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Poisson's ratio of a soft sphere system

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Monte Carlo simulations of soft spheres interacting through inverse power potentials, $u(r) \propto r^{-n}$, have been performed. Poisson's ratio of the soft sphere face-centred cubic crystals were determined using the constant pressure ensemble with variable box shape. It was shown that at high densities, particle motions decrease Poisson's ratio with respect to the static case which corresponds to zero temperature. It was also shown that increasing the exponent *n* in the potential, one can decrease Poisson's ratio.

Key words: *soft sphere; inverse power potential; elastic constant; Poisson's ratio*

1. Introduction

In recent years, quickly growing interest in the systems interacting through the inverse power potential has been observed in the colloid and interface science communities. One of the reasons is that particles of different softness can be used for various applications. In the present work, we study Poisson's ratio of three-dimensional soft spheres in the face-centred cubic phase (fcc). The studied system interacts by the inverse power potential [1–7]:

$$u(r) = \varepsilon \left(\frac{\sigma}{r}\right)^n \quad (1)$$

where r is the separation between two particles, σ is the particle diameter, ε sets the energy scale and $n > 0$ is a parameter determining the potential hardness (the softness is proportional to $1/n$).

This work is a part of a project concentrating on the investigation of Poisson's ratio in various model systems. We expect that studies of simple and well defined models constitute a way to a better understanding and description of a new class of mate-

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rials [8–14] which exhibit anomalous (negative) Poisson's ratio [15]. Such unusual materials are of interest both for the fundamental research and for applications. Searching for mechanisms which can decrease Poisson's ratio of model systems can help in designing new materials with negative Poisson's ratios.

The aim of the paper is to investigate the influence of the exponent n on Poisson's ratio of the fcc soft sphere crystalline phase as well as to determine explicitly the influence of temperature on Poisson's ratio of the hard sphere system.

2. Details of simulation

The Monte Carlo (MC) simulations were performed in the variable box shape (NpT) ensemble by a method following the Parrinello-Rahman idea of averaging strain fluctuations [16] which was further developed in Refs. [17, 18]. The version of this method applied here is based on Refs. [19–21].

The MC simulation was carried out for particles interacting through the inverse power potential (1) for several values of n: 12, 16, 24, 48, 96, 192, 384, 768. In all the simulations reduced units of the energy $E^*=E/\varepsilon$, the dimensionless pressure $p^*=p\sigma^3/\varepsilon$ and the dimensionless temperature $T^*=k_BT/\varepsilon$ were used. A standard interaction cut off of 2.5 for $n \leq 48$, and 2.0 for $n > 48$ was applied.

Two kinds of trial motions were used. The first concerned changes of the sphere positions, and its acceptance ratio was kept close to 30%. The second kind of the motions corresponded to changes of the components of the symmetric box matrix and was tried about $N^{1/2}$ times less frequently than the sphere motions. The box motions determined the size and the shape of the box and their acceptance ratio was close to 20%.

We simulated systems of 256 particles with periodic boundary condition whose $T = 0$ ground state configuration is the fcc. lattice occupying a cubic box of the side $4\sqrt{2}a_0$ (a_0 is the nearest-neighbour distance). It has been shown [22] that simulations of systems as small as $N = 256$ give the elastic constants and Poisson's ratios differing by only a few percent from the results obtained by extrapolation to the $N \to \infty$ limit.

Typical lengths of the runs were equal 5×10^6 trial steps per particle (Monte Carlo cycles), after equilibration of 10^6 MC cycles.

3. Results and discussion

The question concerning the influence of particle motions (i.e. positive temperature) on the elastic properties of the soft sphere system can be answered by considering a static, i.e. zero temperature fcc lattice whose nearest-neighbouring sites (distanced by a) interact by the potential (1). The expressions for pressure, bulk modulus, elastic constants, and Poisson's ratio of such a lattice can be found in Ref. [22]. Here, we only recollect Poisson's ratio of the static model:

$$\nu = \frac{n+6}{3n+6} \tag{2}$$

It is worth noting that Poisson's ratio of a static model equals 1/3 in the limit $n \to \infty$.

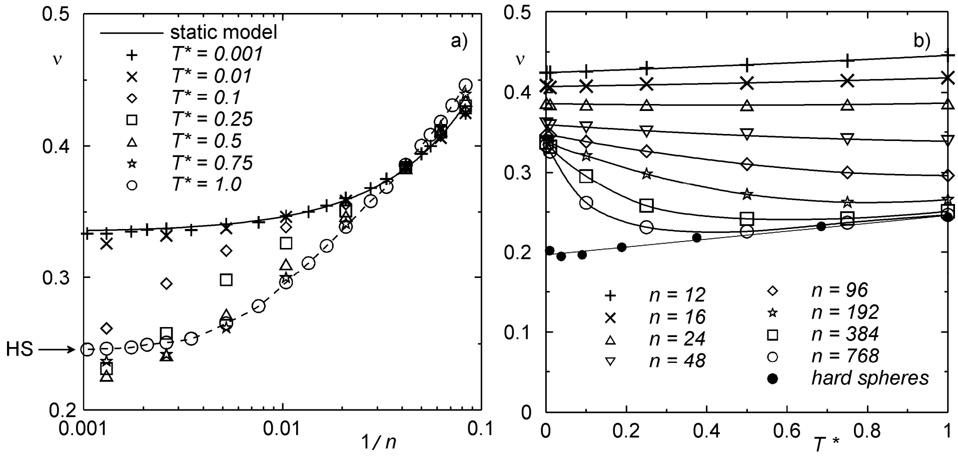

Fig. 1. Poisson's ratio vs. softness (a) and temperature (b) at $p^* = 37.69$; HS – hard spheres

In Figure 1a, Poisson's ratio of the soft sphere systems at the same pressure is plotted versus the softness parameter $1/n$. One can see that when $T^* \to 0$, the limiting values of Poisson's ratio for $n \to \infty$ tend towards the values of the static model. When $T^* \to 1$, Poisson's ratio tends to its value obtained for the hard sphere system at the same pressure. An interesting conclusion which follows from this observation (see also Fig. 1b) is that when $n \to \infty$ there is a discontinuity ("jump") of Poisson's ratio between its value 1/3 obtained for $T = 0$ for any finite n and the value $\nu \approx 0.2$ obtained for $T > 0$ for hard spheres [22]. A detailed analysis of this surprising effect will be made in a separate work. For large n ($n > 384$) and for temperatures in the range $0.25 \le T^* \le 0.75$, the values of Poisson's ratio are lower then those obtained in the hard sphere limit ($n \to \infty$). In the latter case, Poisson's ratio is lower than that for the static system. A similar effect has been observed for the soft disk system in two dimensions [23].

The temperature dependence of Poisson's ratio is shown in Fig. 1b. An increase of the power n in the interaction potential leads to a decrease of Poisson's ratio for soft spheres in the whole temperature range considered. It can be also seen that by increasing the temperature in the range $0 \le T \le 0.2$, one can decrease Poisson's ratio of soft spheres with respect to the static case (i.e. to the zero temperature limit) for $n \ge 25$.

4. Summary and conclusions

Poisson's ratios were determined for a wide range of the softness parameter ($1/n$) of the soft sphere potential and for a wide range of temperatures. These data can be used to construct temperature-softness dependence of this property.

Simulations of the soft spheres indicate that at $T^* = 0.001$, the difference between Poisson's ratio for that model and for the static model is less than 2% when $n \geq 12$. On the other hand, simulations of the soft spheres at $T^* = 1$ show that Poisson's ratio of hard spheres differs by less than 2% from that of the soft sphere system when $n \geq 384$.

We have shown that by introducing particle motions (i.e. by rising the temperature from $T = 0$ to small positive values, $T > 0$), one can decrease Poisson's ratio of the soft sphere system with respect to the static case (i.e. to the zero temperature case) for finite $n \geq 25$. We have also found that by increasing the exponent n in the interaction potential, one can decrease Poisson's ratio at high pressures/low temperatures.

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