Comparison of random configurations of equal disks

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For a variety of "random configurations" of equal disks, the probability distributions of the Voronoi-cell areas are obtained from a computer simulation and a comparison is made in terms of the relation between the regularity of the cell areas and the mean bulk fraction of the area occupied by the disks.

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I. INTRODUCTION

Random assemblies of equal spheres have been playing important roles as simplified fundamental models for a variety of physical systems. In two dimensions, for example, the irreversible adsorption of objects on a surface [1,2] is modeled by random sequential adsorption (RSA). The growth of clusters from metal vapor deposited on amorphous carbon substrates [3] is studied by Monte Carlo simulation. Despite the variety of "random configurations," they have not been compared with each other, so that what "randomness" means is that they remain unknown. To provide a clue, the difference in microstructure of "random configurations" of equal disks is elucidated in this paper.

II. VORONOI STATISTICS

One of the tools in characterizing the geometry of a random disk packing is the statistical distributions of network quantities that may be derived from the different networks possible to be constructed from the positions of the disk centers. The most well known is the Voronoi tessellation: A central disk is supposed to be connected with its neighbors. Each line joining the central disk to its neighbors is bisected by a line; the most inner area enclosed by these lines is the Voronoi polygon. By definition, each polygon or cell contains only one disk. The regularity of cell area r is defined as follows:

$$r=(\langle a\rangle/s)^2,\quad s^2=\langle(a-\langle a\rangle)^2\rangle\ , \tag{1}$$

where a is the cell area and $\langle\ \rangle$ denotes the average. Using the probability distribution function $P(x)$, it becomes

$$r=1/\int_0^\infty (x-1)^2P(x)dx\ ,$$

where $x=a/\langle a\rangle$ and $P(x)$ is normalized. For a Voronoi tessellation defined from completely random points, the Γ distribution was earlier found to fit $P(x)$ [3,4]:

$$P(x)dx=r^rx^{r-1}e^{-rx}dx/\Gamma(r)\ . \tag{2}$$

Γ is the gamma function and the shape of the distribution is determined only by the single parameter r. In what follows, a variety of "random configurations" of equal disks are compared with each other through a relationship between the regularity r and the coverage y or the mean bulk fraction of the area occupied by disks.

A summary of algorithms for generating "random configurations" is listed in Table I. The random-sequential-adsorption model [5–7] was constructed in a square of side 40 in units of the disk diameter. The coverage was $y=0.542$ at the jammed stage, being close to the limit $y=0.5472$ by Hinrichsen, Feder, and Jøssang [8]. For each RSA configuration the Voronoi tessellation was conducted to obtain the regularity of cell areas. The r-versus-y relations are plotted by cross marks in Fig. 1. It is interesting to note that the r increases with increasing y and reaches a saturation point at the limiting coverage $y=0.5472$. The saturation means that the RSA procedure is not able to make the configuration denser.

To make it denser, a RSA configuration was compacted [4] as explained in Table I(b). From the Voronoi tessellation for every iteration of compaction, the r-versus-y relation is obtained as shown by circles in Fig. 1. The dotted line is estimated from the data of Hinrichsen, Feder, and Jøssang [8]. They reported that the coverage reached $y=0.7643$ after 1000 iterations of compaction and its limiting value was $y=0.772$.

Bennett [9] studied the geometry of serially deposited amorphous aggregates. Following his simulation procedure in Table I(c), a random aggregate of 1050 disks was constructed in a computer. The packing fractions were $y=0.839$ and 0.823, respectively, for inner 86 and outer 200 disks of the aggregate. Owing to the finite-size effect, it is a little higher than Berryman's prediction [10], $y=0.82$, for the dense random packing in two dimensions. The Voronoi tessellation for the aggregate yields the r-versus-y relation as depicted by curve c in Fig. 1.

The Monte Carlo simulation [11] outlined in Table I(d) also yields "random configurations," whose Voronoi-statistics study [12] gives the r-versus-y relation as plotted by triangles in Fig. 1. The probability distribution function of cell areas reported in Ref. [3] gives $r=3.57$ at $y=0$, in agreement with the result of the RSA configuration.

Finally, two regular packings with random vacancies explained in Table I(e) and I(f) were constructed for comparison with the configurations mentioned above. The Voronoi tessellation gives the regularity in relation to the coverage as depicted by curves e and f in Fig. 1.

TABLE I. Algorithms for generating random configurations of equal disks.

(a) Random-sequential-adsorption (RSA) model

Equal disks are placed at random in a square with periodic boundary conditions. If the last placed disk overlaps any other ones, it is removed at once. Once a disk has been placed, its position is permanently fixed. When no more disks can be placed without overlapping those already present, the jamming limit has been reached and the process stops.

(b) Random dense packings

Starting with the RSA configuration, the surface is "contracted" homogeneously [4]. One iteration step of the contraction procedure is as follows: First, a Voronoi polygon is constructed around every disk. Each disk center is then moved to the center of the largest inscribed circle in the respective polygons. Then all the disk radii are increased by the same amount until the first disk pair is in contact.

(c) Amorphous aggregate

Emerging from a direction randomly determined, a new disk approaches an initial seed and settles at a stable position after rolling down on disks already in place.

(d) Monte Carlo simulation

n points are placed in a square box using randomly generated coordinates. The Voronoi tessellation is constructed for this configuration, with periodic boundary conditions, and the hard-disk diameter is set equal to the minimum nearest-neighbor distance. A configuration with a higher packing fraction is obtained by compressing a low-packing-fraction configuration. The compression is achieved using the Monte Carlo algorithm with a high applied pressure. The Monte Carlo method allows the disks to move within the system while the high applied pressure gradually squeezes out the free area.

(e) Loosest packing with random vacancies

The prescribed number of disks are eliminated randomly from the regular square packing ($y=0.785$).

(f) Closest packing with random vacancies

The prescribed number of disks are eliminated randomly from the regular closest packing ($y=0.907$).

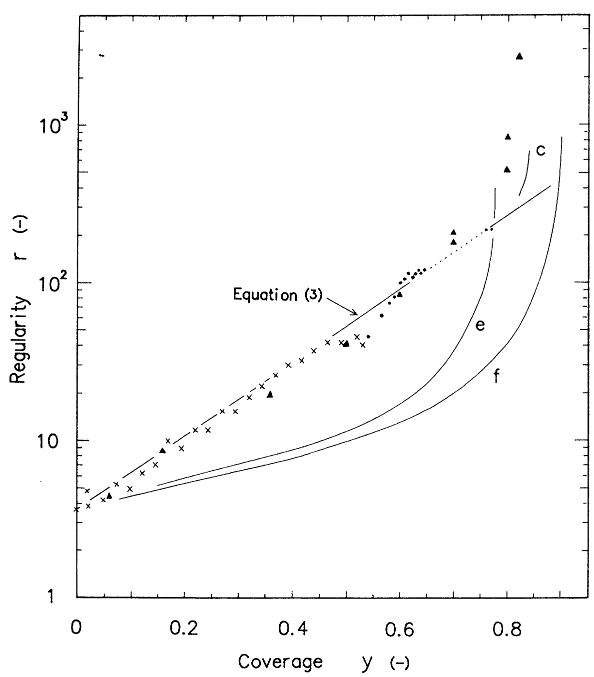

FIG. 1. Regularity r in relation to coverage y. ×, a; ● and $\cdots$, b; ▲, d. Letters a–f correspond to random configurations in Table I.

III. CONCLUDING REMARKS

A variety of "random configurations" of equal disks, as listed in Table I, have been compared with each other in terms of the probability distribution of the Voronoi-cell areas. Figure 1 shows the regularity r in relation to the coverage y. The random sequential adsorption and its compaction model lead to a straight line in Fig. 1, which is expressed by

$$r=3.6\exp(5.4y) . \quad (3)$$

This is a new relation expressing the behavior of the regularity. The limiting value $r=3.6$ at $y=0$ is set equal to the theoretical result $r=2\pi/\sqrt{3}$ explained by Weaire, Kermode, and Wejchert [4]. Two saturation points exist in the regularity r at $y=0.5472$ for the RSA model and $y=0.772$ for the random loose packing [8]. Consider a point lying on the curve, Eq. (3). If we make the corresponding particle assembly partially ordered, the point will move upward from the curve, while if we remove some disks from the assembly, it will move downward. Although existence of the region $y>0.772$ remains unknown, Eq. (3) may stand for the most random configuration for fixed y. In the region higher than Eq. (3), ordered arrangements are apt to exist locally in the configuration, while in the region lower than Eq. (3), empty holes are apt to exist in the configuration.

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