

The coordination number of granular cylinders

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Abstract. – We report the first experimental measurements of the contact number distribution between randomly packed granular right cylinders (rods and disks) as a function of aspect ratio. The average coordination number $\langle z \rangle$ for cylinders varies smoothly with aspect ratio rising from $\langle z \rangle \sim 6$ for aspect ratios close to one to $\langle z \rangle \sim 10$ for large aspect ratio. Additionally, our measurements demonstrate the validity of the random contact model for compacted piles of long granular cylinders.

In any packing of granular material the *coordination* number, or number of touching neighbors per particle, is an important quantity because contacts between particles in a pile provide the necessary mechanical constraints to ensure a stable pile. Although the majority of granular studies concentrate on spheres, in Nature granular material is almost always aspherical, which motivated us to make the first measurements of the coordination number distribution, γ_z , for random packings of right cylindrical granular particles as a function of the rod length (L) to diameter (D), or *aspect* ratio, for both rods ($L/D > 1$) and disks ($L/D < 1$).

The average coordination number is $\langle z \rangle = \sum z \gamma_z$, where n_z is the number of rods with z touching neighbors and $\gamma_z = n_z / \sum n_z$ is the coordination number distribution function, or equivalently, the fraction of rods with z touching neighbors. There is broad consensus that an argument that provides upper and lower limits on $\langle z \rangle$ for both frictional and frictionless spheres based on the enumeration of the number of constraint and force equations [1–3] is correct. While conventional wisdom holds that the enumeration argument is also correct for anisotropic particles [1, 2], this belief has recently been questioned [4–6].

Here we recapitulate the enumeration argument for mechanically stable random packings of hard rods [1, 3] based on the fact that the number of equations must be less than the number of unknowns for sets of linear equations. Upper limits on $\langle z \rangle$ are obtained by noting that hard rods in contact have the constraint that at the contact point their two axes have a separation of one rod diameter. If there are N rods, then there will be $N_c = N \langle z \rangle / 2$ contacts and thus N_c constraint equations that must be satisfied. In three dimensions, each cylindrically symmetric rod requires five variables to specify its location and orientation (3 positions, 2 angles) yielding a total of $5N$ variables that specify the configurations of the rods. The number of constraint equations must be less than or equal to the number of variables, otherwise the coordinates of the rods are overdetermined. Thus $N \langle z \rangle / 2 \leq 5N$ and $\langle z \rangle \leq 10$. Lower limits on $\langle z \rangle$ are

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obtained by considering the mechanical stability condition that the sum of the forces and torques on each rod must be zero. Force balance provides three equations, but for frictionless rods there are only two torque equations per particle because with only normal forces there is no torque about the symmetry axis. Therefore there are 5 force-torque equations per particle giving $5N$ mechanical stability equations. These $5N$ equations determine the magnitude of the N_c contact forces. The number of mechanical stability equations cannot exceed the number of force variables, otherwise the forces are overdetermined. Thus $5N \leq N_c = N\langle z \rangle/2$ or $10 \leq \langle z \rangle$. The upper and lower limits on $\langle z \rangle$ are identical so for frictionless rods $\langle z \rangle = 10$.

When considering friction the number of constraints remains the same so $\langle z \rangle \leq 10$. However, the force balance equations are modified. With friction both normal and tangential forces are allowed so there are now three force and three torque equations per particle giving $6N$ mechanical stability equations. The number of force variables increases to $3N_c$ because there can be two tangential and one normal force at each contact. The number of equations must be less than the number of variables, $6N \leq 3N_c = 3N\langle z \rangle/2$, or $4 \leq \langle z \rangle$. Thus for hard frictional cylinders $4 \leq \langle z \rangle \leq 10$. The same arguments provide limits for hard frictionless spheres in d dimensions; $\langle z \rangle = 2d$, and for hard frictional spheres; $d+1 \leq \langle z \rangle \leq 2d$. While the enumeration arguments provide bounds on $\langle z \rangle$, they say nothing about how $\langle z \rangle$ of anisotropic particles varies between these bounds as a function of friction or shape.

Bernal and Mason [7] measured $\langle z \rangle = 6.4$ for a random packing of frictional spheres. Their method was to pour spheres into a container, pour paint into the container, drain the paint, allow the pile to dry and then count the number of spots on each sphere without any paint. Such spots were identified as touching neighbors. This method does not distinguish between rattlers and jammed particles. Donev *et al.* [4] employed Bernal and Mason's method on frictional oblate ellipsoids with an aspect ratio of 0.5 (M&M's Candies [8]) and measured $\langle z \rangle = 9.8$. This is the only measurement of $\langle z \rangle$ for non-spherical objects in three dimensions. Neither Bernal and Mason [7] nor Donev *et al.* [4] measured or varied friction, but their values of $\langle z \rangle$ were close to the upper limit.

In contrast to experiment, there have been several computational studies of $\langle z \rangle$ of non-spherical frictionless objects as a function of aspect ratio. Donev *et al.* [4] performed simulations of random packings of frictionless ellipsoids showing that $\langle z \rangle$ has a minimum for spheres (aspect ratio one) and increases continuously as spheres are deformed into either prolate or oblate ellipsoids from $\langle z \rangle \sim 6$ for spheres to $\langle z \rangle \sim 10$ for maximally jammed random packings of prolate or oblate ellipsoids at aspect ratios of approximately two and one-half, respectively. These results contradict the constraint and force balance arguments presented above, which predict that $\langle z \rangle$ jumps discontinuously from $\langle z \rangle = 6$ to $\langle z \rangle = 10$ when frictionless spheres are infinitesimally deformed into ellipsoids [5,6]. If the enumeration theory [1] gives too high a value for the lower limit of $\langle z \rangle$, then what is wrong with this theory? Chaikin *et al.* [5] provide an example of ellipses which are locally jammed with fewer contacts than predicted in which the contact normals are correlated such that the normals intersect. A more complete explanation is that near spheres need only $2d$ neighbors to block translations and if the radii of curvature at the point of contact are flat enough then rotations are blocked as well [6]. Thus Donev *et al.* [6] predict for prolate ellipsoids that $\langle z \rangle - 2d \propto \sqrt{L/D - 1}$. Although the lower limit on $\langle z \rangle$ given by the enumeration argument [1,5,6] is wrong for nearly spherical ellipsoids, is the lower limit also wrong for cylinders, which unlike ellipsoids do not have a spherical limit at $L/D = 1$? This question has yet to be addressed theoretically or computationally; here we treat this problem experimentally.

Simulation results for $\langle z \rangle$ of granular rods are contradictory. Some simulations find that $\langle z \rangle$ decreases as the rod aspect ratio increases [9,10], which is opposite to the simulations and theory of Donev *et al.* [4,6].

Unger *et al.* [11] recently performed simulations to measure $\langle z \rangle$ for frictional disks in 2D and found that $3 \leq \langle z \rangle \leq 4$ with increasing friction, which is consistent with theory. No such studies have been performed for non-spherical frictional particles. Parenthetically, it is often stated that shaking a granular pile of frictional particles makes them behave as if they were frictionless. This is based on the observations that granular piles compact upon shaking and by doing so $\langle z \rangle$ increases, and that for Bernal's frictional spheres, $\langle z \rangle \sim 6$, which is the frictionless limit. However, Unger's simulations demonstrate that frictional piles do not always approach the frictionless limit of $\langle z \rangle$. There is a range of friction values for which $\langle z \rangle$ equals the frictionless limit, but there is also a range of values for which $\langle z \rangle$ varies with friction.

Philipse [12] presented experimental data from compacted piles of granular cylinders showing that the product of the pile's volume fraction (ϕ) and the aspect ratio is a constant, $\phi(L/D) = 5.4$, for long, thin rods ($L/D > 15$). One consequence of this scaling is that extremely low volume fractions can be achieved experimentally ($\phi \approx 0.06$ for $L/D = 96$). Materials as diverse as spaghetti, wood, glass, metal, and plastic [13–16] show the same result implying that $\phi(L/D) = 5.4$ is insensitive to the frictional properties of the rods and the precise method of compaction. Philipse [12] argued that this scaling arises as a consequence of the excluded volume between randomly oriented rods in a pile and the assumptions of uncorrelated contacts between rods and uniform density in the pile, which make up the random contact model (RCM). The RCM predicts a relationship between ϕ , $\langle z \rangle$ and the ratio of the excluded volume between particles to the volume of a single particle, $V_{\text{ex}}/V_{\text{p}}$:

$$\phi(V_{\text{ex}}/V_{\text{p}}) = \langle z \rangle. \quad (1)$$

Onsager [17] calculated the excluded volume between two right cylinders (rc) averaged over an isotropic orientational distribution of cylinders: $V_{\text{ex}}^{\text{rc}} = (\pi D/2)[L^2 + (\pi + 3/2)LD + \pi D^2/4]$ and therefore: $(V_{\text{ex}}/V_{\text{p}})^{\text{rc}} = 2\pi + 3 + 2(L/D) + (\pi/2)D/L$. The ratio of excluded volume to particle volume in the limit of long rods ($L/D \gg 1$) is $(V_{\text{ex}}/V_{\text{p}})^{\text{rods}} \sim 2L/D$ and in the limit of thin discs ($L/D \ll 1$) this ratio becomes $(V_{\text{ex}}/V_{\text{p}})^{\text{discs}} \sim (\pi/2)D/L$. Therefore, the RCM predicts $\phi(L/D) = \langle z \rangle/2$ for long rods and $\phi(D/L) = 2\langle z \rangle/\pi$ for thin discs. In order to quantitatively test the predictions of the RCM, ϕ , $\langle z \rangle$ and L/D must be measured independently for a given granular pile.

Compaction experiments were performed to measure ϕ as a function of L/D by pouring rods into a container and then compacting the pile by vertical excitation of the container with a single period of a 50 Hz sine wave at a maximum acceleration of five times gravity. The excitation was repeated at a rate of 1 Hz until the height of the pile reached a quasi-steady state value. Cut pieces of tinned buss wire with diameters ranging from 0.25 mm to 1.4 mm were used for compaction experiments and for the coordination number experiment with $L/D = 3$. A Schleuniger RC 3250 cable cutter cut spools of round wire to make the rods. These wire pieces have $\Delta L/L = 1\%$ polydispersity in length. Each experiment was repeated three times and the volume fraction was taken to be the average of the three trials. A quasi-steady state was reached after typically 500–1000 excitations but further compaction was not systematically investigated. In our experiments the container diameter was always greater than the rod length. In this case, high aspect ratio rods form highly jammed piles in which local particle rearrangements are constrained and rods in the bulk of such piles do not rearrange when the pile is vertically vibrated. The rods in our experiments never aligned in a smectic packing as did the $L/D = 3$ rods in the experiments of Villarruel *et al.* [18], an effect caused by the narrow diameter of their container.

The evolution of the piles' volume fraction as a function of number of excitations is shown in fig. 1a. Plotted on a logarithmic scale, the volume fraction shows evidence of approaching

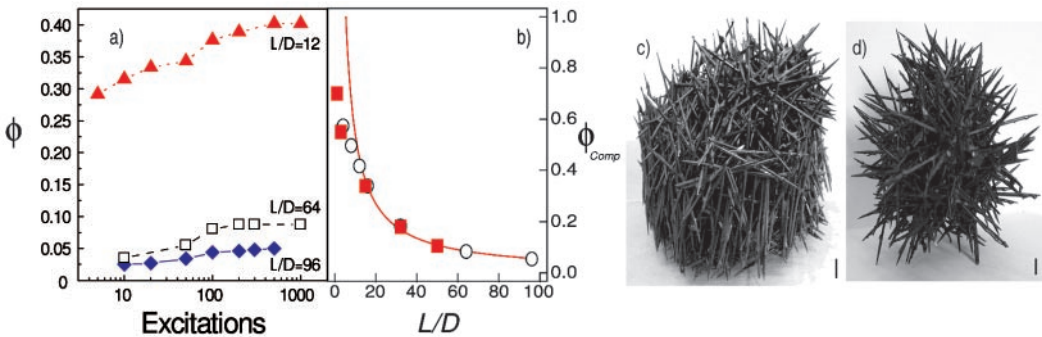


Fig. 1 – a) The volume fraction ϕ of piles of granular rods is shown as a function of the number of vertical excitations for $L/D = 12, 64$ and 96 . b) The dependence of the final, compacted volume fraction (ϕ_{comp}) as a function of L/D . The data from bulk compaction experiments are shown as open circles and the data from coordination number experiments are shown as filled squares. The solid line is $\phi(L/D) = 5.4$. c) The entire compacted pile of $L/D = 32$ rods is shown after painting, drying and removal from the container. d) The pile after the boundary rods have been removed. The scale bars indicate 1 cm.

a limiting value. The volume fraction of the compacted piles scales as $\phi_{\text{comp}}(L/D) = 5.4 \pm 0.3$ as shown in fig. 1b, which is consistent with previous results [12], and for uncompactd piles as $\phi_{\text{uncomp}}(L/D) = 4.2 \pm 0.2$ (data not shown).

In order to measure $\langle z \rangle$ for random rod packings we followed Bernal and Mason's method. Round wooden toothpicks and round bamboo skewers were used as long rods for coordination number experiments. The toothpicks measured 0.2 cm in diameter and 6.5 cm in length with pointed ends. The bamboo skewers measured 0.26 cm in diameter and were cut to 4 and 13 cm lengths to provide $L/D = 15$ and 50 rods. The measured polydispersity in the toothpicks' and skewers' length was 2% and 3%, respectively. Those particles which contacted the container walls or exposed upper surface of the pile were categorized as boundary particles and those which did not were categorized as bulk particles (figs. 1c and d). An example of a measured coordination number distribution is shown in fig. 2a.

Inspired by Donev *et al.*'s [4] choice of materials for low aspect ratio particles we employed Jujube [19] candies as $L/D = 1$ rods. Jujubes approximate the shape of right cylinders of $L/D = 1$. The polydispersity of Jujubes is $\Delta L/L = 20\%$ and $\Delta D/D = 10\%$. Aluminum disks of 1.27 cm diameter were used as rods of aspect ratio $L/D = 0.4$ with a polydispersity of 2% both in length and diameter. It must be noted that the compacted pile of disks displayed local parallel orientational ordering although the entire pile was isotropic [20]. 17% of disks aligned parallel to their neighbors in chains of 2–5 particles forming extended contacts across the circular faces of the disks. As a minimum of three points of contact are needed to constrain a plane, an extended contact between disk faces was counted as three contacts in the coordination number distribution. The fraction of chains of 2, 3, 4, and 5 disks was 0.74, 0.21, 0.03 and 0.02, respectively, showing that the vast majority of chains were made up of two or three disks. The coefficient of static friction (μ) was determined by fixing two parallel rods to a plane and laying a third rod on top of the other two with its long axis oriented perpendicular to the two fixed rods. Then the plane was tilted about a rotation axis parallel to the attached rods until the unattached rod began to slip and the coefficient of friction was determined by $\mu = \tan \theta$, with θ the tilt angle of the plane (table I).

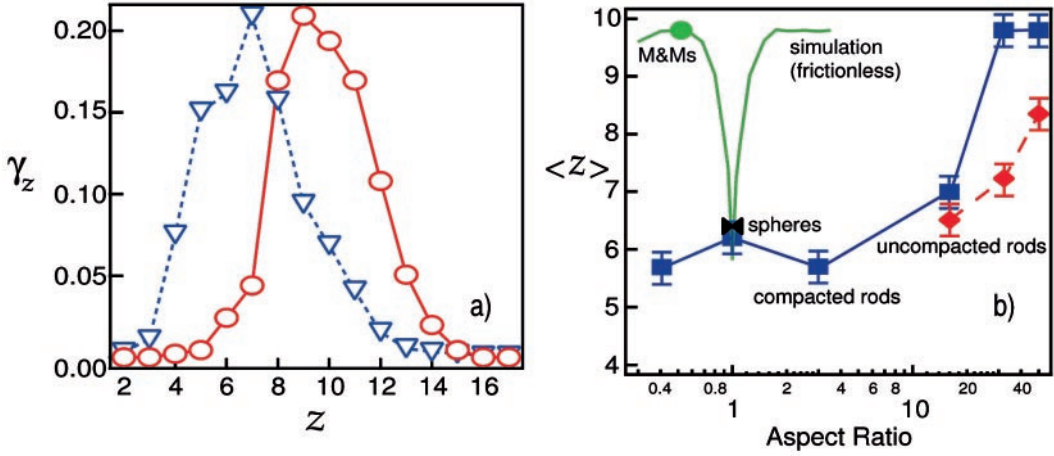


Fig. 2 – a) The coordination number distribution function of 454 bulk particles (open circles) is shown alongside the distribution for the 904 boundary particles (open triangles), for the compacted pile of $L/D = 32$ rods shown in figs. 1c and d. b) $\langle z \rangle$ is shown as a function of the aspect ratio (L/D) on a logarithmic scale. The squares represent our compacted rod piles and the diamonds our uncompacted rod piles. The bowtie represents spheres and is taken from Bernal and Mason [7]. The filled circle represents experimental data on M&M’s and the solid line without symbols represents simulations of frictionless ellipsoids, both taken from Donev *et al.* [4].

Figure 2b shows the dependence of $\langle z \rangle$ on aspect ratio for our experimental data as well as for the data on spheres [7] and on ellipsoids [4]. The average coordination number for random right cylinder packings increases as a function of aspect ratio from $\langle z \rangle \sim 6$ for disks of aspect ratio $L/D = 0.4$ to an asymptotic value of $\langle z \rangle \sim 10$ for rods of $L/D > 30$. The growth of $\langle z \rangle$ with aspect ratio is much slower for frictional rods than for frictionless ellipsoids. As shown in table I we find that $\langle z \rangle$ increases when a random packing of rods is compacted. For compacted piles of long aspect ratio rods the number of touching neighbors, $\langle z \rangle$, approaches the theoretical upper limit for frictional non-spherical particles, $\langle z \rangle = 10$. Intuitively, one expects that rods with higher friction constants should have lower coordination numbers than rods with lower friction, but no such correlation is observed. Rather, as detailed in table I,

TABLE I – The average number of touching neighbors $\langle z \rangle$ and the volume fraction of the pile occupied by rods ϕ are listed as a function of rod aspect ratio L/D . Only the bulk rods are included. The column labelled as “uncomp” corresponds to the uncompacted random rod packings whereas the column labelled as “comp” corresponds to the compacted packings. The material of the rods is listed, as well as the coefficient μ of static friction.

L/D	$\langle z \rangle \pm 0.3$		$\phi \pm 0.04$		Material	μ
	uncomp	comp	uncomp	comp		
0.4	–	5.7	–	0.56	aluminum	0.3
1	–	6.2	–	0.70	Jujubee	0.6
3	–	5.7	–	0.58	tin	0.4
15	6.5	7.0	0.26	0.34	bamboo	0.4
32	7.2	9.8	0.13	0.18	wood	0.8
50	8.3	9.8	0.08	0.10	bamboo	0.4

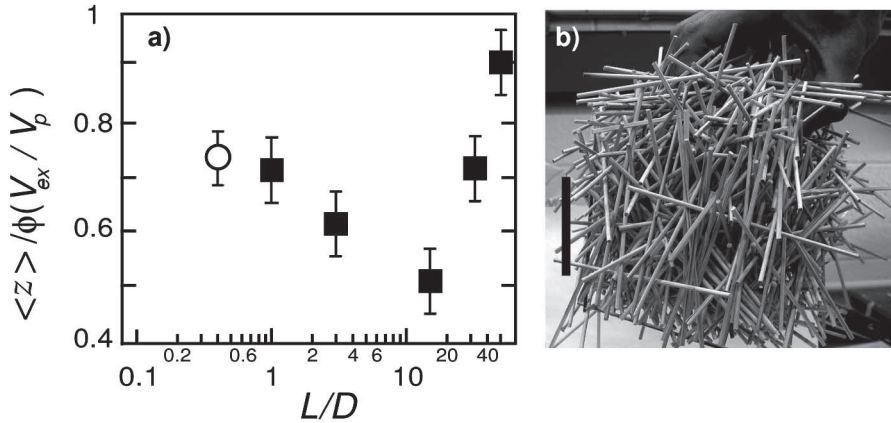


Fig. 3 – a) The RCM’s prediction for eq. (1) is shown for the data for rods (filled squares) and discs (open circle) from co-ordination number experiments as a function of L/D for compacted piles. In the long-rod limit the experimental data tend toward the RCM prediction; $\frac{\langle z \rangle}{\phi(V_{ex}/V_p)} = 1$. b) The plug forming pile of bamboo skewers of $L/D = 50$ is shown after removal from the container. The pile is supported only by the experimenter’s fingers. The scale bar at the left indicates 5 cm.

rods and disks of aspect ratio near one have low values of $\langle z \rangle$ irrespective of their coefficient of friction, while rods with the same friction coefficient have values of $\langle z \rangle$ that increase with aspect ratio. In numerical studies of the effect of friction on $\langle z \rangle$ for spheres in 2D and 3D a gradual evolution of $\langle z \rangle$ between the lower and upper limits was observed [11,21]. In the case of rods we see a new behavior; $\langle z \rangle$ varies as a function of aspect ratio and not as a function of friction, at least for the limited range of the coefficient of friction we studied.

If the geometry of granular cylinders dominates their behavior in compacted piles, then the RCM’s prediction given in eq. (1) should be valid, namely that $\frac{\langle z \rangle}{\phi(V_{ex}/V_p)} = 1$. The data from table I allow us to test this quantitative prediction. In fig. 3a the quantity $\frac{\langle z \rangle}{\phi(V_{ex}/V_p)}$ is plotted as a function of L/D for bulk particles in compacted piles and shows that the RCM limit is approached for high aspect ratio cylindrical particles. This is further evidence that particle geometry and not friction determines the structure of granular rods. The RCM assumes that contacts between rods are uncorrelated, that the excluded volume is given by the value for a pair of particles and is independent of volume fraction, and that rods are randomly oriented. Figure 3a shows deviation from the RCM scaling for short rods and disks implying that some of these assumptions break down. Qualitatively, at least, the assumption of an isotropic angular distribution of rods is borne out experimentally, but we were not able to ascertain whether or not the two other assumptions were valid.

Philipse [12] noted that random rod packings of sufficiently high aspect ratio form solid-like plugs with non-zero bulk extensional modulus. We also consistently observed plug formation for compacted piles composed of rods with $L/D > 44$ in which a plug of rods of volume $\approx L^3$ can be lifted by pulling on only one rod. We measured $\langle z \rangle = 9.8$ for the plug forming pile of bamboo skewers of $L/D = 50$ shown in fig. 3b. The data in table I show that $\langle z \rangle$ is larger for the compacted plug forming pile at $L/D = 50$ than for the uncompact pile, which did not form a solid-like plug. However, this same value of $\langle z \rangle = 9.8$ was also observed for compacted piles that did not form plugs; the rods with $L/D = 32$, as well as the M&M’s with aspect ratio of 0.5 [4]. These observations prove that a high value of $\langle z \rangle$ alone is not sufficient for

plug formation. The mechanism leading to plug formation of granular rods remains unknown, but probably friction and flexibility of the cylinders are important physical variables.

In conclusion, we measured the average coordination number $\langle z \rangle$ for piles of granular cylinders. $\langle z \rangle$ increases gradually with aspect ratio for frictional cylinders ranging from $\langle z \rangle \sim 6$ for $L/D \sim 1$ to $\langle z \rangle \sim 10$ in the large aspect ratio limit, $L/D \geq 30$. $\langle z \rangle$ is not sensitive to friction for the range of values studied. The measured limits, $6 \leq \langle z \rangle \leq 10$, are consistent with theoretical bounds, but the discovery that $\langle z \rangle$ varies with aspect ratio, independent of friction, was previously unsuspected. Notably, the lower limit on $\langle z \rangle$ was observed to be six, rather than four, which is the theoretical lower limit. Is the experimentally observed value of $\langle z \rangle = 6$ for spheres and cylinders of $L/D \sim 1$ a co-incidence or the indication of an unknown connection between these symmetry unrelated particles? Follow-up experiments and simulations would be to determine the aspect ratio dependence of $\langle z \rangle$ as a function of the coefficient of friction over a wider range of values than in our studies and to study other shaped particles, such as ellipsoids. Finally, independent measurements of the volume fraction for these random rod packings coupled with measurements of the coordination number show that the random contact model is within a factor of two of experiment, and that theory and experiment approach each other in the long-rod limit.

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REFERENCES

- [1] ALEXANDER S., *Phys. Rep.*, **296** (1998) 65.
- [2] EDWARDS S. F. and GRINEV D. V., *Phys. Rev. Lett.*, **82** (1999) 5397.
- [3] TKACHENKO A. V. and WITTEN T. A., *Phys. Rev. E*, **60** (1999) 687.
- [4] DONEV A. *et al.*, *Science*, **303** (2004) 990.
- [5] CHAIKIN P. M. *et al.*, *Industrial & Engineering Chemistry Research* (web release: July, 2006) 10.1021/ie060032g.
- [6] DONEV A. *et al.*, <http://lanl.arxiv.org/> (2006) cond-mat/0608334.
- [7] BERNAL J. D. and MASON J., *Nature*, **188** (1960) 910.
- [8] M&M's Candies are a registered trademark of Mars Inc.
- [9] STOKELY K., DIACOU A. and FRANKLIN S. V., *Phys. Rev. E*, **67** (2003) 051302.
- [10] WILLIAMS S. R. and PHILIPSE A. P., *Phys. Rev. E*, **67** (2003) 051301.
- [11] UNGER T., KERTESZ J. and WOLF D. E., *Phys. Rev. Lett.*, **94** (2005) 178001.
- [12] PHILIPSE A. P., *Langmuir*, **12** (1996) 1127.
- [13] MILEWSKI J. V. and KATZ H. S. (Editors), *Handbook of Fillers and Reinforcements for Plastics* (Van Nostrand Reinhold) 1978, pp. 66-78.
- [14] NARDIN M., PAPIRER E. and SCHULTZ J., *Powder Technol.*, **4** (1985) 131.
- [15] PARKHOUSE J. G. and KELLY A., *Proc. R. Soc. London, Ser. A*, **454** (1998) 1889.
- [16] NOVELLANI M., SANTINI R. and TADRIST L., *Eur. Phys. J. B*, **13** (2000) 571.
- [17] ONSAGER L., *Ann. N.Y. Acad. Sci.*, **51** (1949) 627.
- [18] VILLARRUEL F. X. *et al.*, *Phys. Rev. E*, **61** (2000) 6914.
- [19] Jujubes are a registered trademark of The Hershey Company.
- [20] VEERMAN J. A. C. and FRENKEL D., *Phys. Rev. A*, **45** (1992) 5632.
- [21] SILBERT L. E. *et al.*, *Phys. Rev. E*, **65** (2002) 031304.