ELASTIC PROPERTIES OF THE RECTANGULAR CRYSTALLINE PHASE OF PLANAR HARD CYCLIC PENTAMERS

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Abstract: Structural and elastic properties of the densest known solid phase of two-dimensional (2D) system of hard cyclic pentamers (each pentamer is composed of five discs which centres are placed at vertices of a perfect pentagon of sides equal to the disc diameter, σ) are studied by Monte Carlo simulations. The present study confirms that at high densities the pentamers form a 2D solid structure of rectangular lattice with two pentamers (which librate, without rotation, around their mean orientations) in the unit cell. Elastic constants calculated for this structure show that, in contrast to densely packed 2D hard cyclic heptamers (composed of seven discs of centres forming a perfect heptagon of sides equal to the disc diameter σ), the pentamers do not exhibit anomalous Poisson's ratios.

Keywords: elastic constants, Poisson's ratio, hard molecule, anisotropic body, Monte Carlo, computer simulations, close packing, orientational phase transition

1. Introduction

The planar hard cyclic pentamer (see Figure 1), further referred to as pentamer, is the simplest model molecule of pentagonal symmetry. This axis is the lowest symmetry axis forbidden in periodic crystalline phases. As it is interesting, in general, what kinds of order in dense structures can be obtained for molecules of pentagonal symmetry [1–3], the pentamers have been studied both experimentally [1] and by computer simulations [3]. The simulations revealed existence of a fluid phase in the system and three crystalline phases, which differ from each other by orientational ordering, see Figure 1.

The equation of state obtained for the pentamers is similar to the equation of state of planar hard cyclic heptamers which were simulated only recently [4]. Both the systems freeze into solid phases of triangular lattice in which the molecules rotate (almost) freely. The 'atomic' density distribution around the lattice sites shows almost circular symmetry in this phase, see Figure 1c. With increasing density the molecular rotation becomes more and
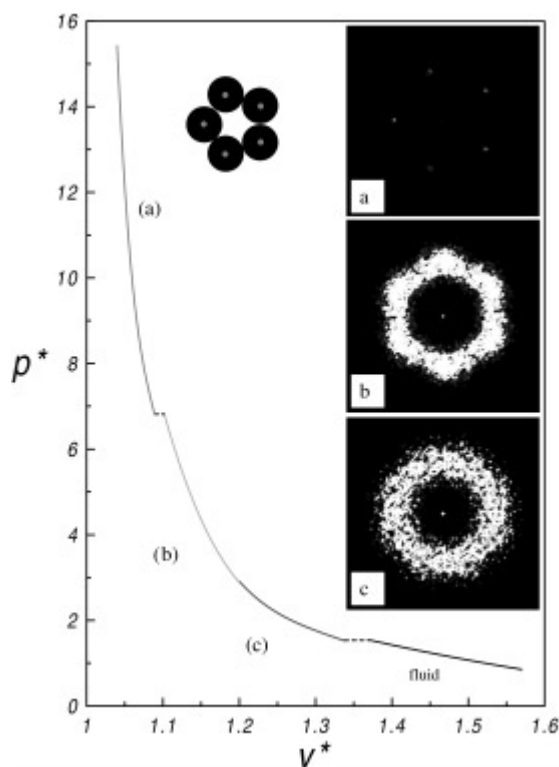
Figure 1. The equation of state and 'atomic' density distributions around a lattice site for
the pentamers. The dimensionless volume v^* is defined as the ratio of the volume
of the system to the volume of the rectangular close packed structure which is the densest known
structure of the pentamers. (The volume per patricle of the close packed rectangular structure
is equal [1] $v_{cp} = (1/4)[3^{1/2}\sin(\pi/5) + \cos(\pi/5) + 1][1 + 4\cos(\pi/5)]/\sin(\pi/5) = 5.0936\ldots)$. The pentamer
molecule is shown in the left upper corner. The inserts on the right show the atomic probability density
around a crystalline lattice site (a) in the rectangular structure ($p^* = 15.0$), (b) in the high-density
rotational phase ($p^* = 4.0$), and (c) in the low-density rotational phase ($p^* = 2.5$), respectively

more hindered and one observes a smooth transition to the atomic patterns of clearly *six-
fold* symmetry, see Figure 1b. Presence of such symmetry of the atomic density distribution
proves that there exists a strong coupling between the translational and orientational motions
of the molecules in this phase [3]. At further increase of the density, the molecular rotation
'freezes' (the molecules can only librate around their preferred orientations, but they do
not rotate) and the atomic density patterns seem to exhibit the molecular symmetry (which
is the five-fold one for pentamers, see Figure 1a, and the seven-fold one for heptamers).
Closer inspection shows, however, that this symmetry is only approximate [3].

　　　In the system of heptamers at least three structures without molecular rotation are
stable or metastable at the highest densities. It has been shown that two of them show
anomalous (negative) Poisson's ratios [4]. The Poisson's ratio, v_α, can be measured by
introducing an infinitesimal change of the stress along a certain direction α whereas other
components of the stress tensor are kept fixed. v_α is defined as the negative ratio of the
transverse strain change to the strain change along the direction α [5]. The Poisson's rations
of typical materials are positive [5]. It is worth to add here that an anomalous Poisson's ratio

has been also found in the dense phase of hard cyclic hexamers which are composed of six identical discs which centres for a perfect hexagon of sides equal to the disc diameter [6]. It has been suggested that certain phases of anisotropic (non-convex) hard bodies can exhibit anomalous Poisson's ratio at high densities [6]b. Thus, being an anisotropic, hard and non-convex body, the pentamer is an interesting model molecule from the point of view of elastic properties of its dense solid phase(s).

It should be stressed that systems of negative Poisson's ratio are not just theoretical curiosities [6, 7] but have a lot of interesting applications. They have been manufactured more than a decade ago [8] and since that time they have been a subject of very intensive studies [9].

The main aim of this paper is to determine elastic properties of the *defect-free*, dense crystalline phase of pentamers (*i.e.* in absence of vacancies, dislocations, disclinations, *etc.*) by applying the strain-fluctuation method [10–12] and to test the convergence of this method. This study extends the amount of available data concerning systems consisted of anisotropic molecules interacting through highly anharmonic potentials. Such data are useful to construct various theoretical approximations and necessary to test them.

The paper is organized as follows. Section 2 concerns searching for the densest (stable or metastable) structures of the pentamers. In Section 3 the elastic constants of the densest known crystalline structure of the pentamers are discussed, in absence of defects. Section 4 contains summary and conclusions.

2. Close packed structures of planar pentamers

In the case of hard-body systems the configuration of the densest packing can be thought of as the ground state structure. The densest configuration is usually expected to be directly related to the structure of the densest phase of the system. In three dimensions this is typically a translationally ordered phase (periodic crystal). In two dimensions, the situation is more complicated because of the well known problem of translational ordering [13]. At high densities, however, the samples typically studied by computer simulations in periodic boundary conditions can be thought of as periodic crystals. For the latter ones the theoretical description is much easier than for phases showing other kinds of long-range order.

We searched for the densest periodic packing of the pentamers. We should add here that, except the simplest cases like hard discs [14] or hard spheres [15], the densest structures of hard body systems are not known in general. One of the most natural, simple and efficient ways to search for dense packings of hard bodies is computer simulation. In the case of pentamers, to search for the structure of the densest thermodynamically stable crystalline phase, we applied constant pressure Monte Carlo method with variable shape of the periodic box [16]. We used various initial structures and various initial dimensionless pressures (defined as $p^* = p\sigma^2/kT$, where p is the pressure, T is the temperature, and k is the Boltzmann constant) which were increased during the simulations up to $p^*_{max} = 10^7$ (which can be thought of as infinity). The search for the densest packing of the pentamers was performed in a few directions described below.

The studies were started by a few series of runs, initiated by various configurations representing the thermodynamically stable triangular phase with (almost free) rotation. In each series the dimensionless pressure in subsequent runs was increased up to p^*_{max}. In all the cases the final configuration represented the rectangular phase without rotation found

earlier both in experiment [1] and in computer simulations [3]. The obtained structure is shown in Figure 2a. It can be seen there that pentamers are arranged in parallel rows along one of the molecular symmetry axes, and in neighbouring rows the molecular orientations differ by $\pi/10$. First order phase transition between this phase and a phase of hexagonal lattice and of 6-fold symmetry atomic density patterns around the lattice sites. The phase transition was accompanied by a small hystheresis, and no other phase was observed above this transition.
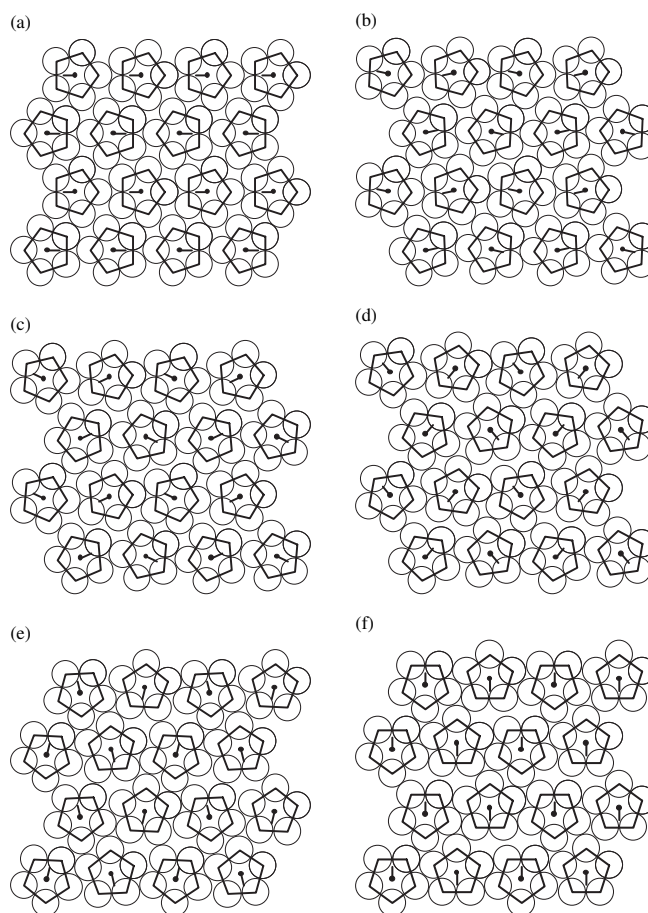

Figure 2. A few examples of close packed structures used as the initial structures in searching for the densest thermodynamically stable crystalline phase of the pentamers. The neighbouring pentamers in a row are slightly rotated, by the 'tilt' angle φ, in opposite directions with respect to the rectangular close packed structure (for which $\varphi = 0$). The vertical shifts of the pentamers in a row and the relative positions of neighbouring rows are such that they minimize the volume at the chosen tilt angle. (In the case of heptamers simulations of analogous structures result in a structure which has the highest known density at close packing.) The tilt angles of the presented pentamer structures are: (a) $\varphi = 0$, (b) $\varphi = \pi/72$, (c) $\varphi = \pi/36$, (d) $\varphi = \pi/18$, (e) $\varphi = 61\pi/720$, (f) $\varphi = \pi/10$

Although the above result strongly suggests that the rectangular phase is the only crystalline phase without molecular rotation, we did not restrict our searches to these simulations. This is because the simulations of hard cyclic heptamers showed that analogous

result is obtained even when the rectangular phase is not the densest one [4]. The densest of presently known structures of heptamers contains not two but four molecules in a unit cell [4]. The latter structure can be obtained from a rectangular structure similar to that shown in Figure 2a by rotating pairs of the neighbouring pentamers in a row, in opposite directions, and slightly shifting them perpendicularly to the direction of the row.

Guided by the results of simulations of planar heptamers we considered various close packed structures of pentamers, some of which are shown in Figure 2. Using such structures as the initial configurations in the constant pressure simulations with variable shape of the box, and increasing the dimensionless pressure from various initial values (above the pressure corresponding to orientational freezing) up to p^*_{max}, we have always obtained the rectangular structure with two molecules per unit cell. It can be seen in Figure 3 that for pentamers the latter structure is the densest amongst the considered structures of four pentamers per unit cell.
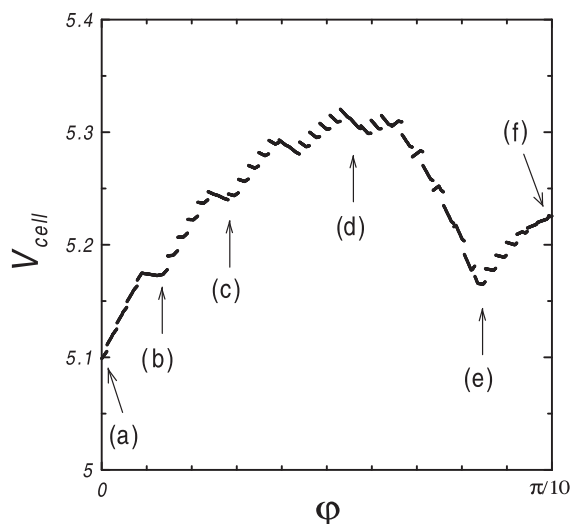

Figure 3. The minimum volume per particle of a unit cell as a function of the tilt angle, φ. The angles of the structures shown in Figure 2 are marked by arrows

The same result as in the above cases was also obtained when a system of $N = 16$ pentamers was first rapidly compressed from well equilibrated configurations representing the hexagonal phase with (almost free) molecular rotation. In the first part of such simulations the molecular orientations were kept frozen at their initial (practically random) values corresponding to the equilibrium hexagonal phase. The orientations were relaxed when the simulated system reached a density plateau corresponding to a chosen high pressure (pressure values $p_{relax} = 10$, 10^2, 10^3, 10^4, 10^5 were used) and the system was then equilibrated at this pressure. The final configurations always corresponded to the rectangular phase.

Thus, the results above confirm the conjecture formulated in [1] that the maximum density structure of planar pentamers is the rectangular lattice shown in Figure 2a. In the next section we discuss the elastic properties of this phase.

3. Elastic properties of the rectangular crystalline phase

Computations of elastic properties of the pentamer crystalline structures were performed by the strain-fluctuation method [10–12]. We will not describe details of this method here; they can be found in [10–12]. It is worth to stress, however, that the version of this method described in [12] allows one to compute both the reference state (the equilibrium structure) and all the elastic compliances in a single run.

In the simulations a (variable) periodic box which is described by the *symmetric* box matrix, h_{ij}, the columns of which are formed by the components of the edge-vectors of the box. In such a case the (Lagrange) strain tensor, ε_{ij}, can be written as [12]:

$$\underline{\varepsilon} = \left(\underline{h}_0^{-1} \underline{h} \underline{h} \underline{h}_0^{-1} - \underline{I} \right)/2 \ , \tag{1}$$

where the zero index denotes the reference state. In the constant pressure simulations, it is convenient to define the reference state as the equilibrium state corresponding to the simulation pressure, $\underline{h}_0 = <\underline{h}>_p$ [11, 12]. The components of the tensor of the elastic compliances can be expressed by fluctuations of the components of the strain tensor as follows [10–12]:

$$\frac{\langle V \rangle_p}{kT} < \varepsilon_{ij} \varepsilon_{kl} > = \bar{S}_{ijkl} \ . \tag{2}$$

For two-dimensional hard-body systems it is convenient to use dimensionless elastic compliances defined as:

$$S_{ijkl} = \bar{S}_{ijkl} kT/\sigma^2 \tag{3}$$

For the rectangular phase of planar pentamers they are collected in Table 1 and their volume dependence is shown in Figure 4. It is worth to add here that the symmetry of the crystalline structure studied implies $S_{xyyy} = S_{yxxx} = 0$. This equality can be used as one of tests of the convergence of the applied computational method.
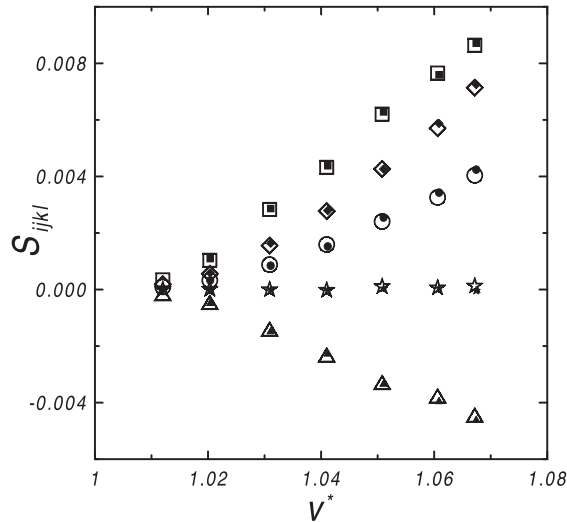
Figure 4. The relative volume dependence of the elastic compliances for the defect-free rectangular solid structure of the pentamers. The following components of the compliance tensor are shown: S_{xxxx} (squares), S_{yyyy} (diamonds), S_{xxyy} (triangles), S_{xyxy} (circles), and S_{xyyy} (stars). The results obtained for S_{yxxx} are not shown as they are indistingushable from S_{xyyy}. The full symbols correspond to $N = 56$ and the open symbols to $N = 224$. The errors do not exceed the sizes of the symbols

Table 1. The dimensionless elastic compliances of the defect-free rectangular structure for various system sizes (N is the number of the pentamers). The lengths of the runs (measured in trial steps per particle, M) depend on the system size as follows: $N = 16, 30, 36 - M = 2 \times 10^6$; $N = 56, 64 - M = 3 \times 10^6$; $N = 120, 144 - M = 5 \times 10^6$; $N = 224 - M = 10^7$; $N = 400, 480 - M = 1.5 \times 10^7$; $N = 896 - M = 2.5 \times 10^7$. The stars in the first column indicate the shape of the samples used. Single star corresponds to a periodic box containing $2r$ rows of $2r$ molecules (r is a natural number). Double star represents a periodic box of $6r$ rows, each containing $5r$ molecules. Triple star indicates a periodic box of $8r$ rows of $7r$ molecules. The molecular rows are parallel to the x-axis

N	p^*	v^*	S_{xxxx}	S_{yyyy}	S_{xxyy}	S_{xyxy}	S_{xyyy}	S_{xxxy}
30*	9	1.06780(6)	0.00894(10)	0.00754(10)	−0.00466(6)	0.00433(9)	0.00015(8)	−0.00013(9)
36**	9	1.06782(8)	0.00863(16)	0.00709(11)	−0.00430(11)	0.00419(9)	−0.00013(3)	0.00007(5)
56***	9	1.06741(6)	0.00871(17)	0.00722(20)	−0.00462(15)	0.00424(7)	−0.00005(8)	0.0001(16)
120*	9	1.06733(5)	0.00863(16)	0.00720(14)	−0.00450(11)	0.00407(9)	−0.00004(4)	0.00007(5)
224***	9	1.06716(4)	0.00864(14)	0.00714(18)	−0.00444(20)	0.00404(5)	0.00002(6)	0.00009(8)
480*	9	1.06721(6)	0.00872(23)	0.00697(19)	−0.00437(20)	0.00398(9)	−0.00006(7)	0.00002(9)
∞	9	1.06711(6)	0.00863(20)	0.00703(19)	−0.00442(20)	0.00399(9)		
56***	10	1.06086(12)	0.00759(25)	0.00588(22)	−0.00397(21)	0.00343(8)	0.00004(5)	−0.0001(4)
224***	10	1.06058(6)	0.00765(39)	0.00576(32)	−0.00380(28)	0.00326(12)	0.00006(3)	−0.0000(2)
56***	12	1.05105(5)	0.00628(13)	0.00426(12)	−0.00335(9)	0.00255(23)	0.00003(3)	−0.0001(2)
224***	12	1.05080(1)	0.00620(13)	0.00427(10)	−0.00329(8)	0.00241(21)	0.00010(6)	−0.00011(8)
36**	15	1.04134(3)	0.00427(9)	0.00277(9)	−0.00225(6)	0.00157(3)	−0.00005(3)	0.00006(4)
64**	15	1.04119(3)	0.00430(9)	0.00277(4)	−0.00228(5)	0.00157(3)	0.00009(4)	−0.00011(4)
144**	15	1.04101(3)	0.00438(10)	0.00283(7)	−0.00236(7)	0.00158(4)	−0.00003(4)	0.00005(6)
400**	15	1.04096(3)	0.00427(10)	0.00275(7)	−0.00224(6)	0.00156(6)	0.00002(5)	0.00007(9)
∞	15	1.04092(3)	0.00433(9)	0.00279(8)	−0.00230(7)	0.00157(5)		
30*	15	1.04147(5)	0.00470(12)	0.00301(11)	−0.00256(9)	0.00161(5)	−0.00002(4)	0.00004(4)
120*	15	1.04106(3)	0.00441(9)	0.00281(7)	−0.00234(7)	0.00157(4)	0.00000(3)	−0.00002(5)
480*	15	1.04094(2)	0.00429(9)	0.00275(8)	−0.00226(7)	0.00160(4)	0.00002(8)	0.00004(9)
∞	15	1.04091(2)	0.00428(9)	0.00274(8)	−0.00225(7)	0.00158(4)		
56***	15	1.04117(4)	0.00437(11)	0.00280(5)	−0.00231(7)	0.00152(4)	−0.00003(4)	0.00000(4)
224***	15	1.04099(3)	0.00432(9)	0.00278(7)	−0.00231(5)	0.00159(5)	−0.00003(6)	−0.00004(7)
896***	15	1.04092(2)	0.00423(9)	0.00271(9)	−0.00222(9)	0.00162(4)	0.00003(8)	−0.00007(8)
∞	15	1.04091(2)	0.00425(9)	0.00273(9)	−0.00225(8)	0.00162(4)	0.00002(9)	−0.00003(9)
56***	20	1.03107(2)	0.00286(5)	0.00162(4)	−0.00149(7)	0.00085(2)	−0.00001(1)	0.00000(1)
224***	20	1.03089(3)	0.00284(4)	0.00157(3)	−0.00141(8)	0.00087(2)	−0.00001(1)	0.00003(3)
56***	30	1.02037(2)	0.00108(3)	0.00059(1)	−0.000480(23)	0.000319(21)	0.00000(1)	0.0000(1)
224***	30	1.02030(1)	0.00105(2)	0.00057(1)	−0.000454(21)	0.000325(15)	0.00001(1)	0.00001(1)
30*	50	1.01212(3)	0.000352(5)	0.000188(3)	−0.000146(3)	0.0000966(12)	−0.0000012(11)	0.0000004(26)
36**	50	1.01211(1)	0.000345(6)	0.000191(3)	−0.000148(4)	0.0000966(8)	−0.000001(13)	0.0000016(13)
56***	50	1.01204(2)	0.000341(12)	0.000186(3)	−0.000145(6)	0.000092(2)	−0.000001(11)	−0.0000012(17)
120*	50	1.01201(1)	0.000331(6)	0.000183(3)	−0.000135(4)	0.000095(2)	0.000001(2)	−0.000002(2)
224***	50	1.01198(1)	0.000339(11)	0.000186(4)	−0.000140(6)	0.000093(2)	0.000001(1)	0.000002(1)
480*	50	1.01198(1)	0.000332(11)	0.000181(6)	−0.000137(6)	0.000094(2)	−0.000001(2)	0.000003(2)
∞	50	1.01196(1)	0.000331(8)	0.000182(6)	−0.000136(6)	0.000093(2)		

Table 2. The Poisson's ratios in the *x* and *y* directions for the defect-free rectangular phase of pentamers

N	p^*	v^*	n_{xy}	n_{yx}
30*	9	1.06780(6)	0.521(7)	0.618(8)
36*	9	1.06782(8)	0.498(11)	0.606(12)
56*	9	1.06741(6)	0.530(14)	0.640(19)
120*	9	1.06733(5)	0.521(11)	0.625(14)
224*	9	1.06716(4)	0.514(16)	0.622(22)
480*	9	1.06721(6)	0.501(18)	0.627(23)
∞	9	1.06711(6)	0.513(19)	0.629(23)
56*	10	1.06086(12)	0.523(22)	0.675(21)
224*	10	1.06058(6)	0.497(24)	0.660(22)
56*	12	1.05105(5)	0.533(13)	0.786(21)
224*	12	1.0508(1)	0.531(12)	0.770(18)
36*	15	1.04134(3)	0.527(13)	0.812(24)
64*	15	1.04119(3)	0.530(12)	0.823(15)
144*	15	1.04101(3)	0.539(14)	0.833(22)
400*	15	1.04096(3)	0.525(13)	0.815(22)
∞	15	1.04092(3)	0.532(13)	0.826(22)
30*	15	1.04147(5)	0.544(16)	0.85(3)
120*	15	1.04106(3)	0.531(14)	0.833(23)
480*	15	1.04094(2)	0.527(14)	0.822(25)
∞	15	1.04091(2)	0.526(14)	0.822(24)
56*	15	1.04117(2)	0.529(15)	0.825(20)
224*	15	1.04099(4)	0.535(12)	0.831(20)
896*	15	1.04092(2)	0.525(16)	0.819(24)
∞	15	1.04091(2)	0.529(16)	0.824(24)
56*	20	1.03107(2)	0.521(17)	0.919(33)
224*	20	1.03089(3)	0.496(18)	0.898(34)
56*	30	1.02037(2)	0.444(17)	0.813(26)
224*	30	1.0203(1)	0.432(14)	0.796(25)
30*	50	1.01212(3)	0.415(9)	0.776(14)
36*	50	1.01211(1)	0.429(12)	0.775(16)
56*	50	1.01204(2)	0.425(16)	0.779(22)
120*	50	1.01201(1)	0.408(11)	0.738(17)
224*	50	1.01198(1)	0.413(16)	0.753(24)
480*	50	1.01198(1)	0.413(16)	0.757(29)
∞	50	1.01196(1)	0.411(16)	0.748(30)

In Figure 5 the results obtained for a few system sizes and shapes are shown at $p^* = 15.0$. These data were used to estimate the thermodynamic limit, $N \to \infty$, at this pressure (see Table 1). It can be seen that the results obtained for systems as small as $N = 56$ approximate the thermodynamic limit within a few percent accuracy.

Knowledge of the elastic compliances allows one to calculate all the elastic properties of the system, including the Poisson's ratio. As the studied structure of the pentamers is anizotropic, the Poisson's ratio depends on the direction, in general, and will be indexed by the direction of the infinitezimal change of the stress. In Table 2 the computed Poisson's ratios at a few pressures are collected for the *x* and *y* directions. As it is easy to see, the Poisson's ratio is positive everywhere, what is in contrast to the results obtained for the
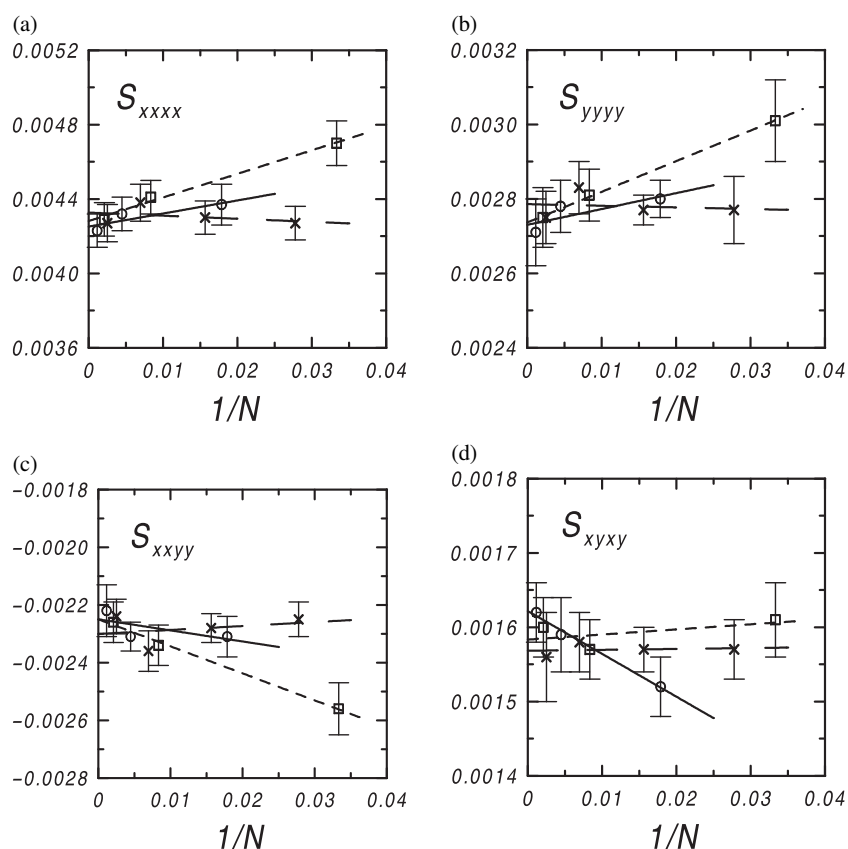
Figure 5. Number dependencies of the elastic compliances of the pentamers
at the dimensionless pressure $p^* = 15.0$: (a) S_{xxxx}, (b) S_{yyyy}, (c) S_{xxyy}, (d) S_{xyxy}.
The short-dash (squares), long-dash (crosses), and continuous lines (circles) correspond
to structures marked in the Table 1 by one, two, and three stars, respectively

densest phase of the planar heptamers [4]. It can be also seen in this table that within the
present experimental accuracy the Poisson's ratios are well approximated by their values
obtained for systems as small as $N = 56$.

4. Final remarks

The performed simulations confirm earlier results [1, 3] concerning the structure of
the dense crystalline phase of the pentamers. At high pressures the molecular rotation is
frozen and the pentamers form a solid phase with two molecules in a unit cell of rectangular
shape.

Elastic compliances of pentamers in the defect-free rectangular solid phase have been
computed by using the strain-fluctuation method [12]. It follows from the results obtained
that neither the anizotropy of the studied structure nor the anizotropy of the intermolecular
interactions of the pentamers cause any complications for using this method. The method
is sufficiently well convergent to give results within a few percent accuracy for systems as
small as $N = 56$. This encourages one to apply it to more complex systems.

The Poisson's ratios which have been computed for the rectangular phase in the x and y directions do not exhibit anomalous behaviour found in the highest density phases of planar hard cyclic heptamers [4]. It is worth to stress that within the present four-percent accuracy the Poisson's ratios obtained for $N = 56$ are equal to the values estimated in the thermodynamic limit.

Acknowledgements

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