol{v}^*,t^*)f_0^*(\boldsymbol{r}'^*,\boldsymbol{v}'^*,t^*) + \xi f_0^*(\boldsymbol{r}^*,\boldsymbol{v}^*,t^*)f_1^*(\boldsymbol{r}'^*,\boldsymbol{v}'^*,t^*) + \xi f_0^*(\boldsymbol{r}'^*,\boldsymbol{v}'^*,t^*)f_1^*(\boldsymbol{r}^*,\boldsymbol{v}^*,t^*) + \xi^2 f_1^*(\boldsymbol{r}^*,\boldsymbol{v}^*,t^*)f_1^*(\boldsymbol{r}'^*,\boldsymbol{v}'^*,t^*). \tag{53}$$

By evaluating Eq. (52) with Eq. (53), the expression for $\boldsymbol{\tau}^{D*}$ can be obtained. After some mathematical manipulation, the expression for $\boldsymbol{\tau}^{D*}$ can finally be obtained as

$$\boldsymbol{\tau}^{D*} = \frac{\gamma^* n_0^{*2}}{15}[R^{*2}w]\cdot\frac{1}{2}\left\{\frac{\partial}{\partial \boldsymbol{r}^*}\boldsymbol{u}^* + \left(\frac{\partial}{\partial \boldsymbol{r}^*}\boldsymbol{u}^*\right)^t\right\}. \tag{54}$$

Hence, the expression for the viscosity η^{D*} due to dissipative forces can be written as

$$\eta^{D*} = \frac{\gamma^* n_0^{*2}}{30}[R^{*2}w] = \frac{2\pi}{1575}n_0^{*2}\gamma^*. \tag{55}$$

5. EVALUATION OF VISCOSITY BY SIMULATIONS

The Green-Kubo expressions for transport coefficients are widely used for evaluating them for a molecular system by means of molecular simulations. The viscosity is evaluated from the integration of the mean values of the correlation function [12,13]:

$$\eta_{yx} = \frac{1}{kTV}\int_0^\infty \left\langle J_{yx}(t)J_{yx}(0)\right\rangle dt, \tag{56}$$

in which

$$J_{yx}(t) = \sum_{i=1}^N \left\{mv_{iy}(t)v_{ix}(t) + y_i(t)F_{ix}(t)\right\} = \sum_{i=1}^N mv_{ij}(t)v_{ix}(t) + \sum_{i=1}^N\sum_{\substack{j=1\\(i<j)}}^N y_{ij}(t)F_{ijx}(t), \tag{57}$$

and F_{ijx} is the x-component of the force vector $\mathbf{F}_{ij}$.

The theory of the non-equilibrium molecular dynamics method [13] for a molecular system is applicable to the present case, if a simple shear flow is considered as a flow field. In this case, the viscosity η_{yx} is evaluated from the following equation in simulations [12,13]:

$$\eta_{yx} = -\frac{1}{V\dot{\gamma}}\left\langle J_{yx}\right\rangle_{\mathrm{ne}}, \tag{58}$$

in which $\dot{\gamma}$ is the shear rate, $\langle J_{yx}\rangle_{\mathrm{ne}}$ is the time average of J_{yx} under circumstances of a simple shear flow, which is assumed to act in the x-axis direction.

6. RESULTS

Figures 1 shows the influence of the values of γ^* on the viscosity, which were obtained by the non-equilibrium dynamics method. Similar results are shown in Figs. 2, which were obtained from the Green-Kubo expression by means of equilibrium simulations.

It is seen from Fig.1 that the results obtained by the non-equilibrium dynamics simulations are in good agreement with the theoretical solutions shown in Eq. (55) for both cases of $\alpha^*=\gamma^*/10$ and $\alpha^*=\gamma^*$. However, for the cases of small number densities such as $n_0^*=0.5$, the simulation results have significant errors and, therefore, qualitative properties are relatively difficult to be notified. That the number density n_0^* is smaller than unity means that a sufficiently large number of particles do not exist around an arbitrary particle within the range of the radius r_c from its center. In this situation, the accuracy of the viscosity data is strongly dependent on

whether or not there are other particles which interact with the particle of interest. Hence such a situation causes significant errors of the simulation results of viscosity, which has been seen for n_0^*=0.5 in Fig.1. We may conclude from this fact that it is desirable to take the number density as $n_0^* \gg 1.0$ in simulating a flow problem by means of the dissipative particle dynamics method. It is clearly seen from Fig. 2 that the simulation results of η^{D*}, which were obtained by the Green-Kubo expression, are significantly smaller than the theoretical solutions. This dependence becomes more significant with increasing the values of number density. As shown before, the viscosity due to dissipative forces is evaluated by the integral of the average of the time correlation according to the Green-Kubo method. In the dissipative particle dynamics method, since random forces are included in the equation of motion and, therefore, have influence on the motion of dissipative particles, the time correlation of dissipative forces are presumed to decrease more significantly with time than in the case of no random forces. We may conclude that this causes more significant discrepancy between the simulation and theoretical results with increasing the values of number density.

7. CONCLUSIONS

In order to investigate the validity of the dissipative particle dynamics method, which is a mesoscopic simulation technique, we have derived the expression for transport coefficients such as viscosity, from the equation of motion of the dissipative particles. In the concrete, we have shown the Fokker-Planck equation in phase space, and macroscopic conservation equations such as the equation of continuity and the equation of momentum conservation. The basic equations of the single-particle and pair distribution functions have been derived using the Fokker-Planck equation. The solutions of these distribution functions have approximately been solved by the perturbation method under the assumption of molecular chaos. The expression of the viscosity due to dissipative forces has been obtained using the approximate solutions of the distribution functions. Also, we have conducted non-equilibrium dynamics simulations to investigate the influence of the parameters, which have appeared in defining the equation of motion in the dissipative particle dynamics method. The results obtained here are briefly summarized as follows. The theoretical values of the viscosity due to dissipative forces are in good agreement with the simulation results obtained by the non-equilibrium dynamics method, except in the range of small number densities. The results obtained from the Green-Kubo expression by equilibrium simulations are significantly smaller than the theoretical ones.

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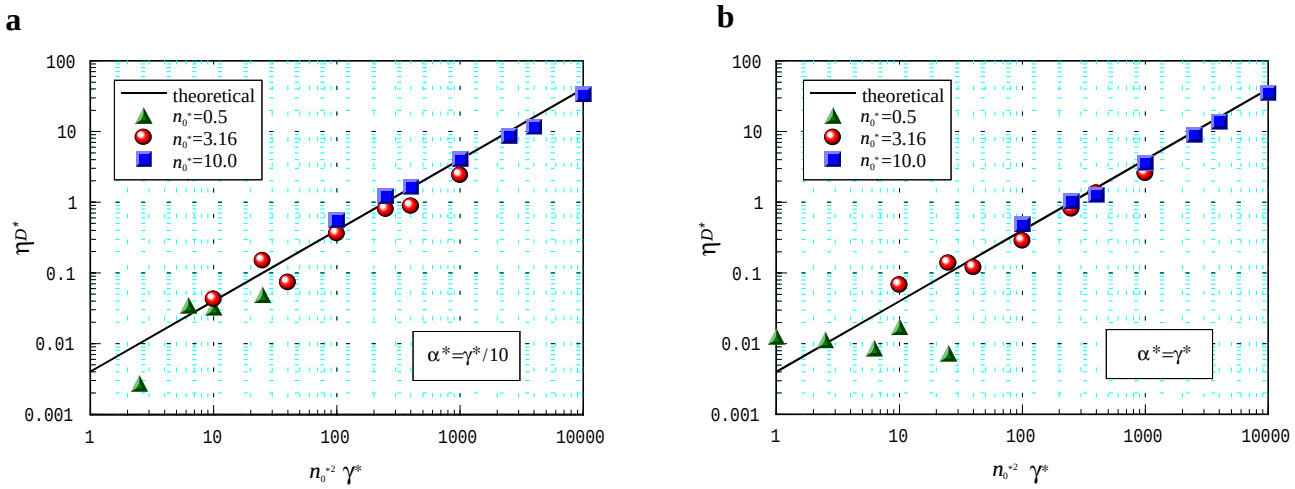

FIG. 1 Influence of γ^* on viscosity due to dissipative forces obtained by non-equilibrium dynamics method: (a) for $\alpha^*=\gamma^*/10$ and (b) for $\alpha^*=\gamma^*$ (Error bars: $\Delta h^{D^*}_{error}$ =±(5.2, 1.5) for $n_0^{*2}\gamma^*$ =(10000,1000), respectively, for n_0^* =10, ±(1.5, 0.32) for $n_0^{*2}\gamma^*$ =(1000,100), respectively, for n_0^* =3.16, and ±(0.049, 0.022) for $n_0^{*2}\gamma^*$ =(25,2.5), respectively, for n_0^* =0.5, in Fig. 1(a); similar errors are included in Fig.1(b)).

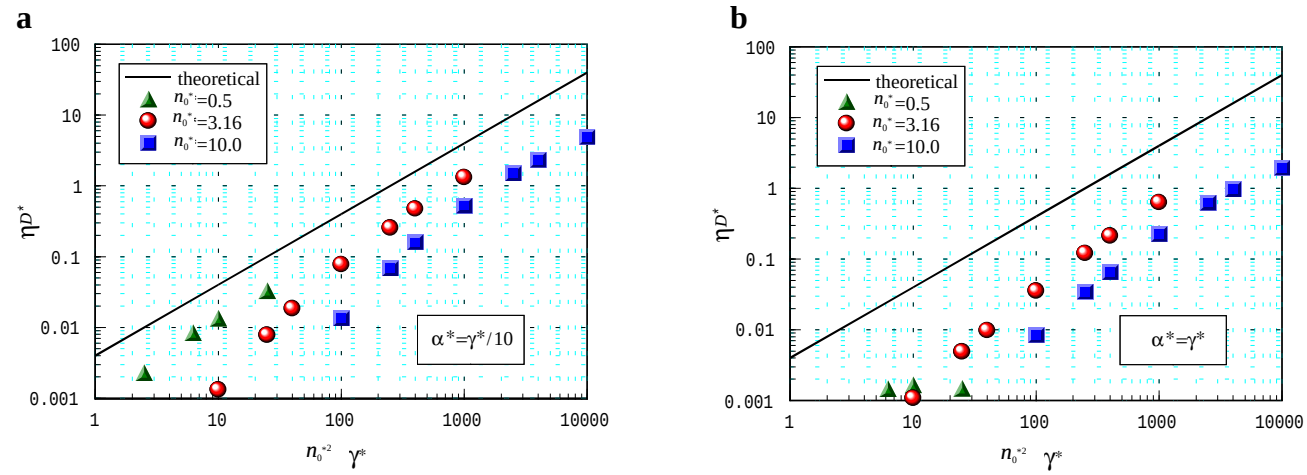

FIG. 2 Influence of γ^* on viscosity due to dissipative forces obtained by Green-Kubo expression: (a) for $\alpha^*=\gamma^*/10$ and (b) for $\alpha^*=\gamma^*$ (Error bars: $\Delta h^{D^*}_{error}$ =±(0.015,0.0033) for $n_0^{*2}\gamma^*$ =(10000,1000), respectively, for n_0^* =10, ±(0.0052,0.00055) for $n_0^{*2}\gamma^*$ =(1000,100), respectively, for n_0^* =3.16, and ±(0.00012, 0.000016) for $n_0^{*2}\gamma^*$ =(25,2.5), respectively, for n_0^* =0.5, in Fig. 2(a); similar errors are included in Fig.2(b)).