Philosophical Magazine,
Vol. 87, Nos. 3–5, 21 January–11 February 2007, 425–431

Taylor & Francis
Taylor & Francis Group

Enumeration of distinct mechanically stable disk packings in small systems

G.-J. GAO†, J. BLAWZDZIEWICZ†, and C. S. O'HERN*†‡

†Department of Mechanical Engineering, Yale University,
New Haven, CT 06520-8286
‡Department of Physics, Yale University, New Haven,
CT 06520-8120

(*Received 2 May 2006; in final form 29 May 2006*)

We create mechanically stable (MS) packings of bidisperse disks using an algorithm in which we successively grow or shrink soft repulsive disks followed by energy minimization until the overlaps are vanishingly small. We focus on small systems because this enables us to enumerate nearly all distinct MS packings. We measure the probability of obtaining an MS packing at packing fraction ϕ and find several notable results. Firstly, the probability is highly non-uniform. When averaged over narrow packing fraction intervals, the most probable MS packing occurs at the highest ϕ and the probability decays exponentially with decreasing ϕ. Even more striking, within each packing-fraction interval, the probability can vary by many orders of magnitude. By using two different packing-generation protocols, we show that these results are robust and the packing frequencies do not change qualitatively with different protocols.

1. Introduction

Inherent structures or potential energy minima are important for determining the mechanical and dynamical properties of supercooled liquids and glasses [1]. Recently, a host of computational studies have attempted to relate thermodynamic quantities in supercooled liquids to the number of inherent structures and vibrational motions about them [2–4]. It is often assumed in these calculations that all inherent structures at a given energy are equally probable. Similarly, statistical descriptions of granular media assume that all stable particle packings at a particular volume are equally likely [5, 6]. Thus, it is important to examine under what conditions and to what extent inherent structures in glassy systems and jammed packings of granular materials are equally probable. In this short article, we begin to address this question by enumerating nearly all mechanically stable (MS) packings in small two-dimensional bidisperse systems.

An innovative feature of this work and our other recent study [7] is that we focus on systems containing small numbers of disks. We note that related studies of small hard disk systems have been carried out previously, but these have not investigated the

*Corresponding author. Email: corey.ohern@yale.edu

Philosophical Magazine
ISSN 1478–6435 print/ISSN 1478–6443 online
http://www.tandf.co.uk/journals
DOI: 10.1080/14786430600851760

MS packing probabilities [8, 9]. We confine our studies to small two-dimensional systems for two key reasons. Firstly, we are able to generate nearly all of the mechanically stable disk packings in these systems. The number of MS disk packings grows exponentially with the number of particles N, but is finite for any finite N. In small systems, we are able to accurately determine the probability with which each MS packing occurs. In contrast, in large systems, only the most frequent MS packings are found. Secondly, we believe that understanding small jammed systems is crucial to developing a theoretical explanation for slow stress and structural relaxation in large glassy and amorphous systems [10]. Our view of the relationship between jamming in small systems and glassy behaviour in large systems will be more fully developed in a future publication.

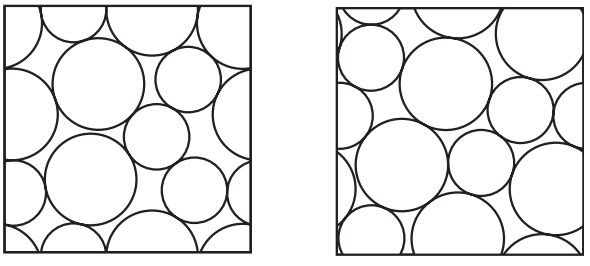
We discuss several important results below. Firstly, we find that the frequency with which mechanically stable packings occur is not uniform; instead it can vary by many orders of magnitude over the range of packing fractions where MS packings exist. This large variation in frequency occurs even though we do not target specific packings. Moreover, MS packings can have frequencies that differ by many orders of magnitude even over narrow packing-fraction intervals and there are no striking structural differences between rare and frequent MS packings at similar ϕ as shown in figure 1. Thus, it is not immediately obvious what variables set the frequency of MS packings. Also, we show below that even when we significantly alter the protocol used to generate the MS packings, the most frequent packings remain frequent and the rare ones remain rare. Thus, we suggest that although it is clear that the particular protocol chosen to generate the MS packings plays some role in determining the frequency distribution of MS packings [11], prominent geometrical features of the configuration space can also strongly influence the frequency distribution.

2. Simulation methods

2.1. *Generation of mechanically stable packings*

We study mechanically stable packings of $N = 10$ disks that interact via the finite-range, pairwise additive, purely repulsive spring potential

$$V(r_{ij}) = \frac{\epsilon}{2}(1 - r_{ij}/\sigma_{ij})^2 \Theta(\sigma_{ij}/r_{ij} - 1). \tag{1}$$



(a) (b)

Figure 1. Snapshot of (a) a MS packing at $\phi \approx 0.82$ and (b) another MS packing $\phi \approx 0.83$ that is 10^6 times more frequent.

Here ϵ is the characteristic energy scale, r_{ij} is the separation between particles i and j, $\sigma_{ij} = (\sigma_i + \sigma_j)/2$ is their average diameter, and $\Theta(x)$ is the Heaviside step function. We study 50–50 binary mixtures of particles with diameter ratio 1.4 to inhibit crystallization [7, 12–14]. The particles have equal mass m and are confined to a square unit cell with periodic boundary conditions. We chose the small particle diameter σ and $\sigma\sqrt{m/\epsilon}$ as the reference length and time scales.

Our focus is on configurations that are at a potential energy minimum with infinitesimal overlaps. Since these configurations are in mechanical equilibrium and possess vanishingly small overlaps, we term them mechanically stable (MS) packings. MS packings with no overlaps are equivalent to collectively jammed states [15] of hard disks.

We employ a class of packing-generation protocols that involve successive compression or decompression steps followed by energy minimization [7, 16, 17]. The process is initiated by choosing random initial positions for the particles at packing fraction $\phi = 0.60$, which is well below the minimum packing fraction at which MS packings occur in two dimensions. The system is decompressed when the potential energy of the system at a local minimum is non-zero; otherwise, the system is compressed. The increment by which the particle packing fraction is changed at each compression or decompression step is gradually decreased. After a sufficiently large number of steps, an MS packing with infinitesimal overlaps is obtained. This process is performed for a large number of independent starting conditions to generate an ensemble of MS packings. In this way, we can measure the probability of obtaining an MS packing at a given ϕ.

We employ two energy-minimization methods: (a) conjugate-gradient (CG) minimization algorithm or (b) molecular dynamics (MD) with dissipation proportional to local velocity differences. The conjugate-gradient method is a numerical scheme that begins at a given point in configuration space and moves the system to the nearest local potential energy minimum without traversing any energy barriers [18]. In contrast, molecular dynamics with finite damping is not guaranteed to find the nearest local potential energy minimum since kinetic energy is removed from the system at a finite rate. The system can thus surmount a sufficiently low energy barrier. In the molecular dynamics method, each particle i obeys Newton's equations of motion

$$m\vec{a}_i = \sum_{j \neq i} \Theta(\sigma_{ij}/r_{ij} - 1)\left[\frac{\epsilon}{\sigma_{ij}}\left(1 - \frac{r_{ij}}{\sigma_{ij}}\right) - b\vec{v}_{ij} \cdot \hat{r}_{ij}\right]\hat{r}_{ij}, \tag{2}$$

where $\vec{a}_i$ is the acceleration of particle i, $\vec{v}_{ij}$ is the relative velocity of particles i and j, $\hat{r}_{ij}$ is the unit vector connecting the centres of these particles, and $b = 0.5$ is the damping coefficient. Note that in our previous studies [7, 13, 14] we used only the CG method.

2.2. *Classification of mechanically stable packings*

In our numerical simulations we distinguish distinct mechanically stable disk packings by the lists of eigenvalues of their dynamical matrices. For a pairwise additive,

rotationally invariant potential (1) the dynamical matrix is given by the expressions [19]

$$M_{i\alpha,j\beta} = -\frac{t_{ij}}{r_{ij}}\left(\delta_{\alpha\beta} - \hat{r}_{ij\alpha}\hat{r}_{ij\beta}\right) - c_{ij}\hat{r}_{ij\alpha}\hat{r}_{ij\beta}, \quad i \neq j, \tag{3}$$

and

$$M_{i\alpha,i\beta} = -\sum_{j\neq i} M_{i\alpha,j\beta}, \tag{4}$$

where $t_{ij} = \partial V/\partial r_{ij}$ and $c_{ij} = \partial^2 V/\partial r_{ij}^2$. In the above relations, the indices i and j refer to the particles, and $\alpha, \beta = x, y$ represent the Cartesian coordinates. For a system with N_f rattlers and $N' = N - N_f$ particles forming a connected network the indices i and j range from 1 to N', because the rattlers do not contribute to the potential energy.

The dynamical matrix is symmetric and has dN' rows and columns, where $d = 2$ is the spatial dimension. Thus it has dN' real eigenvalues $\{m_i\}$, d of which are zero due to translational invariance of the system. In an MS disk packing, no set of particle displacements is possible without creating an overlapping configuration; therefore the dynamical matrix has exactly $d(N' - 1)$ non-zero eigenvalues. In our simulations we use the criterion $|m_i| > m_{\min} = 10^{-6}$ for non-zero eigenvalues.

We consider two MS packings to be the same if they have the same list of eigenvalues of the dynamical matrix. The eigenvalues are considered to be equal if they differ by less than the noise threshold $m_{\min}$ for our calculations. Using the CG and MD methods, we have identified ≈ 1600 distinct MS packings for systems with 10 particles. Packings with rattlers have been included in this count.

It is generally not true that each distinct MS packing possesses a unique packing fraction ϕ. However, we find that for these systems only at most a few percent of distinct MS packings share the same packing fraction. Thus, in the following we will associate a unique ϕ with each MS packing to simplify the discussion.

3. Results

The principal result of this work is that the frequency with which MS packings occur can vary dramatically, by many orders of magnitude from one packing to another. In figure 2, we show the probability $P(\phi) = n(\phi)/N_t$ to obtain a given MS packing at ϕ for the MD energy minimization method. $n(\phi)$ is the number of MS packings obtained at ϕ out of N_t trials performed. For $N = 10$, we ran more than 30×10^6 trials for both energy minimization methods and obtained results that do not depend on N_t.

We notice several interesting features in figure 2. Firstly, the probability distribution is not uniform. The most probable MS packings occur at large $\phi \approx 0.83$ and the least probable occur for $\phi < 0.75$. When averaged over narrow packing-fraction intervals, the probability distribution decays exponentially with decreasing ϕ [7]. Even more striking, the probability is not monotonic in packing fraction and is in fact noisy and difficult to predict. In the inset to figure 2, we find that even over a

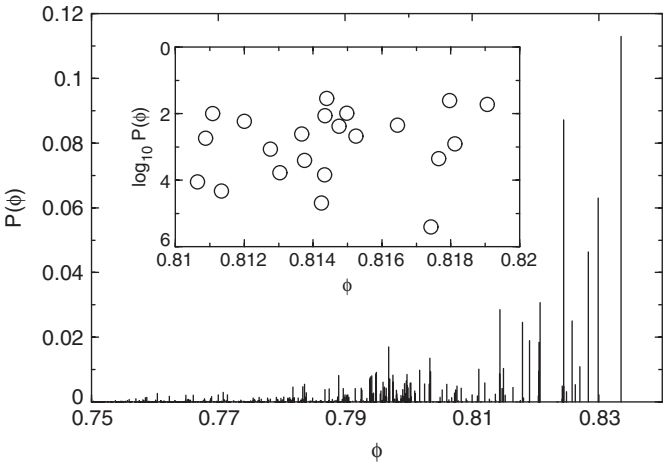


Figure 2. The probability of obtaining an MS packing at packing fraction ϕ for $N = 10$ particles using the MD method. The inset shows a magnified view of the probability on a logarithmic scale over a narrow packing-fraction interval between 0.81 and 0.82.

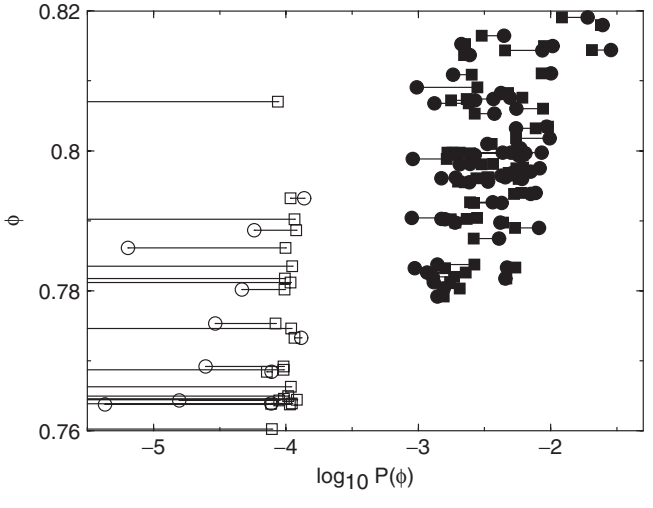


Figure 3. The probabilities for the most frequent MS packings obtained from the CG packing-generation algorithm (filled squares) are compared to the probabilities for the same MS packings obtained from the MD method (filled circles). A similar comparison of less frequent MS packings obtained from the CG (open squares) and MD (open circles) methods is also shown.

narrow range $\Delta\phi$, the probability varies by more than five orders of magnitude, and this occurs over the entire range of ϕ.

To understand the influence of the packing-generation protocol on our results, we have examined the probabilities for obtaining each MS packing using two energy

minimization methods. We compared the 100 most frequent MS packings obtained from the CG method to the 100 most frequent packings from the MD method. We find that $\sim$80% of the MS packings were common to both sets; these are shown as filled symbols in figure 3. A similar comparison of probabilities for obtaining less frequent MS packings using the MD and CG methods is also displayed (using open symbols) in figure 3. We make several important observations. Firstly, significant shuffling of frequent and rare packings does not occur – frequent packings remain frequent and rare ones remain rare. Secondly, within each probability grouping (i.e. filled versus open symbols) the more frequent MS packings in the CG method become more frequent in the MD method, while the less frequent packings from the CG method become more rare in the MD method. Although these results were obtained for small systems, we expect similar findings for large systems.

The result that frequent packings become more frequent and rare ones become more rare when switching from CG to MD energy minimization can be explained in part by considering the rate at which energy is dissipated in the system. The MD energy minimization method utilizes a finite rate of energy dissipation. Thus, at various points during the packing generation process, the system can in principle possess enough kinetic energy to jump out of a shallow basin corresponding to a rare MS packing and into the basin of a more frequent packing. This suggests that understanding the topography of configuration space surrounding MS packings is crucial to understanding the frequency of MS packings.

Also, the result that frequent MS packings remain frequent and rare ones remain rare when switching from the MD to CG methods implies that geometrical features of configuration space strongly influence the frequency of MS packings. Correlations between the frequency with which MS packings occur and the shape and volume of basins near each MS packing is a topic of our current investigations.

4. Conclusion

We have enumerated nearly all of the distinct MS in small systems composed of 50–50 mixtures of bidisperse disks. This has allowed us to accurately measure the probability of obtaining each MS packing. We find that the probability is not uniform – packings with large ϕ are exponentially more likely than those at low ϕ. Moreover, even over narrow packing-fraction intervals, distinct MS packings occur with frequencies that differ by many orders of magnitude. We have varied the packing-generation protocol and shown that these results do not change qualitatively, which suggests that geometrical features of configuration space strongly influence the packing frequencies. These results suggest that further work should be carried out to explicitly test the Edwards assumption that stable grain packings are equally probable and similar assumptions about inherent structures. Another intriguing possibility is that only the most frequent MS packings are relevant for slow dynamics in glassy and jammed systems. However, even if this were true, we must first understand what determines MS packing frequencies in order to identify correctly the relevant set of frequent MS packings.

Acknowledgements

Financial support from NSF grant numbers CTS-0348175 (GG,JB), DMR-0448838 (GG,CSO), and CTS-0456703 (CSO) is gratefully acknowledged. We also thank Yale's High Performance Computing Center for generous amounts of computer time.

References

[1] F.H. Stillinger, Science **267** 1935 (1995).
[2] M.S. Shell and P.G. Debenedetti, Phys. Rev. E **69** 051102 (2004).
[3] E. LaNave, S. Mossa and F. Sciortino, Phys. Rev. Lett. **88** 225701 (2002).
[4] M.S. Shell and P.G. Debenedetti, J. Phys. Chem. B **108** 6772 (2004).
[5] S.F. Edwards and R.B.S. Oakeshott, Physica A **157** 1080 (1989).
[6] H.A. Makse and J. Kurchan, Nature **415** 614 (2002).
[7] N. Xu, J. Blawzdziewicz and C.S. O'Hern, Phys. Rev. E **71** 061306 (2005).
[8] R.K. Bowles and R.J. Speedy, Physica A **262** 76 (1999).
[9] R.K. Bowles and I. Saika-Voivod, Phys. Rev. E **73** 011503 (2006).
[10] G. Adam and J.H. Gibbs, J. Chem. Phys. **43** 139 (1965).
[11] S. Torquato, T.M. Truskett and P.G. Debenedetti, Phys. Rev. Lett. **84** 2064 (2000).
[12] R.J. Speedy, J. Chem. Phys. **110** 4559 (1999).
[13] C.S. O'Hern, S.A. Langer, A.J. Liu *et al*., Phys. Rev. Lett. **88** 075507 (2002).
[14] C.S. O'Hern, L.E. Silbert, A.J. Liu *et al*., Phys. Rev. E **68** 011306 (2003).
[15] S. Torquato and F.H. Stillinger, J. Phys. Chem. B **105** 11849 (2001).
[16] H.A. Makse, D.L. Johnson and L.M. Schwartz, Phys. Rev. Lett. **84** 4160 (2000).
[17] H.P. Zhang and H.A. Makse, Phys. Rev. E **72** 011301 (2005).
[18] W.H. Press, B.P. Flannery, S.A. Teukolsky *et al*., *Numerical Recipes in Fortran 77* (Cambridge University Press, New York, 1986).
[19] A. Tanguy, J.P. Wittmer, F. Leonforte *et al*., Phys. Rev. B **66** 174205 (2002).