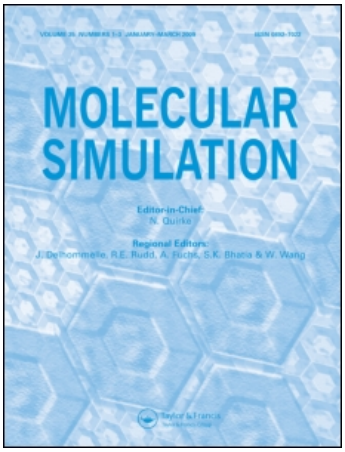

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Dielectric screening effects in molten AgI-AgBr system

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Dielectric screening effects in molten AgI–AgBr system

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The screened effect in molten AgI–AgBr system is discussed by the inverse dielectric function $1/\varepsilon(q)$, which is newly obtained in terms of the charge–charge structure factor $S_{ZZ}(q)$ by the re-examined theory of dielectric screening in molten salts. $S_{ZZ}(q)$ and in due course, $1/\varepsilon(q)$ are obtained from structural properties of molten AgI–AgBr system by molecular dynamics (MD) simulations. The obtained $1/\varepsilon(q)$ is multiplied onto the attractive part in the inter-ionic potential between cation and anion to obtain the screened potential. The total screened potential is examined in terms of the potential of mean force.

Keywords: Dielectric screening; Charge–charge structure factor; Noble-metal halide; Molecular dynamics simulation

1. Introduction

Superionic conductors are a group of substances that exhibit high values of ionic conductivity while in the solid state. The mechanism of high ionic conductivity in these substances has been of considerable interest because of their novel physical behavior and technological importance [1]. It is well known that silver iodide is one of the superionic conductors in its alpha phase, i.e. α-AgI, in which silver ions statistically distribute around the iodine bcc cubic. On the other hand, AgBr has a rock salt structure in its solid state and does not exhibit high conduction, though it is also one of the silver halides. We have investigated the effect of dissolving AgBr into AgI on the structural and transport properties in superionic and molten phases by molecular dynamics (MD) simulations [2].

On the other hand, the dielectric screening properties in molten salts have eagerly been investigated [3,4]. There is a close relationship between the dielectric screening properties and the charge fluctuation of the constituents of the substances. The charge–charge structure factor, or $S_{ZZ}(q)$, indicates the charge fluctuation in a molten salt, which can be easily obtained from their partial structure factors by diffraction experiments or simulation [5]. In fact, the dielectric screening function $\varepsilon(q)$ of a monovalent molten salt has been represented by $S_{ZZ}(q)$ in the momentum representation, as follows,

$$\frac{1}{\varepsilon(q)} = 1 - \left\{ \frac{(4\pi e^2 \beta n S_{ZZ}(q))}{q^2} \right\} \tag{1}$$

where $\beta = 1/k_B T$ and n is the number density of constituent ions.

Several attempts have been carried out at deriving the dielectric screening functions from these experimentally obtained structure factors. However, the obtained results indicate a negative sign in the small q region. This fact suggests the difficulty in appropriate explanation of equation (1). In these circumstances, we have proposed the new theory of expression of the dielectric functions in molten salts and we have applied the theory to alkali-halides, i.e. NaCl and RbBr [6]. In this study, we apply this theory to molten AgI–AgBr system as an example of a pseudo-binary system, in which ions are thought to be considerable order. Accordingly, it is interesting to discuss the dielectric screening effects in this system and whether plausible and useful results are obtainable or not.

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2. Brief summary of charge–charge structure factors in a molten salt

The theory of the dielectric screening in molten salt has been re-examined using $S_{ZZ}(q)$ in the previous work [6]. We briefly summarize it as follows. To simplify the argument, we consider a typical binary molten salt system $A_\nu B_\mu$, where N_ν and N_μ stand for number of particle species + and −. If N is the total number of particles, the concentration of species ν is $x_\nu = N_\nu/N = 0.5$. The densities of particles are $n^+ = n^- = n/2$ and $n = N/V$, where V is the volume of the system. The effective charge of ions are $z^+ = -z^- = z$. The charge–charge structure factor $S_{ZZ}(q)$ defined by Hansen and McDonald [7] are written as follows,

$$S_{ZZ}(q) = \frac{\left\langle \rho_q^Z \rho_{-q}^Z \right\rangle}{N} = \sum\nolimits_\nu \sum\nolimits_\mu z_\nu z_\mu S_{\nu\mu}(q) \tag{2}$$

where $S_{\nu\mu}(q)$ is a partial structure factor, which is expressed as,

$$S_{\nu\mu}(q) = \left[x_\nu \delta_{\nu\mu} + n x_\nu x_\mu \int_0^\infty \left(\frac{\sin qr}{qr} \right) \{ g_{\nu\mu}(r) - 1 \} 4\pi r^2 \mathrm{d}r \right] \tag{3}$$

If a charge $e\rho_{\mathrm{ext}}(\mathbf{r})$ is introduced from outside into this system at the position $\mathbf{r}$, then there occurs an induced charge $e\rho_{\mathrm{ind}}(\mathbf{r})$ at its position. Therefore, we have the following Poisson equations in the electrostatic unit,

$$\mathrm{div}\, \mathbf{D}(\mathbf{r}) = 4\pi e \rho_{\mathrm{ext}}(\mathbf{r}) \tag{4}$$

$$\mathrm{div}\, \mathbf{E}(\mathbf{r}) = 4\pi e \{ \rho_{\mathrm{ext}}(\mathbf{r}) + \rho_{\mathrm{ind}}(\mathbf{r}) \} \tag{5}$$

where $\mathbf{D}(\mathbf{r})$ and $\mathbf{E}(\mathbf{r})$ are the electric displacement and the electric field, respectively.

The electric potential $\phi(\mathbf{r})$ due to this external charge density is given by

$$\mathbf{E}(\mathbf{r}) = -\mathrm{grad}\, \phi(\mathbf{r}) \tag{6}$$

Using equation (5), we have

$$\nabla^2 \phi(\mathbf{r}) = -\left\{ \frac{4\pi e \rho_{\mathrm{ext}}(\mathbf{r})}{\varepsilon} \right\} \tag{7}$$

$$= -4\pi e \{ \rho_{\mathrm{ext}}(\mathbf{r}) + \rho_{\mathrm{ind}}(\mathbf{r}) \}$$

$$= -4\pi e \rho_{\mathrm{ext}}(\mathbf{r}) \left[1 + \left\{ \frac{\rho_{\mathrm{ind}}(\mathbf{r})}{\rho_{\mathrm{ext}}(\mathbf{r})} \right\} \right] \tag{8}$$

where ε is the dielectric constant, but it may be extended to an isotropic r-dependent term written as $\varepsilon(r)$. Hansen and McDonald [7] took partly $\varepsilon(r) = 1$ for the dielectric function in molten salts and obtained the formula expressed as shown in equation (1).

We express each quantity $\varepsilon(r)$, $\phi(\mathbf{r})$ and $\rho_{\mathrm{ext}}(\mathbf{r})$ in this equation as the following Fourier representations,

$$\varepsilon(r) = \sum_q \varepsilon(q)\, \mathrm{e}^{\mathrm{i}\mathbf{q}\cdot\mathbf{r}}, \quad \phi(\mathbf{r}) = \sum_q \phi(q)\, \mathrm{e}^{\mathrm{i}\mathbf{q}\cdot\mathbf{r}},$$

$$\rho_{\mathrm{ext}}(\mathbf{r}) = \sum_q \rho_{\mathrm{exp}}(q)\, \mathrm{e}^{\mathrm{i}\mathbf{q}\cdot\mathbf{r}}$$

and

$$\rho_{\mathrm{ind}}(\mathbf{r}) = \sum_q \rho_{\mathrm{ind}}(q)\, \mathrm{e}^{\mathrm{i}\mathbf{q}\cdot\mathbf{r}} \tag{9}$$

Putting some of these into equation (7) and taking $\mathbf{r} = 0$, then we have,

$$q^2 \varepsilon(q) \underline{\phi}(\mathbf{q}) = 4\pi e \underline{\rho}_{\mathrm{ext}}(\mathbf{q}) \tag{10}$$

where $\underline{A}(\mathbf{q}) = \{A_x(\mathbf{q}), A_y(\mathbf{q}), A_z(\mathbf{q})\}$. We assume that $\varepsilon(q)$ is isotropic, for simplicity.

Since $e\rho_{\mathrm{ind}}(\mathbf{r})$ is a charge fluctuation by the insertion of the external charge $e\rho_{\mathrm{ext}}(\mathbf{r})$, it might be expressed in the following form by using the linear charge response function $\chi_{ZZ}(q)$,

$$e\underline{\rho}_{\mathrm{ind}}(\mathbf{q}) = \chi_{ZZ}(q)\, e\underline{\phi}_{\mathrm{ext}}(\mathbf{q}) \tag{11}$$

Based on the fluctuation dissipation theorem, $\chi_{ZZ}(q)$ is expressed in terms of $S_{ZZ}(q)$ as follows,

$$\chi_{ZZ}(q) = -\beta n S_{ZZ}(q) \tag{12}$$

Compared equation (11) with equation (12), the inverse dielectric function $1/\varepsilon(q)$ is expressed as follows,

$$\frac{1}{\varepsilon(q)} = \frac{\mathrm{FT}\{\mathrm{div}\, \mathbf{E}(\mathbf{r})\}}{\mathrm{FT}\{\mathrm{div}\, \mathbf{D}(\mathbf{r})\})} = \frac{\{\mathbf{q}\cdot\underline{\mathbf{E}}(q)\}}{\{\mathbf{q}\cdot\underline{\mathbf{D}}(q)\}} = 1 + \frac{\{\underline{\rho}_{\mathrm{ind}}(\mathbf{q})\}}{\{\underline{\rho}_{\mathrm{ext}}(\mathbf{q})\}} \tag{13}$$

where FT means the Fourier component.

Putting equations (10) and (11) into equation (13) and using equation (12), we have

$$\frac{1}{\varepsilon(q)} = 1 + \left\{ \frac{4\pi e^2 \chi_{ZZ}(q)}{\varepsilon(q) q^2} \right\}$$

$$= 1 - \left\{ \frac{4\pi e^2 \beta n S_{ZZ}(q)}{\varepsilon(q) q^2} \right\} \tag{14}$$

that is,

$$\frac{1}{\varepsilon(q)} = \frac{1}{\left\{ 1 + (\kappa_s^2/q^2) S_{ZZ}(q) \right\}} \tag{15 - a}$$

where

$$\kappa_s^2 = 4\pi e^2 \beta n \tag{15 - b}$$

It should be specially emphasized that equation (15-a,-b) is the new relation between $1/\varepsilon(q)$ and $S_{ZZ}(q)$.

On the other hand, the inverse dielectric function in the long wavelength limit is already well known by the theory of classical one component plasma [7,8]. Starting from the continuity equation relating to the charge and taking Fourier transforms under the condition of long wavelength

limit, the relation between $\rho_{ind}(q)$ and $\rho_{ext}(q)$ is expressed as follows,

$$\rho_{ind}(q) = \frac{-\rho_{ext}(q)}{\left\{1 + \left(q^2/\lambda_s^2\right)\right\}} \tag{16}$$

where

$$\lambda_s^2 = 4\pi e^2 n^2 \chi_T \tag{17}$$

where χ_T being the isothermal compressibility.

If an external point charge ze is put at the position r, then we have the well-known Thomas–Fermi type screening potential using equation (16), which indicates that the inverse dielectric function near the long wavelength limit is written as follows,

$$\frac{1}{\varepsilon(q)} = \frac{1}{\left\{1 + \left(\lambda_s^2/q^2\right)\right\}} \tag{18}$$

As shown in equation (18), $1/\varepsilon(q)$ in its higher q-region and very lower q-region is expressed by a similar form, although their screening constants are quite different. In the intermediate region, $1/\varepsilon(q)$ exhibits an oscillating behavior due to the effect of $S_{ZZ}(q)$. Equation (15-a,-b) is useful to derive $1/\varepsilon(q)$ from experimental results of the partial structure factors and also equation (3) is applicable for deriving $1/\varepsilon(q)$ by a computer simulation.

It is apparent that equation (18) is equal to zero at $q = 0$. And, therefore, $1/\varepsilon(q)$ has the following relation for any positive values of $S_{ZZ}(q)$,

$$0 \leqq \frac{1}{\varepsilon(q)} \leqq 1 \tag{19}$$

It is, therefore, possible to derive $1/\varepsilon(q)$ if $S_{ZZ}(q)$ or pair distribution functions $g_{\nu\mu}(r)$ are known by either the experimental method or computer simulation. In the following sections, we will show the result for $1/\varepsilon(q)$ by using $S_{ZZ}(q)$ obtained by simulation. Though the consideration so far is for the equi-charged binary salts, the theory is easily extendable to the equi-charged pseudo binary molten salts, i.e. AgI–AgBr, and equation (15-a,-b) is also applicable to them, which we will discuss in the following sections.

3. Inverse dielectric function of molten AgI–AgBr system obtained by molecular dynamics simulation

In this section, we will derive $1/\varepsilon(q)$, from the structure factors obtained by MD simulation. The procedure of the simulation is essentially same as the previous work, which we briefly describe as follows [2]. The used pair potential sets for i and j ions are written as,

$$V_{ij}(r) = \frac{H_{ij}}{r^{nij}} + \frac{z_i z_j e^2}{r} - \frac{P_{ij}}{r^4} \tag{20}$$

in which the third term is charge–dipole interactions. The parameters are listed in Ref. [2]. The MD calculations are performed for $Ag(Br_xI_{1-x})$ $(x = 0.20)$ using 864(432Ag + 86Br + 346I) atoms, which are placed in a cubic cell. The periodic boundary conditions are used, and the Coulomb interaction is calculated by the *Ewald* method. The particles are allocated to the initial position of the crystal structure of alpha phase. Initial velocities are allocated with the *Maxwellian* distribution at a specified temperature, which is kept constant using Nosé method [9]. At first, the temperature of the system is equilibrated just below the melting point, then moved to arbitrary temperature. Then, the calculation of structure is carried out on *NVE* constant condition. One time step $\Delta t = 2.0 \times 10^{-15}$ s is used in Verlet's integration algorithm. The structural properties are obtained as the average of 2000 time steps.

As mentioned in Section 1, $S_{ZZ}(q)$ is related to structure factors and pair distribution functions, as

$$S_{ZZ}(q) = \sum_{\nu}\sum_{\mu} z_\nu z_\mu S_{\nu\mu}(q) \tag{21}$$

where summation is taken for species Ag, Br and I.

The obtained $S_{ZZ}(q)$ at 903 K is shown in figure 1. We can see a significant peak in $S_{ZZ}(q)$ at about 1.7 Å^{-1} and a plateau around 4.0 Å^{-1} corresponding to the oscillations of partial structure factors [2]. We have the inverse dielectric function $1/\varepsilon(q)$ by putting obtained $S_{ZZ}(q)$ into equation (15-a), which is shown in figure 2 with that calculated by equation (18) as comparison. It is clearly recognized that $1/\varepsilon(q)$ satisfies the condition (19). We can see the significant minimum at around 1.7 Å^{-1} corresponding the large maximum of $S_{ZZ}(q)$, which shows the large charge fluctuation. This fact may be attributed to the effect that an ion at the origin is susceptible to be surrounded by ions of opposite sign at position r, which may yield the large charge fluctuation and screening effect.

4. Screening effect for Coulomb potential in molten AgI–AgBr system

In a molten salt having with the charges of $z^+ = -z^- = z$, the effective potential between a cation

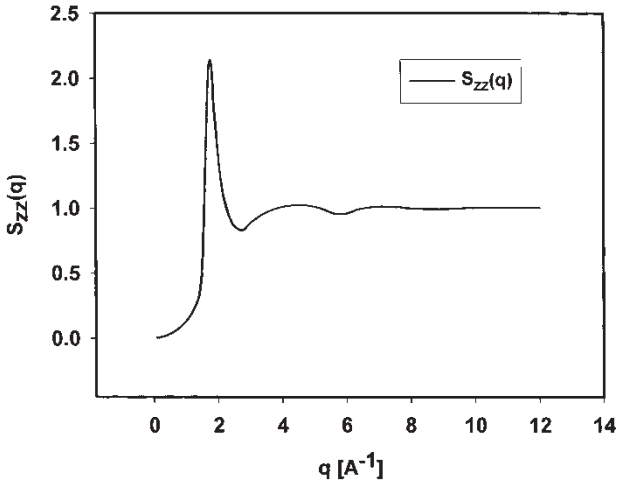

Figure 1. The charge–charge structure factor $S_{ZZ}(q)$ of molten $Ag(Br_xI_{1-x})$ $(x = 0.20)$ at 903 K obtained by MD.

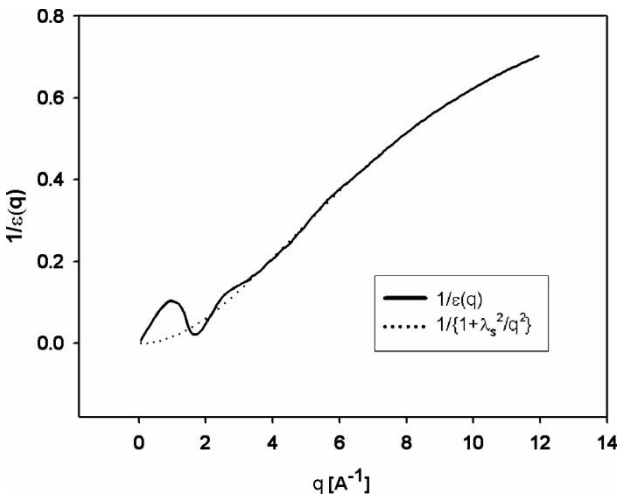

Figure 2. The inverse dielectric function $1/\varepsilon(q)$ obtained by equation (15-a,-b) (solid line) together with that obtained by equation (18) (dotted line).

and an anion at a distance of r, ϕ^{+-} effective(r), may be divided into two parts as follows,

$$\phi^{+-}\,\text{screened}\,(r) = \phi^{+-}\,\text{repulsive screened}\,(r) + \phi^{+-}\,\text{attractive screened}\,(r) \quad (22)$$

Here ϕ^{+-} repulsive screened (r) is the direct repulsive potential between cation and anion influenced by a small amount of screening effect in the short-range distance and ϕ^{+-} attractive screened (r) is the attractive screened potential in the long range.

Equation (12) is a poor approximation for the repulsive potential because of its highly non-linear functional form and therefore, the screening effect for the direct repulsive potential should be treated in a different way.

The attractive screened potential ϕ^{+-} attractive screened (r) is effectively screened by the existence of other ions, though its bare-potential may be mainly ascribed to the form of Coulomb interacting potential. Let put an ion of point charge $z^{+}e$ at the origin and then another ion of point charge $z^{-}e$ at r in the region of attractive Coulomb potential feels the following potential,

$$\phi^{+-}\text{attractive}\,(r) = -\frac{z^2e^2}{r} \quad (23)$$

Therefore, the screened attractive potential in q-space is written as follows,

$$\phi^{+-}\,\text{attractive screened}\,(q) = \frac{-4\pi z^2e^2}{\varepsilon(q)q^2} \quad (24)$$

The numerical result for ϕ^{+-} attractive screened (r) is given by the inverse Fourier transformation FT{ϕ^{+-} attractive screened (q)}.

In the region of $S_{ZZ}(q) \sim 1$, equation (16) is applicable and therefore we have,

$$\phi^{+-}\,\text{attractive screened}\,(q) = -\left(\frac{4\pi z^2e^2}{q^2}\right)\left\{\frac{q^2}{(q^2+\kappa_s^2)}\right\} = -\frac{4\pi z^2e^2}{(q^2+\kappa_s^2)} \quad (25)$$

This equation is easily converted to the r-dependent expression as

$$\phi^{+-}\,\text{attractive screened}\,(r) = -\frac{z^2e^2}{r}\exp(-\kappa_s r) \quad (26)$$

A simple consideration for the screening effect for the repulsive potential is the introduction of parameter multiplier α, which can be written as,

$$\phi^{+-}\text{screened}\,(r) = \alpha\left(\frac{B}{r^n}\right) - \left(\frac{z^2e^2}{r}\right)\exp(-\kappa_s r) \quad (27)$$

Then, the effective potential between cation and anion in the region of $S_{ZZ}(q) \sim 1$ is then expressed as follows,

$$\phi^{+-}\text{screened}\,(r) = \alpha\left(\frac{B}{r^n}\right) - \left(\frac{z^2e^2}{r}\right)\exp(-\kappa_s r) \quad (28)$$

It is emphasized that it is not necessary to apply the dielectric function in the procedure of the computer simulation, because the simulation itself involves automatically the screening behaviors and only the utilization of appropriate bare inter-ionic potentials is required.

Under this situation, it is interesting to obtain the screened potential between Ag^+ and Br^- in molten AgI–AgBr system, because the pair distribution function $g_{BrAg}(r)$ is obviously different from $g_{IAg}(r)$. This fact may be attributed to the larger screened effect by Ag^+ ions around Br^- [2]. Using the obtained $1/\varepsilon(q)$ and taking $\alpha = 0.73$, the screened potential together with the original one between Ag^+ and Br^- in molten $Ag(Br_xI_{1-x})$ ($x = 0.20$) is shown in figure 3. The reduction of the depth of potential by screening effect is obviously recognized.

5. Discussion

To examine the result of screened potential between Ag^+ and Br^-, we calculate the pair distribution function by the potential mean force $U^{+-}(r)$, which is defined by the following equation incorporating with the pair distribution function $g_{+-}(r)$ [7],

$$g_{+-}(r) = \exp\left[\frac{-U^{+-}(r)}{k_BT}\right] \quad (29)$$

We can take ϕ^{+-} screened (r) as $U^{+-}(r)$, because equation (29) is originally suggested by weak interacting materials. We have proved that ϕ^{+-} screened (r) and $U^{+-}(r)$ are mathematically equivalent in large r region based on Ornstein–Zernike equation [6].

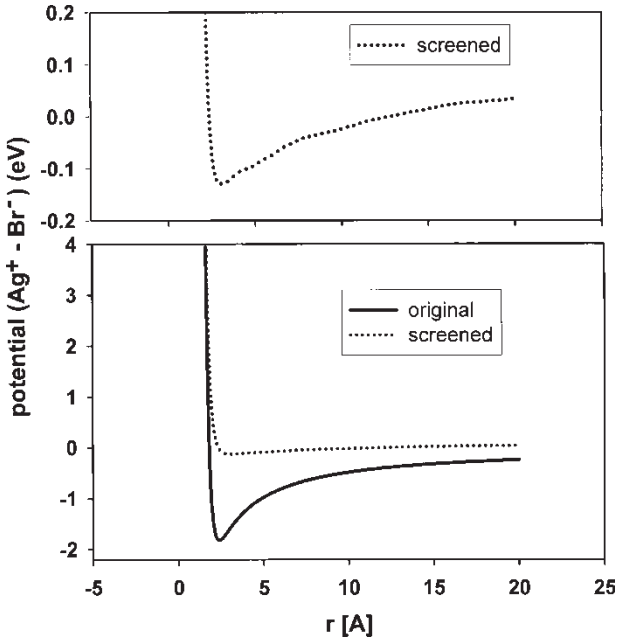

Figure 3. The screened potential between Ag^+ and Br^- (dotted line) together with original one (solid line) (bottom). The screened potential is also shown with different scale (top).

The pair distribution function $g_{ij}(r)$ obtained by inserting the calculated ϕ^{+-} screened (r) instead of $U^{+-}(r)$ into equation (29) together with $g_{ij}(r)$ obtained directory by MD is shown in figure 4. The first peak position and its height almost agree well, though the first peak obtained by equation (29) is broader. This fact may suggest that the screening effect is expected to be considerable in small r region, i.e. the distance to the first nearest neighbors.

The discrepancy in the intermediate region between $g_{ij}(r)$'s are attributed to the difference between ϕ^{+-} sreened (r) and $U^{+-}(r)$, which may be caused by several reasons, besides a margin of calculation error in Fourier transformation. One reason is that only Coulomb attractive potential is used to derive ϕ^{+-} screened attractive (r) instead of the attractive part of RVP type potential used in MD simulation. Another expected reason is that the non-symmetric structure in solid phase remains in molten phase, and may obstruct the screening effect in molten phase. In previous work, these tendencies of $g_{ij}(r)$'s were also observed in alkali halides, though the oscillatory feature of ϕ^{+-} screened (r) was a little more obvious, which may suggest the structural difference between molten alkali halides and silver halides [6].

In spite of above facts, however, it may be recognized that the calculated result for $\phi^{+-}_{\text{screened}}(r)$ so as to carry on the above treatment is physically significant and affected by screening effect in molten AgI–AgBr. It is expected that the screened effects in molten pseudo-binary salt affects on transport properties. This problem will be treated in future work.

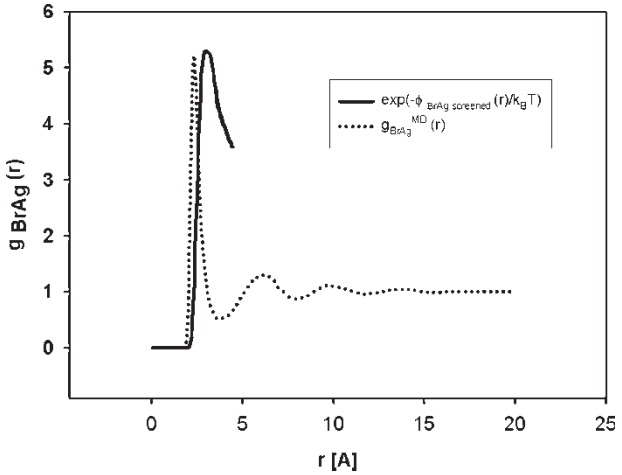

Figure 4. The pair distribution function $g_{ij}(r)$ calculated using screened potential (solid line) together with that obtained directly by MD (dotted line).

6. Conclusion

The theory of dielectric screening in molten salt has been reexamined to obtain the new relation between $S_{ZZ}(q)$ and $1/\varepsilon(q)$. The theory has been applied to molten AgI–AgBr pseudo-binary system. Screening effect in molten AgI–AgBr has been investigated in connection with $S_{ZZ}(q)$ and $1/\varepsilon(q)$ obtained by MD. Screened attractive potential between Br^- and Ag^+ has been obtained by inverse Fourier transformation of that in q-space. The estimated screened potential has been examined by taking it as a potential mean force to obtain $g_{\text{BrAg}}(r)$, which agreed well with that obtained by MD in small r region.

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