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## On solid–liquid transition in plane disc systems

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**Abstract.** Structural, mechanical and thermodynamical properties of close packed binary systems of discs with hard, elastic and Lennard-Jones potentials of interaction are considered. Using the method of molecular dynamics the transition from crystal melting to glass softening with increasing relative dispersity in disc size from 0 to 0.23 is investigated. A single particle mean-field model is proposed, which allows us to obtain straightforwardly the constitutive equation and shear modulus of the systems considered.

### 0. Introduction

At present there are different viewpoints on the nature of crystal melting and glass softening ('glass transition') processes. Besides a simple Lindeman criterion relating the melting process to an amplitude of lattice vibrations [1], Born's theory based on the assumption that the shear modulus turns to zero at the melting point [2], and theoretical models based on the dislocation mechanism of crystal melting have been proposed (for example, [3, 4]). However none of these approaches provides a clear understanding of microscopic processes responsible for crystal melting. The same thing relates to the glass transition, which is considered as a purely kinetic phenomenon or a thermodynamic phase transition of second or first order [5–7].

Essential progress in understanding these processes on the molecular level can provide the analysis of a two-dimensional system of discs which are now under intensive investigation as a convenient model for a wide range of problems [8–11]. Specific interest in these systems results from studying thin films on the surface. Today properties of one-component assemblies of discs with different interaction potentials are rather well understood. Particularly, it is shown that the melting of a crystal in the plane comprises two subsequent phase transitions of infinite order (without any jumps in derivative values) in a narrow temperature range. An intermediate metastable phase (hexatic) shows an orientation order and no translational one [7].

The binary assembly of discs in the plane is the simplest polydisperse system allowing us to control the gradual transition of a crystal to the amorphous solid (glass) by changing the relative difference in size of two disc types and their concentrations. The effect of the system composition on its structure in solid state (at zero temperature) is discussed in [9–11]. Thermodynamic properties of polydisperse systems are much less studied. Thus, in the assemblies of Lennard-Jones (LJ) elastic and hard discs a liquid–solid transition takes place, the structure of the solid state being dependent on the system composition [12]. Mechanical parameters of a system of LJ discs of relative difference in sizes being equal approximately to 0.47 are described in [13]. However up to now the effect of the system properties (interaction

potential, fraction size and concentration) on the parameters of solid–liquid transition has not been elucidated.

In this paper microscopic mechanisms of crystal melting and glass softening are discussed on the base of molecular dynamics (MD) analysis of a two-component two-dimensional system of discs of different interaction potentials. In computer simulations the solid state usually differs from the liquid state by the presence of self-diffusion in the latter case which disappears upon liquid–solid transition. However the shear resistance is known to be the main characteristic feature of the solid state. The difference between these definitions is the most evident in the assemblies of hard discs without attraction at zero temperature in the absence of both self-diffusion and shear resistance. Hence, in this paper special interest is paid both to self-diffusion and shear resistance.

In the first section a model system is presented, as well as some details of numerical simulations being described. In the second section the temperature driven solid–liquid transition in the system is analysed.

The third section is devoted to the theoretical estimation and computer simulation of the system mechanical properties. The main results obtained are briefly discussed in section 4.

### 1. Model and method of computer simulation

Systems of elastic or LJ discs of two types have been considered in a cell with periodic boundary conditions. The overall number of particles was from 1000 to 120 000, the numbers of particles of each type being identical.

For elastic discs the interaction potential was expressed as:

$$U(r_{ij}) = \begin{cases} k(r_{ij} - R_i - R_j)^2/2 & r_{ij} \leq (R_i + R_j) \\ 0 & r_{ij} > (R_i + R_j) \end{cases}$$

where  $R_i$ ,  $R_j$  are particle radii,  $r_{ij}$  the distance between centres of  $i$ th and  $j$ th particles and  $k$  the stiffness of particles. At  $k/P \rightarrow \infty$  ( $P$  is external pressure) the system can be considered as a model of absolutely hard discs (HD model).

For the Lennard-Jones model (LJ model) the interaction of particles was defined by LJ potential of finite interaction radius:

$$U(r_{ij}) = \begin{cases} U_{LJ}(r_{ij}) - U_{LJ}(2.5\sigma_{ij}) & r_{ij} \leq 2.5\sigma_{ij} \\ 0 & r_{ij} > 2.5\sigma_{ij} \end{cases}$$

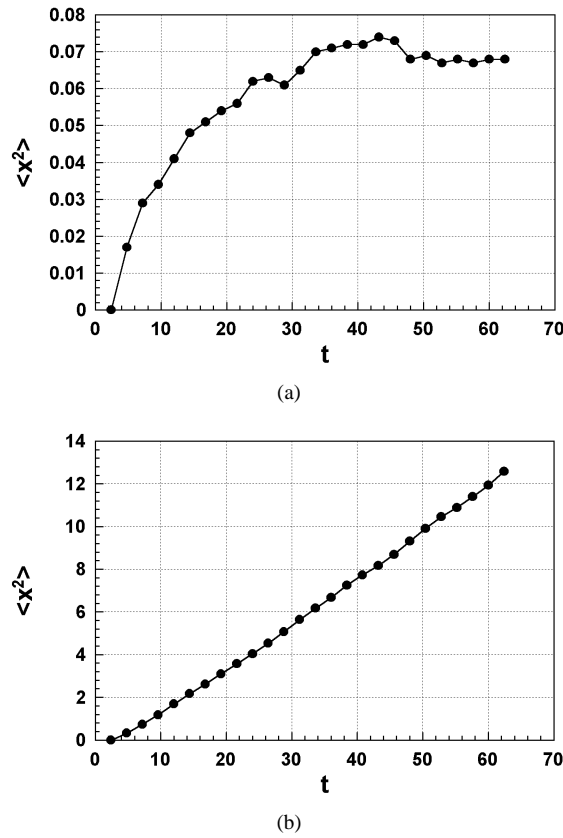
$$U_{LJ}(r_{ij}) = 4\epsilon \left[ \left( \frac{\sigma_{ij}}{r_{ij}} \right)^{12} - \left( \frac{\sigma_{ij}}{r_{ij}} \right)^6 \right]$$

where  $\sigma_{ij} = 0.5(\sigma_i + \sigma_j)$ ,  $\sigma_i$  is the size parameter of  $i$ th particle.

All calculations were accomplished in a system of units where the Boltzmann constant, particle mass, and small disc diameter ( $2R_1$  or  $\sigma_1$ ) were equal to 1.

The initial packing represents an ideal hexagonal crystal of identical discs (at given pressure). To obtain a binary system the radii of 50% of randomly located discs were gradually increased up to a given value of  $\delta$ :  $\delta = (R_2 - R_1)/R_1$ ,  $R_2 > R_1$ , or  $\delta = (\sigma_2 - \sigma_1)/\sigma_1$ ,  $\sigma_2 > \sigma_1$  for elastic and LJ discs, respectively. The system relaxation by density was carried out simultaneously at constant pressure. As was shown earlier, this procedure provides formation of nearly the densest packing [11].

The Berendsen algorithm was used to simulate the NPT ensemble,  $x$ - and  $y$ -components of pressure being given independently, which made it possible to simulate both bulk stress,  $P_\tau = (P_x + P_y)/2$  and shear stress,  $P_\tau = (P_x - P_y)/2$  [14, 15]. The system heating up

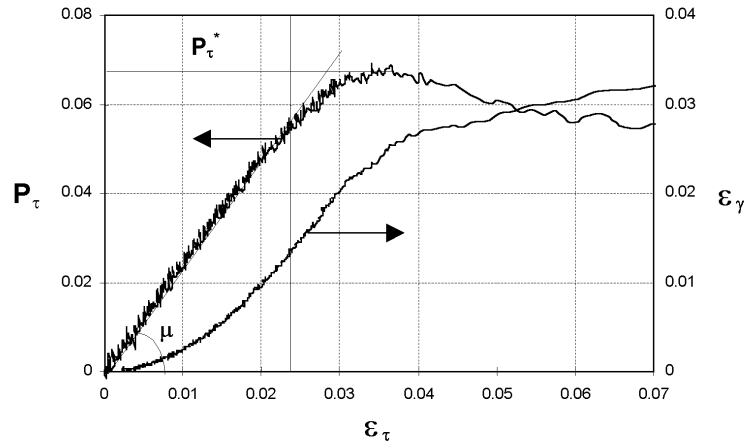


**Figure 1.** Typical dependences of mean square displacement ( $\langle x^2 \rangle$ ) versus time  $t$  at different temperatures: (a)  $T = 0.01$  (solid), (b)  $T = 0.08$  (liquid),  $N = 4096$ ,  $P = 0.2$ ,  $k = 1000$ ,  $\delta = 0.5$ .

to a given temperature was carried out gradually, the temperature being increased by the step of 0.001 of temperature unit with the relaxation of density and energy at each step. This procedure of numerical simulation made it possible to obtain continuous temperature dependences of the system parameters, particularly, to evaluate the thermal expansion coefficient,  $P\Delta S/\Delta T$ .

Each run length consisted of 100–1000 of time units that allowed measurement of the system packing fraction and self-diffusion coefficient to a good accuracy. The packing fraction was defined by the ratio between the area occupied by the discs and the mean (by time) area of the calculated cell. The self-diffusion coefficient was determined as a slope of the plot of the mean-square deviation of particles, versus time at high time values where this dependence was a linear one (figure 1(a),(b)).

Diagrams of biaxial compression were obtained at constant  $P$  and constant rate of  $P$  change ( $dP/dt = 0.000\,03\text{--}0.001$ ) and values of volume ( $\varepsilon_\gamma$ ) and shear ( $\varepsilon_\tau$ ) deformations were measured:  $\varepsilon_\gamma = (\varepsilon_x + \varepsilon_y)/2$ ,  $\varepsilon_\tau = (\varepsilon_x - \varepsilon_y)/2$ , where  $\varepsilon_x = A_x/A_{x0}$ ,  $\varepsilon_y = A_y/A_{y0}$ ,  $A_{x0}$  and  $A_{y0}$  are dimensions of the calculated cell in the undeformed state and  $A_x$  and  $A_y$  are dimensions of the cell under deformation conditions. The typical diagram is given in figure 2. As shown, at low  $\varepsilon_\tau$  the plot of  $\varepsilon_\tau$  versus  $P_\tau$  is linear and the shear modulus,  $\mu = P_\tau/\varepsilon_\tau$  can be calculated, as well as the yield stress  $P_\tau^*$  (the maximum shear stress).



**Figure 2.** Typical dependence of shear stress  $P_\tau$  and volume deformation  $\varepsilon_\gamma$  on shear deformation  $\varepsilon_\tau$ . Bulk stress  $P_\gamma = P = \text{const}$ . System of units—see text,  $P_\tau^*$ —yield stress,  $\mu$ —shear modulus.

As known, the numerical simulation in binary systems can be accompanied by system separation in fractions differing by particle size. The separation degree on the local scale was controlled as follows: the numbers of different triads of neighbour discs were calculated for a system with random distribution and the system discussed. Then the parameter that differentiates this system from a random one was calculated [11]:

$$\xi = \frac{\sqrt{\sum (N_i - N_{ic})^2}}{\sqrt{N}}$$

where  $N_i$  and  $N_{ic}$  are measured and calculated numbers of triads of different type and  $N$  the total number of particles in the system. For a random packing  $\xi \sim 1$  and for a fully separated system  $\xi \sim \sqrt{N}$ . As shown, for all the systems considered the value of  $\xi$  parameter was less than 3 and was practically constant in the course of numerical simulation, which suggests the absence of separation in fractions. So all the systems considered are metastable in the simulated time scale.

The degree of system ordering was determined by analysing the orientation correlation function  $g_6(r)$ :

$$g_6(|r - r_0|) = \langle \psi(r) \psi(r_0) \rangle$$

$$\psi(r_j) = \frac{1}{z} \sum_{k=1}^z e^{i6\theta_{kj}}$$

where  $z$  is the number of nearest neighbours of the  $j$ th particle and  $\theta_{ij}$  the angle between the line connecting the centres of  $i$ th and  $j$ th particles and a fixed axis, the averaging being carried out over all the particles.

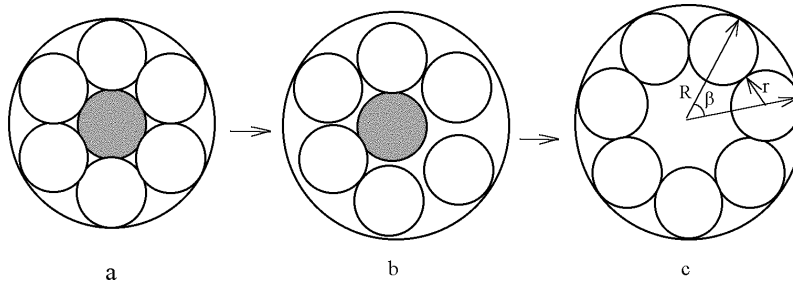
In crystalline systems at great distances  $g_6(r)$  tends to a value differing from zero (in the ideal hexagonal crystal  $g_6(r) = 1$ ) whereas in liquid and glass at  $r \rightarrow \infty$   $g_6(r) \rightarrow 0$  [16].

## 2. Temperature driven solid-liquid transition

### 2.1. Theoretical model

The phase transition of the first order (melting) in crystals is usually related to the nucleation and mobility of structural defects (dislocations and disclinations) [17]. The nature of glass transition is not so evident because of ambiguous identification of structural defects in glass [18]. However in the system of hard discs considered the simulation data demonstrate a continuous transition from the crystal melting to the glass softening. This fact suggests that the model to explain transitions in these systems must be the same.

The key concept of such a model is that all the properties of the system considered are governed by local geometrical disorder; from the geometrical point of view near the melting point ( $T_{lr}$ ) the free interchange of the discs becomes possible. For the case of hard discs this approach can be developed using simple calculations.



**Figure 3.** Melting of hexagonal crystal of hard discs—illustrative scheme:  $R$ —cell radius,  $r$ —disc radius; (a)  $T = 0$ , (b)  $0 < T < T_{lr}$ , (c)  $T = T_{lr}$ .

Let us consider a system of six identical discs surrounding the central one (figure 3). The interchange is possible if the system density is low enough to allow the central disc ‘to enter’ the circle of its nearest neighbours (see figure 3(c)). If all the seven discs form the ring of minimum radius, it can be expressed as follows (see symbols in figure 3):

$$R = r + \frac{r}{\sin(\beta/2)} = 3.31r \quad \beta = \frac{2\pi}{7} \approx 51.4^\circ.$$

The relative change of the cell volume can be roughly estimated as follows:

$$\frac{\Delta S}{S} = \frac{\pi R^2 - 9\pi r^2}{9\pi r^2} \approx 0.214.$$

The relative density corresponding to this change of volume is expressed by:

$$\rho^* = \frac{0.907}{1.214} \approx 0.75. \quad (1)$$

Thus the minimum additional volume of the cell is evaluated when local changes in topology of bonds between a particle and its neighbours are possible. This interchange in neighbours can result in initiation of topological structure defects of minimum intensity in glasses [17–19] and vacancies in crystals.

In binary systems the relative volume change upon melting will be different due to difference in sizes of neighbour particles. The calculation for different neighbour types shows that the volume change becomes lower at increasing relative difference in particle size. On the other hand, the increase in  $\delta$ -values results in reduction of density at  $T = 0$ . As a result, the density at the melting point is changed moderately.

## 2.2. Constitutive equation

Let us consider a system of hard discs. The discs oscillate near their equilibrium states within the boxes formed by the nearest neighbours at temperatures below the melting point. Since the self-diffusion in the solid state is low, the effect of discs interchange between the boxes is negligible. Thus the interparticle interaction reduces to fully elastic collisions with the nearest neighbours, which allows us to apply a one-particle model of the mean field (where each disc is suggested to be 'locked' in an immobile box with rigid walls) to the system of hard discs. The box size must be chosen so that the ratio between the disc area and the box area is equal to the mean density of the system.

A similar approach was first used in the well known paper [20] while studying the phase diagrams and melting of molecular systems. The difference is that we do not use any phenomenological parameters. It allows us to obtain straightforwardly the constitutive equation. As will be shown in section 3 this model with certain additions can be used for the analysis of mechanical properties also.

Let us consider the motion of a disc of radius  $r_0$  in the box of radius  $R$ . It can be easily seen that for elastic collisions this motion is completely described by the motion of the disc centre within the circle of radius  $r = R - r_0$ . If  $\phi$  is the angle between the velocity vector of the disc centre and the circle radius in the point of collision, the momentum transmitted to the circle boundary in one collision is equal to:

$$\Delta p = 2mv \cos \phi$$

where  $v$  is disc velocity and  $m$  disc mass. Then the average time between the consecutive collisions can be estimated as follows:

$$\tau = \frac{r \cos \phi}{v}.$$

The average pressure of the disc on the box boundary can be expressed as follows:

$$P = \frac{\Delta p}{2\pi R\tau} = \frac{mv^2}{2\pi Rr}.$$

The temperature in the system being defined by the following simple relationship (the Boltzmann constant is suggested to be equal to 1):

$$mv^2 = 2T$$

the constitutive equation may be written as follows:

$$PS/T = 1/(1 - \sqrt{S_0/S}).$$

If the condition  $(R - r_0)/R \ll 1$  is met, the constitutive equation can be finally written in the following form:

$$P(S - S_0) = 2T \quad (2)$$

where  $S = \pi R^2$ ,  $S_0 = \pi r_0^2$ . When comparing the results obtained using this equation to the experimental data, account must be taken of the fact that the initial density  $\rho_0$  is not equal to 1 and thus the ratio  $S_0/\rho_0$  must be used instead of  $S_0$ .

The relative temperature of the solid-liquid transition can be estimated using the constitutive equation:

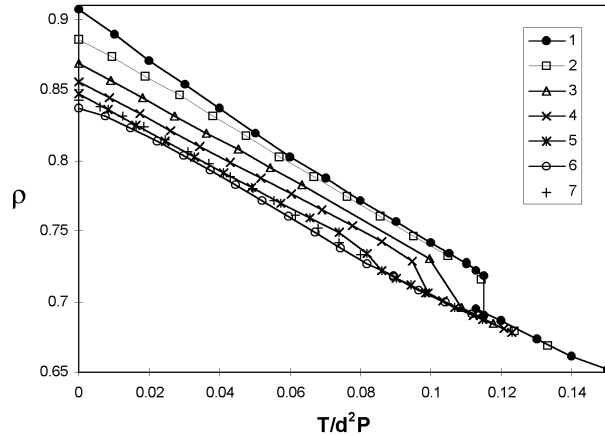
$$\left(\frac{T}{P}\right)^* = \frac{\pi r_0^2}{2} \left(\frac{1}{\rho^*} - \frac{1}{\rho_0}\right)$$

where  $\rho_0 = 0.9069$  is the packing fraction of the ideal hexagonal crystal. Substituting  $\rho^*$  from equation (1) gives the temperature value:

$$\left(\frac{T}{P}\right)^* = 0.094. \quad (3)$$

### 2.3. Results of computer simulations

In figure 4 (curve 1) typical plots of packing fraction versus temperature are shown for a system of elastic discs with  $k/P = 5000$  (this system can be considered as an HD model). The analogous dependences take place for both elastic and LJ discs. It turned out that in the systems of hard, elastic and LJ discs of identical size a sharp jump in density was observed at a given temperature. The analysis of mechanical property measurements shows that the solid–liquid transition takes place in the range of the above density jump. The melting process of solid crystals from discs is accompanied by yield stress and elastic modulus reducing to zero at the melting point (figure 5(a)). By contrast, the self-diffusion coefficient increases above the melting point.



**Figure 4.** Plot of density  $\rho$  versus reduced temperature  $T/d^2P$  in binary systems of hard discs ( $P_\tau = 0$ ):  $\delta = 0$  (1);  $\delta = 0.05$  (2);  $\delta = 0.1$  (3);  $\delta = 0.15$  (4);  $\delta = 0.2$  (5);  $\delta = 0.3$  (6);  $\delta = 0.5$  (7).

The experiments on crystallization and melting demonstrate the difference of the temperatures to be less than 5%. So, the difference between the melting point and the point of loss of stability is lower than the accuracy of our calculation, which allows to detect the melting point unambiguously.

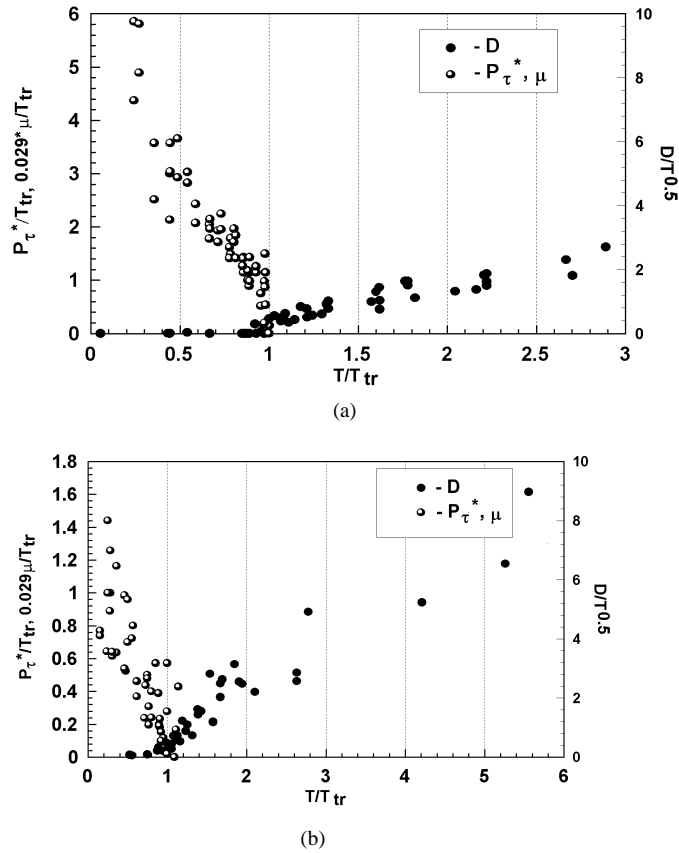
At zero temperature a long-range orientation order is observed in the system of identical discs, i.e. the function  $g_6(r)$  attains a limit differing from zero at large distances. When increasing temperature the value of this limit lowers and beyond the range of density jump the long-range order is not observed in the system (figure 6(a)).

Upon the system melting the density jump persists with  $\delta$  increase, but the jump value decreases (figure 4, curves 2–7) and disappears at the critical value of  $\delta^* = 0.23$ . At  $\delta > 0.23$  the jumps in values of density and coefficient of thermal expansion disappear. The temperature dependences of yield stress, elastic modulus and self-diffusion coefficient of the systems considered (crystals from identical discs and systems with  $\delta > \delta^*$ ) are similar (figure 5(a),(b)).

At zero temperature in the systems with  $\delta$ -values differing from zero the gradual decrease of ordering degree is observed when  $\delta$ -values growing. At  $\delta$ -values corresponding to the absence of a density jump upon solid–liquid transition the long-range orientation ordering does not take place (figure 6(b)).

These regularities are valid for particles with elastic and LJ interaction potentials. As shown, the plots of density jump versus relative difference in disc radii are similar and critical values of  $\delta^*$  corresponding to zero density jump for these systems are in good accordance (figure 7).



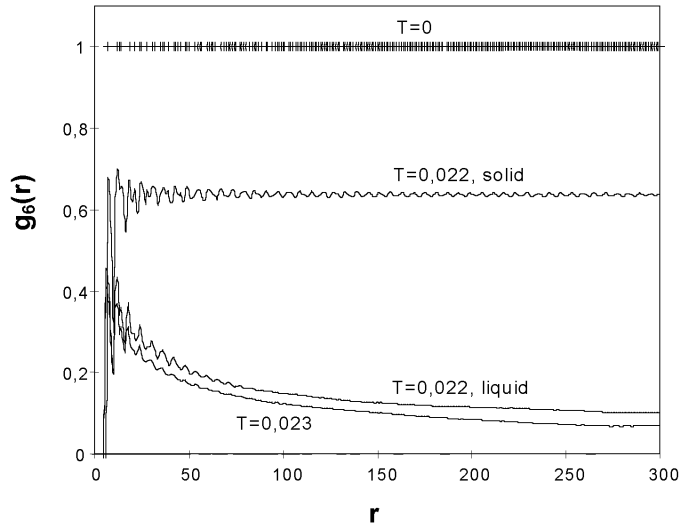


**Figure 5.** Plot of self-diffusion coefficient  $D$ , yield point  $P_{\tau}^*$  and shear modulus  $\mu$  versus reduced temperature  $T/T_{tr}$ : (a) crystal ( $\delta = 0$ , hard discs  $P = 0.2, 2, 5, k = 100$ , LJ discs  $P = 2, 10, 50$ ,  $\varepsilon = 1$ ); (b) binary glass ( $\delta = 0.5$ , hard discs  $P = 0.2, 2, 5, k = 100$ , LJ discs  $P = 10, 50, \varepsilon = 1$ ).

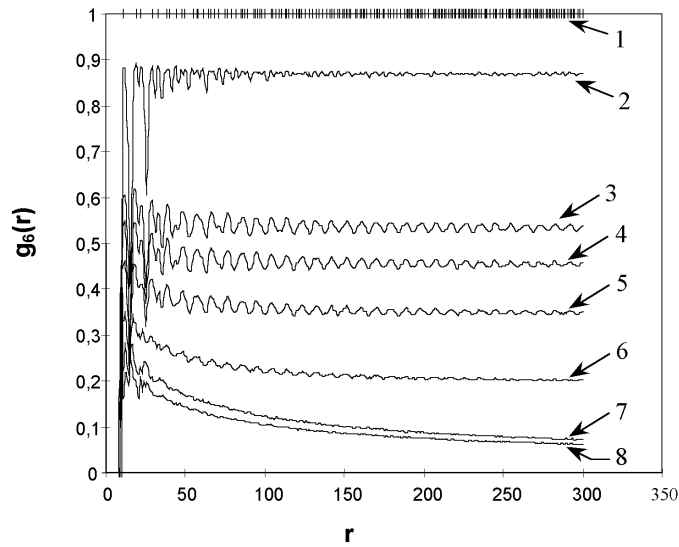
The density of a solid at phase transition point is weakly dependent on the difference in particle sizes up to the confluence point ( $\delta \approx 0.23$ ) whereas the density of a liquid shows nearly linear growth with  $\delta$  and reaches the density of a solid at the confluence point; beyond this point both densities of the solid (glass) and the liquid grow. It should be noted that in the same  $\delta$  range (from 0 to 0.23) the gradual drop of density at  $T = 0$  (the maximum packing fraction) is observed. The close value of  $\delta^*$  at equal disc concentrations was given in [12].

The value of packing fraction corresponding to the phase transition at  $\delta = 0$  is  $\rho^* \approx 0.73$  and the coincidence with the theoretical value  $\rho^* = 0.747$  (equation (1)) is satisfactory. The results obtained correspond to a known crystallographic rule that the cocrystallization of structurally similar compounds can take place at a difference in molecule size not exceeding a given value [21]. Thus the results obtained should be the first demonstration of a surprising similarity in the structural transition (melting) and aggregate transformation (glass transition).

In the assemblies of hard discs the temperature of transition (melting or glass transition),  $T_{tr}$ , is proportional to pressure; for the ideal crystal from hard discs  $T/Pd^2 \approx 0.1-0.11$ . Substitution of  $P^* = P/(\varepsilon\sigma^2)$  and  $T^* = T/\varepsilon$  leads to a common linear dependence of  $T_{tr}$  versus  $P$  for all LJ systems, which coincides with the analogous dependence for elastic discs.



(a)

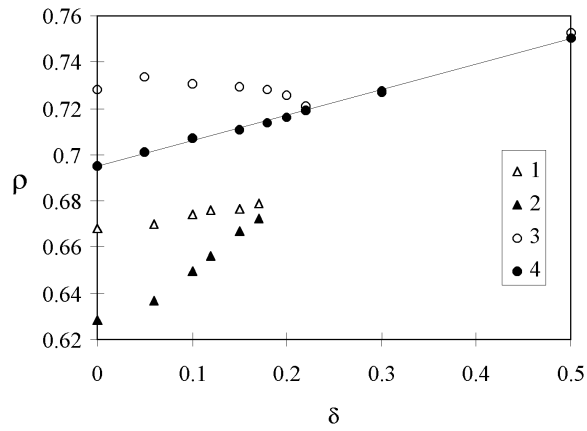


(b)

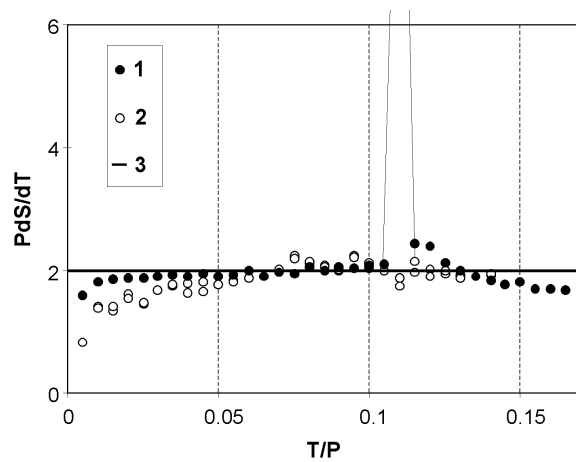
**Figure 6.** Plot of orientational correlation function  $g_6(r)$  at different temperatures (equal discs,  $\delta = 0$ ) (a) and different values of relative difference in disc size  $\delta$  (b):  $\delta = 0$  (1);  $\delta = 0.1$  (2);  $\delta = 0.2$  (3);  $\delta = 0.22$  (4);  $\delta = 0.25$  (5);  $\delta = 0.3$  (6);  $\delta = 0.4$  (7);  $\delta = 0.5$  (8), elastic discs,  $N = 4096$ ,  $k = 1000$ ,  $P = 0.2$ .

The differences between the systems with elastic and LJ interaction potentials arise from the presence of an attraction component in the latter case. As a result, the melting point is different from zero at zero external pressure and the temperature dependence of the system parameters is more strongly expressed.

The peculiar behaviour of the coefficient of thermal expansion,  $P \, dS/dT$ , is observed near the melting point. For the crystal of absolutely hard identical discs  $P \, dS/dT = 2$  (equation (2)), this value being constant in the whole solid region and in the liquid just above the melting



**Figure 7.** Plot of density in solid and liquid state near transition area versus relative difference in disc size  $\delta$ : LJ, solid (1); LJ, liquid (2); HD, solid (3); HD, liquid (4).



**Figure 8.** Coefficient of thermal expansion  $P dS/dT$  as a function of reduced temperature in systems of hard discs:  $\delta = 0$  (1),  $\delta = 0.3$  (2) and theoretical estimation (3).

point (figure 8). For elastic discs and/or binary assemblies with  $\delta < 0.23$   $P dS/dT \approx 2$  and this value is temperature dependent, but the jump of  $P dS/dT$  at the transition point is absent.

In the systems with LJ potential at high pressures ( $P > 10\varepsilon_0/d^2$ ) the  $dS/dT$ -jump at the transition point is also absent at any  $\delta$ -values. The  $dS/dT$ -jump at the melting point ( $\delta < 0.23$ ) takes place at low pressures only ( $P < 2\varepsilon_0/d^2$ ) when the strong temperature dependence of  $dS/dT$  is observed.

In these systems the temperature dependence of  $P dS/dT$  and the  $dS/dT$ -jump in the presence of the density jump is related to the attraction branch in the curve of potential energy and to the dependence of attraction force on the density, i.e. mean interparticle distance. At high mean distances the attraction value decreases with the mean interparticle distance, i.e. with temperature rise and density drop. The continuous smooth plots of  $P dS/dT$  versus density observed in all cases confirm this explanation.

### 3. Analysis of mechanical properties

#### 3.1. Shear modulus estimation

The calculation of the shear modulus is based on the same assumptions as were used for calculating the constitutive equation. The only additional detail to be taken into account is the anisotropy related to shear stress. This anisotropy is taken into account in the mean field model using the assumption that the ‘effective box’ has elliptic rather than circular shape and the difference between axes of these ellipses is defined by the shear deformation level.

However this model is rather difficult to analyse, since the motion of a disc in the ellipse with elastic walls (‘elliptic billiard with balls of finite size’) is very complicated from the mathematical viewpoint.

To simplify the model the motion of a square ‘particle’ in a rectangle of larger size can be considered, the difference between the rectangle sides being related to the shear deformation. It can be easily seen that this model is identical to the ‘circle in an ellipse’ model from the physical point of view, because the latter results in the same constitutive equation in the isotropic case.

Let us consider the square with side  $l$  which moves with velocity  $v$  in the rectangle with vertical side being equal to  $L + \Delta$  and horizontal side being equal to  $L - \Delta$ , where  $L, l \gg \Delta$ . The average force acting on the unit of length in the horizontal direction is expressed by:

$$P_x = \frac{mv^2}{2(L + \Delta)(L - l - \Delta)}$$

and in the vertical direction:

$$P_y = \frac{mv^2}{2(L - \Delta)(L - l + \Delta)}.$$

The shear deformation may be written as follows:

$$\varepsilon_\tau = \frac{\Delta}{L}.$$

The shear modulus can be calculated as follows:

$$\mu = \frac{P_x - P_y}{2\varepsilon_\tau} = \frac{T Ll}{2L^2(L - l)^2}.$$

Taking into account the constitutive equation governing the system, the following equation can be obtained:

$$\mu = \frac{P}{2} \left( S_0 \frac{P}{T} + 1 \right). \quad (4)$$

#### 3.2. Analysis of volume shear deformation

To calculate the volume deformation under shear conditions let us first calculate the trace of stress tensor for the deformed ‘mean-field box’. The pressure value in the deformed box is expressed as follows:

$$P_{def} = \frac{P_x + P_y}{2} = T \frac{L(L - l) - \Delta^2}{(L^2 - \Delta^2)((L - l)^2 - \Delta^2)}.$$

When returning to the extensive parameters we finally obtain:

$$P_{def} = \frac{2T}{S - S_0} \left[ \frac{1 - 2S\varepsilon_\tau^2/(S - S_0)}{1 - 4SS_0\varepsilon_\tau^2/(S - S_0)^2} \right]$$

where  $\varepsilon_\tau = \Delta/L$ .

In the case of constant pressure in the system the volume change (relative volume deformation) according to the constitutive equation can be estimated as follows:

$$\varepsilon_\gamma = \frac{\Delta S}{S} \approx \frac{S - S_0}{S} \frac{\Delta P}{P}$$

where  $\Delta P = P_{def} - P$ .

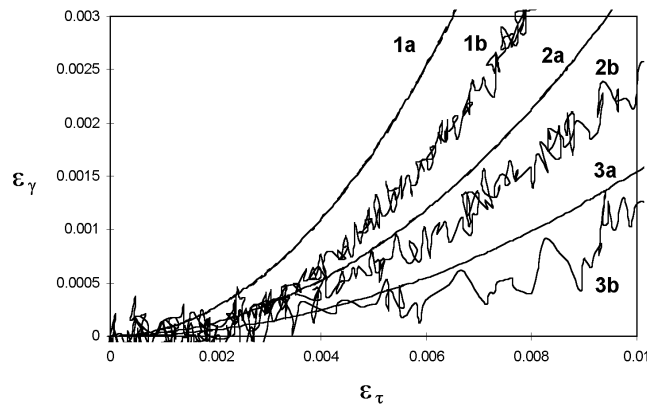
Substituting the expression for the change of average pressure we finally obtain:

$$\varepsilon_\gamma = \frac{2T}{PS} \left[ \frac{1 - 2S\varepsilon_\tau^2/(S - S_0)}{1 - 4SS_0\varepsilon_\tau^2/(S - S_0)^2} - 1 \right]. \quad (5)$$

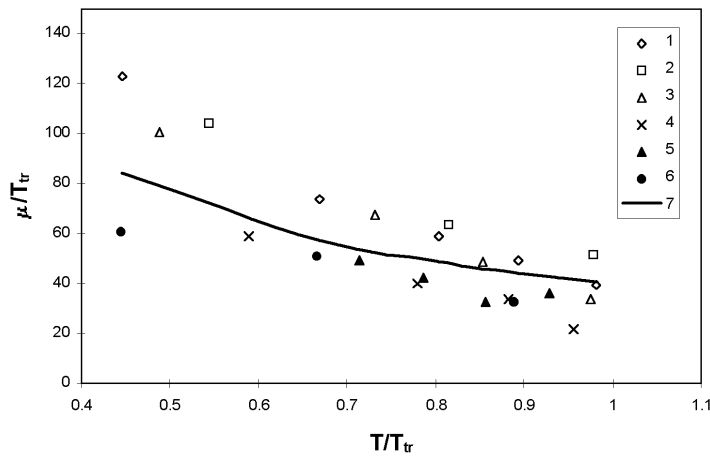
### 3.3. Numerical simulation results

All the biaxial compression diagrams at low temperatures are typical for solids (initial elastic part, maximum stress followed by its reduction). As known, the shear deformation in a solid (both elastic deformation and plastic one) is accompanied by dilation proportional to the yield stress. At high temperatures the shear deformation (flow of liquid above the transition point) takes place at constant volume. The shear modulus and yield stress for the systems of hard discs are proportional to the external pressure both for crystals and glasses. The absolute values of shear modulus and yield stress for a crystal from identical discs ( $\delta = 0$ ) are higher by a factor of four as compared to the values for glass ( $\delta = 0.5$ ). The change in mechanical properties with difference in particle size takes place in the same range where the change in packing fraction values is observed ( $0 < \delta < 0.23$ ). The constant ratio of yield stress and shear modulus values,  $P_\tau^*/\mu = 0.032 \pm 0.008$  is valid for all systems studied.

Thus the mechanism of shear resistance for the above solids is determined by the volume increase at shear, i.e. work against the external pressure and work against the attraction forces for the systems with LJ potential. The theoretical relationship between the volume and shear deformation (equation (5)) is in good accordance with the data of numerical simulations (figure 9). The comparison of the simulation data on shear modulus for a crystal of identical discs to the calculation results obtained with (equation (4)) is presented in figure 10 suggesting that the theoretical predictions are rather reliable. The behaviour of the shear modulus in glasses ( $\delta > 0.23$ ) is more complicated and will be analysed elsewhere.



**Figure 9.** Plot of volume deformation versus shear deformation in systems of hard discs,  $T/P = 0.02$  (1),  $T/P = 0.05$  (2),  $T/P = 0.1$  (3); theoretical estimations (a) and data of computer simulation as parametric dependences  $\varepsilon_\tau(P_\tau)$  and  $\varepsilon_\gamma(P_\tau)$  (b) are represented.



**Figure 10.** Plot of shear modulus  $\mu/T_{tr}$  versus relative temperature  $T/T_{tr}$  in systems of equal discs: HD,  $P = 0.2$  (1); HD,  $P = 2$  (2); HD,  $P = 5$  (3); LJ,  $P = 2$  (4); LJ,  $P = 10$  (5); LJ,  $P = 50$  (6); theoretical estimation (7).

#### 4. Conclusions

The results of molecular dynamics simulation suggest that a two-dimensional system of plane discs is the simplest system for studying basic thermodynamic and mechanical regularities which are characteristic for solids. At the same time, the theoretical system description based on very simple estimations turns to be possible. From a certain viewpoint the system of plane discs can be considered as an alternative to the quasiharmonic crystal in the region of strong anharmonism. For the system considered the simple one-particle statistical models make it possible to forecast both mechanical (shear modulus) and thermodynamic properties (temperatures of crystal–liquid and glass–liquid transitions) with tolerable accuracy.

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