Materials Science-Poland, Vol. 26, No. 4, 2008

Influence of size polydispersity on the elastic constants of fcc crystals of static soft spheres

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Elastic constants of three-dimensional systems of soft spheres, interacting through *n*-inverse power potential and exhibiting aperiodicity (caused by the size polydispersity of the spheres), have been determined at 0 K by computer simulations. It has been shown that Poisson's ratio, as well as other elastic constants, increase with increasing disorder in the system at a fixed number density of spheres.

Key words: *elastic constants; polydispersity; modelling; simulation; mechanical properties*

1. Introduction

Knowledge of the role of various mechanisms influencing elastic properties of model systems is important for accurate description, better understanding and precise predictions of properties of real materials. In this paper, we present preliminary data on the influence of structural aperiodicity introduced to the model of soft spheres by the size polydispersity of the spheres, on elastic constants of the fcc crystalline structure of the model studied. This research can help in understanding properties of real, man-made systems of micro-, mezo- and macroparticles [1, 2] which usually exhibit some amount of polydispersity of particle sizes.

Results of computer simulations, presented in this paper, show a significant influence of the polydispersity on the equation of state and elastic constants of the model. Poisson's ratio dependence on polydispersity is also shown explicitly, as this quantity is the crucial one for so called auxetic materials which have been a subject of increasing research interest [3].

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2. Poisson's ratio

For anisotropic systems, Poisson's ratio, defined as the negative ratio of transverse strain to longitudinal strain when only the longitudinal component of the stress tensor is infinitesimally changed, depends, in general, both on the longitudinal and the transverse direction. For the cubic symmetry, studied in this work, Poisson's ratios along two high-symmetry longitudinal directions ([100] and [111]) do not depend on the choice of the transverse direction [4] and can be expressed by the elastic constants, C_{ij}, and pressure, p, in the form [5]:

$$\nu_{[100]} = \frac{C_{12} + p}{C_{11} + C_{12}} \tag{1}$$

$$\nu_{[111]} = \frac{1}{2}\frac{C_{11} + 2C_{12} - 2C_{44} + 3p}{C_{11} + 2C_{12} + C_{44}} \tag{2}$$

In the present paper, Poisson's ratios along the longitudinal direction [110] and two transverse directions $[1\bar{1}0]$ and [001] have also been computed:

$$\nu_{[110],\,[1\bar{1}0]} = \frac{C_{11}^2 - 2C_{12}^2 - \left(5C_{12} - 2C_{44} + 4p\right) + C_{11}\left(C_{12} - 2C_{44} + p\right)}{C_{11}^2 - 2C_{12}^2 + C_{11}\left(C_{12} + 2C_{44} - 3p\right) - \left(5C_{12} + 2C_{44}\right)p} \tag{3}$$

$$\nu_{[110],\,[001]} = \frac{4\left(C_{44} - p\right)\left(C_{12} + p\right)}{C_{11}^2 - 2C_{12}^2 + C_{11}\left(C_{12} + 2C_{44} - 3p\right) - \left(5C_{12} + 2C_{44}\right)p} \tag{4}$$

3. The polydisperse soft sphere model

The model considered is the system of N soft polydisperse spheres forming a nearly perfect fcc lattice (Fig. 1). The spheres interact through the potential of the form:

$$u(d_i, d_{j,} r_{ij}) = u_0 \left(\frac{d_{ij}}{r_{ij}} \right)^n \tag{5}$$

each only with its twelve nearest neighbours. d_{ij} is the average diameter of a pair of interacting spheres and r_{ij} is the distance between their centres, u_0 is the energy unit and n is the exponent of the potential. One can notice that when n tends to infinity, the above potential tends to the hard-body potential which is widely used in computer simulations and condensed matter physics [6]. Thus, the exponent n can be treated as the hardness parameter.

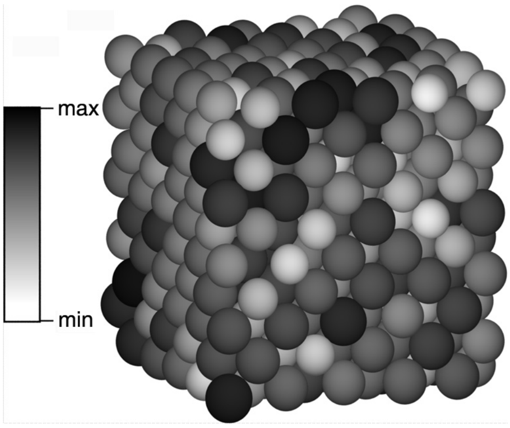

Fig. 1. Typical structure of polydisperse soft spheres studied in this paper. The structure shown consists of 500 particles with the polydispersity parameter (defined in the text) equal to 5%. The scale on the left shows the dispersion of diameters. The smallest particles are drawn in white and those of maximum diameters are drawn in black

The system was studied in the static case (i.e., the temperature of the system was 0 K). To minimize the influence of the boundaries of the (finite) samples studied and to improve convergence of the simulations with increasing size of the samples, periodic boundary conditions we applied. The diameters of the spheres were generated randomly according to the Gaussian distribution with the average equal to <*d*> and a fixed standard deviation δ

$$\delta = \frac{\sqrt{\langle d_i^2 \rangle - \langle d_i \rangle^2}}{\langle d_i \rangle^2} \tag{6}$$

which will be treated as the polydispersity parameter.

In the case of zero polydispersity ($\delta = 0$), one can analytically obtain all the elastic constants describing the system. The formulae for such a case [7] read:

$$p^0 = 2^{2/3} n a^{-(n+3)}, \quad C_{11}^0 = \left(\frac{n}{2} + 1\right) p^0, \quad C_{12}^0 = C_{44}^0 = \frac{1}{2} C_{11}^0 \tag{7}$$

where a is the distance between the interacting particles. The present study was performed by the simulation technique described elsewhere [8].

4. Results

Four different values of δ were investigated ($\delta = 0.001$, 0.003, 0.01 and 0.03) with the hardness parameter ranging from 3 (soft interactions) to 1000 ("hard" interactions). Most of the studied systems consisted of 500 particles. It is worth to add that systems of different sizes ($N = 108$, 256, 864, 1372) were also studied to determine the influence of the size of the sample on the results. No statistically significant influence of the size of the sample was observed for $N > 256$ and, hence, systems of $N = 500$ were typically simulated.

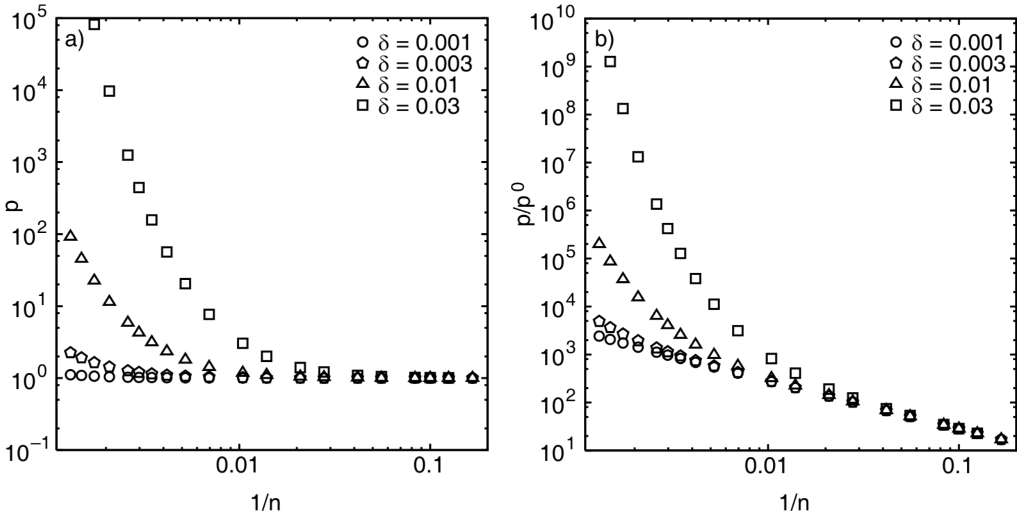

Fig. 2. Pressure p in the polydisperse system (a) and the relative pressure (p divided by the pressure of the reference system of spheres of equal diameters) against the inverse of the exponent n (b)

In Figures 2–4 the obtained results are shown. One can see that both the pressure and all the elastic constants increase when interactions tend to the hard potential. The higher the polydispersity, the larger (and more rapid increase of) elastic constants can be observed (see Figs. 2, 3).

In Figure 4, one can see the plots of Poisson's ratio in three different (longitudinal) directions [100], [111] and [110]. For the last direction, the response of the system was measured in two transverse directions $[1\bar{1}0]$ and [001]. In the hard interaction limit, one can see an increase of Poisson's ratio with increasing hardness of interactions in each of the presented plots. As can be noticed, in most cases (a, b, c) the increasing polydispersity is responsible for the increase of Poisson's ratio in the whole range of n studied. This is in contrast to Fig. 4d where one can notice the opposite behaviour, i.e. higher polydispersity corresponding to lower Poisson's ratio, for the range of n where Poisson's ratio shows negative values. This interesting behaviour will be a subject of further studies.

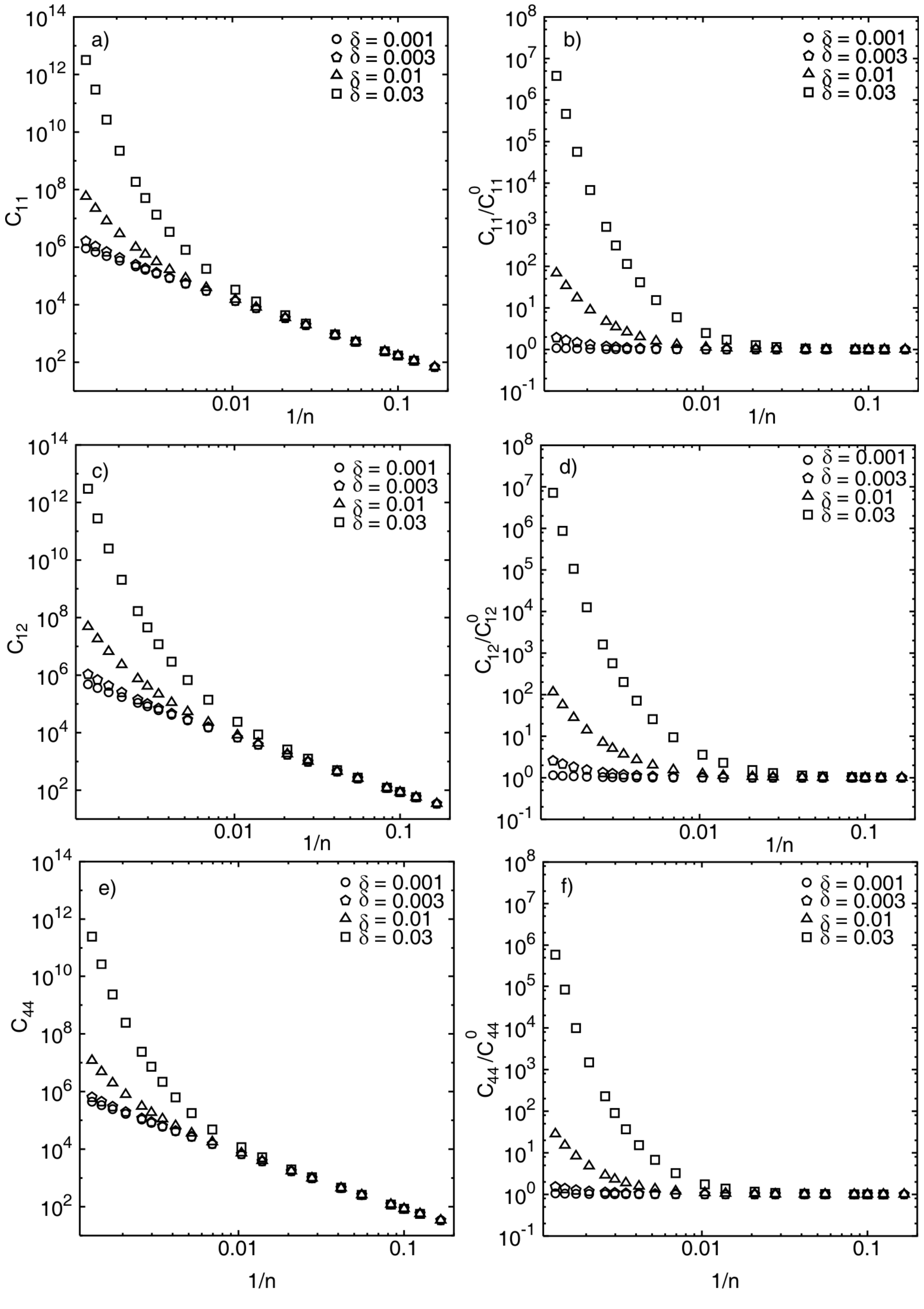

Fig. 3. Plots of elastic constants C_{ij} of the polydisperse spheres (a, c, e) and the relative elastic constants (C_{ij} divided by the corresponding elastic constants of the reference spheres) (b, d, f) against the inverse of the hardness parameter

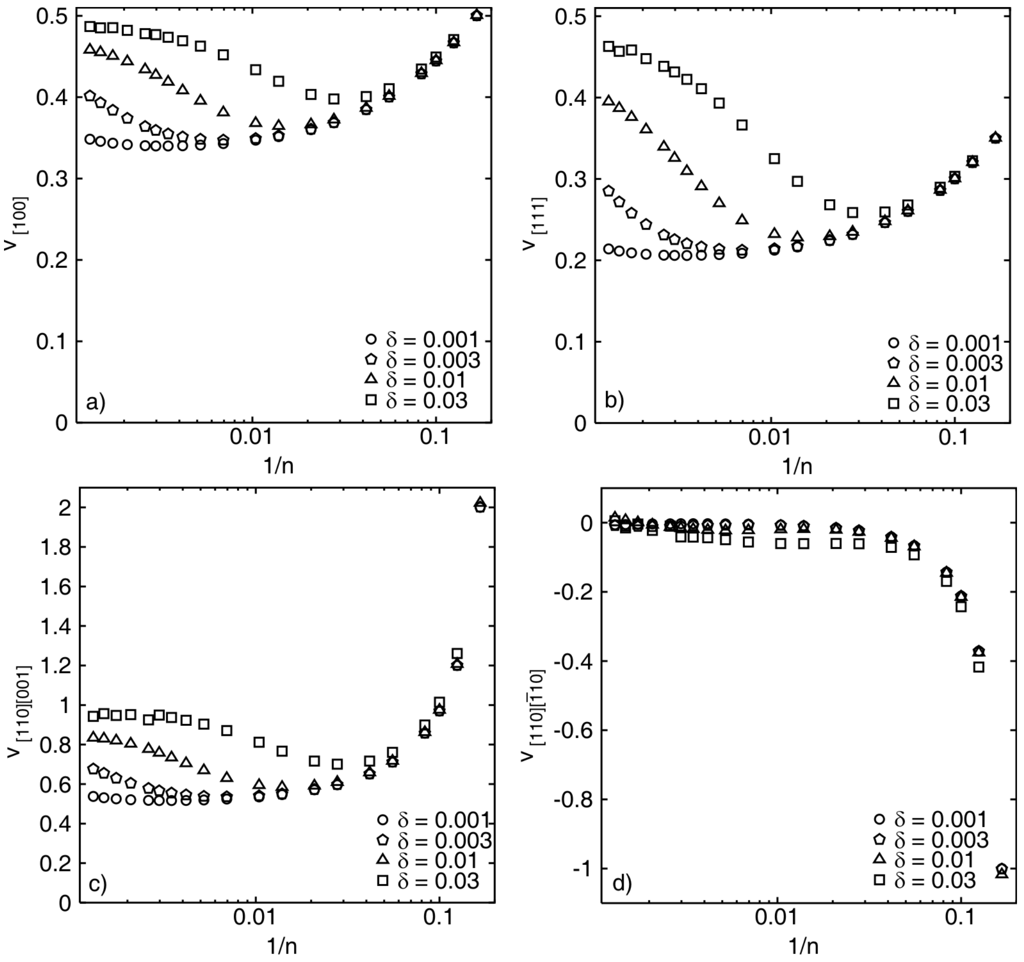

Fig 4. Plots of Poisson's ratio against the inverse of the hardness parameter in the following longitudinal directions: a) [100] b) [111] and c, d) [110] where the transverse directions are c) [001] and d) $[1\bar{1}0]$]

5. Conclusions

The presented numerical studies reveal that disorder (in the form of size polydispersity) has essential influence on the elastic properties of the soft sphere systems. All the elastic constants grow with increasing polydispersity parameter as well as with increasing hardness of the interparticle interactions.

It is interesting to extend similar research to other three-dimensional systems of spherical particles and 'molecules' formed of them. It is also of interest to determine the influence of other types of structural disorder (e.g., degeneracy of the ground states of such systems [9]) on the elastic constants. Such studies will be a subject of our future work.

Acknowledgements

This work was supported by the Polish Office for Science and Higher Education, grant No. N20207032 /1512 (2007–2010).

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Received 7 May 2007
Revised 30 September 2007