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Structure factor of suspended polystyrene macroions using Sogami-Ise potential

Abstract

The modified mean spherical approximation MMSA structure factor obtained for the polystyrene macroions suspended into water using Sogami-Ise SI potential have been well compared with the rescaled mean spherical approximation RMSA structure factors found with the screened coulomb potential SCP. Face centered cubic FCC type of liquid orderings have been obtained amongst the polystyrene macroions suspended into water. Difference for the values of excess energy per macroion and compressibility in the limit of zero momentum transfer for both the potentials has also been reported.

Key Words

Structure factor; SI-potential.

INTRODUCTION

A suspension of polystyrene balls ranging in sizes from 50 Å -10000 Å[1-3] to follow Brownian motion and bear ionizable surface charges of the order of 10^2-10^5 in electronic unit[4] is the colloidal suspension. Each of the polystyrene balls particles acquires large electrostatic negative surface charges into water like solvents and thus, becomes itself negatively charged particles called polystyrene macroions[2-5]. These polystyrene macroions arrange themselves in the suspension due to their electrostatic interaction. Several workers[6-11] have studied structural behavior of mono- and bi-dispersed systems using screened coulomb potential SCP, a repulsive component of the Derjaguin, Landau, Verwey and Overbeek DLVO potential[5], developed between macroions due to their surface charges, which is assumed to monitor the ordered arrangement of macroions in the suspension.

Sogami[12] and his workers[13] have expostulated repulsive nature of the SCP theory, which has long been one of the central foundations of stability of suspended macroions, as it fails to explain the experimental evidences of the existence of two-state structures in dilute macroionic suspension of high charge density. The existence of two-state structure suggests the subsistence of columbic attraction between like macroions mediated through the intermediate counterions. Sogami[12] and Sogami and Ise[13] have established another interaction potential between macroions, called coulomb attractive potential CAP or Sogami-Ise SI potential, that contains attractive component at large distances and repulsive component at small distances in it.

Overbeek[14,15] and Belloni[16] have criticized that the attractive component of the SI-potential results due to erroneous thermodynamical treatments, which is cancelled when contribution of solvent molecules is taken into account. Smalley[17] and Smalley and Sogami[18] have refuted the criticism as it contravenes the Gibbs–Duhem relation.

In a study of structural behavior of charged colloidal suspensions, Tata *et al.*[19] have employed SI-potential for calculation of structure factor using Brownian Dynamics Simulation BDS method and reported that SI-potential leads to structure factor in agreement with the experimental data. Using Baxter factorization method[20], Yasutomi and Ginoza[21] have derived an analytical solution to the Ornstein-Zernike OZ equation[22] for the potential similar to SI-potential under mean spherical approximation MSA[23]. In a different approach, Pandey and Tripathi[24] have derived an analytical solution to the OZ equation for the SI-potential under modified mean spherical approximation MMSA[25] using bipolar convolution theorem[26] and applied successfully to explain ordered structures amongst plasmas and macroions[27]. Recently, Pandey[28,29] has used the analytical solution derived by Pandey and Tripathi[24] to study the structural formation amongst biomacroions suspended into water and plasmas.

In the present paper, modified mean spherical approximation MMSA structure factor has been calculated for the polystyrene macroions suspended into water using expression derived by Pandey and Tripathi[24] for SI-potential. The results obtained have been well compared with the rescaled mean spherical approximation RMSA results found using SCP. It has been reported that besides SCP, SI-potential is also a plausible potential between polystyrene macroions and can be used to study the ordered structures prevailing amongst polystyrene macroions suspended into water in terms of the attractive potential if equally other attractive potential between macroions is not possible or available.

THEORY AND CALCULATIONS

The coulomb attractive pair interaction potential i.e. SI-potential between two polystyrene macroions of diameter σ derived by Sogami[12] in its dimensionless form is given by

$$\beta U(x) = (\gamma_1 - \gamma_2 x)\, \exp(-kx)/x, \qquad x > 1; \tag{1a}$$

$$= \infty, \qquad x < 1; \tag{1b}$$

where $k = \kappa\sigma$, $x = r/\sigma$, $\beta = 1/k_B T$; $\gamma_1 = \beta z^2 e^2 (\sinh(k/2)/k)^2 (2 + k\coth(k/2))/2\pi\varepsilon\varepsilon_0\sigma$; $\gamma_2 = k\gamma_1 / (2 + k\coth(k/2))$

r is the centre-to-centre distance between two macroions, z is the charge on the macroions, ε is the dielectric constant of the solvent, $\kappa = \sqrt{(\beta z^2 e^2 \rho / \varepsilon\varepsilon_0)}$ and ρ is the concentration of macroions.

The expression for the structure factor $S(Q)$ is given by[10]

$$S(Q) = 1/[1 - 24\eta c(Q)] \tag{2}$$

where $Q = K\sigma$ is the dimensionless momentum transfer, $K = 4\pi\sin(\theta/2)/\lambda$ is the wavevector, $\eta = \pi\rho\sigma^3/6$ is the volume fraction and $c(Q)$ is the Fourier transform of $c(x)$ given by[27,30]

$$\begin{aligned} c(Q) = {} & A\, Q^{-3}(\sin Q - Q\cos Q) + B\, Q^{-4}[2Q\sin Q - (Q^2-2)\cos Q - 2] \\ & + C\,[4Q^3\sin Q - Q^4\cos Q - 12\{2Q\sin Q - (Q^2-2)\cos Q - 2\}]Q^{-6} \\ & + D\,[k\sin Q\cosh k - Q\cos Q\sinh k]\, Q^{-1}(Q^2+k^2)^{-1} \\ & + E\,[k\sin Q\sinh k - Q(\cos Q\cosh k - 1) + Q^{-1}(Q^2+k^2)(\cos Q - 1)]Q^{-1}(Q^2+k^2)^{-1} \\ & + F\,[\{Q(Q^2+k^2)^2\}^{-1}\{(Q^2-k^2)\sin Q\cosh k + 2kQ\cos Q\sinh k \\ & - (Q^2+k^2)(Q\cos Q\cosh k - k\sin Q\sinh k)\}] \\ & - \gamma_1 \exp(-k)\, Q^{-1}(Q^2+k^2)^{-1}(Q\cos Q + k\sin Q) \\ & + \gamma_2 \exp(-k)\, Q^{-1}(Q^2+k^2)^{-2}\{(Q^2+k^2)(k\sin Q + Q\cos Q) + (k^2 - Q^2)\sin Q + 2kQ\cos Q\} \end{aligned}$$

The coefficients *A, B, C, D, E* and *F* have been evaluated elsewhere[24].

The expression for the excess energy per polystyrene macroion can be obtained[24] as

$$E_{ex} = \frac{1}{2}\left(\kappa_1^2 U - \kappa_2^2 V\right) \tag{3}$$

Isothermal thermodynamic compressibility χ has also been calculated using the relation[24,31]

$$\chi = \lim_{Q \to 0} S(0) \tag{4}$$

All calculations have been carried out in double precession on the ACER COPMUTER using FORTRAN 77 Compiler.

RESULTS AND DISCUSSION

The MMSA structure factor $S(Q)$ has been calculated for the aqueous suspension of polystyrene macroions of σ=50 Å, z=20e, $\rho = 4.58\times10^{24}\,\mathrm{m}^{-3}$ and T=25° C using SI-potential and the results have been compared with RMSA results obtained using SCP for the same input data in Figure 1. The height of the first peak is smaller and its position lies at lower values of Q in $S(Q)$-Q curve in case of the SI-potential than that of the SCP. The difference in the size and position of peaks is obviously because of the difference in the nature of the two potentials. Like that obtained using SCP, the shape and size of the first peak in $S(Q)$-Q curve for the SI potential shows the liquid like ordering to exist amongst polystyrene macroions suspended into water as its height is less than Hansen and Verlet's[32] criteria *i.e.*, $S(Q) \le 2.85$ above which the polystyrene macroions freeze in the suspension.

The excess energy per polystyrene macroion is found to be –15.35 with the SI-potential whereas this value is equal to –20.36 with the SCP.

The isothermal thermodynamic compressibility χ has been calculated in the limit $Q \to 0$. Its value is 0.047 in the present study using SI-potential and it is equal to the 0.018 in case of the SCP. Large value of compressibility indicates the weakening in the bond strength between ordered suspended polystyrene macroions as it is reflected with shorter peak in $S(Q)$-Q curve for the SI-potential in Figure 1. This may be perhaps due to the competition between attractive and repulsive components in SI-potential.

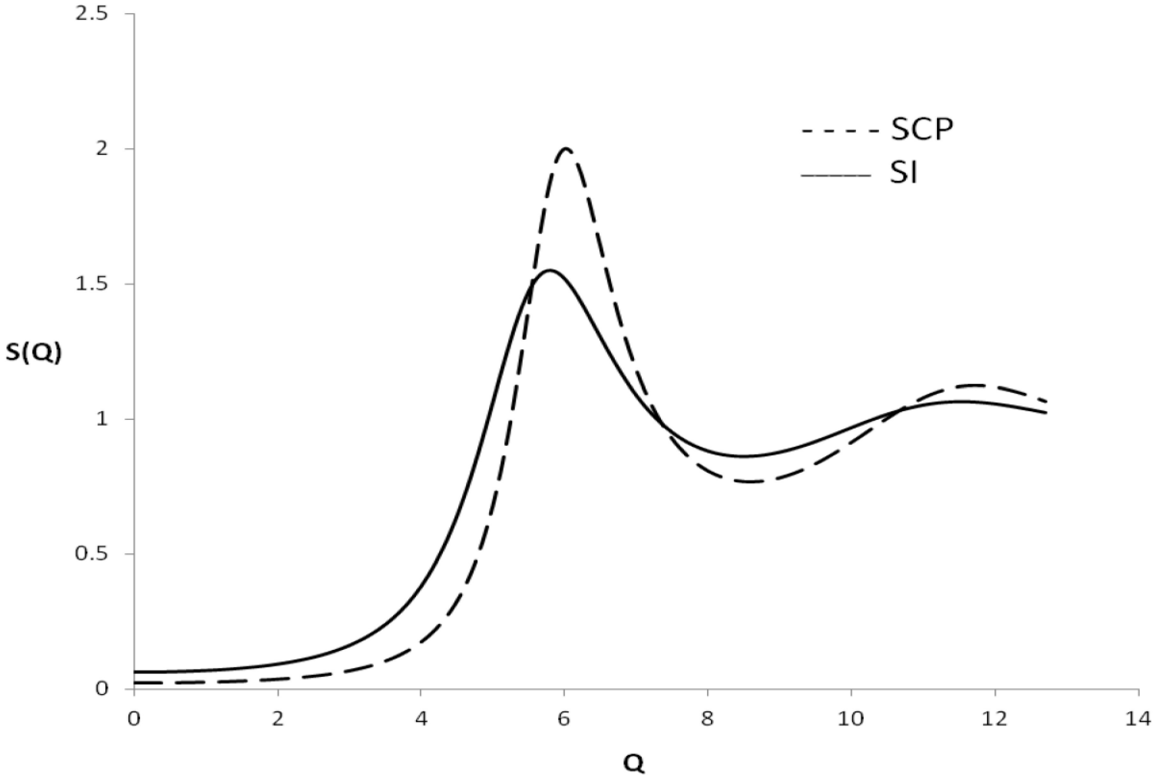

Figure 1 : Variation of structure factor with dimensionless momentum transfer

CONCLUSIONS

Like SCP, SI-potential is also a plausible potential between polystyrene macroions, which can also be used to study ordered structures prevailing amongst suspended polystyrene macroions in terms of the attractive potential if equally other attractive potential for such system is not possible or available.

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