Symmetry, shape, and order

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Packing problems have been of great interest in many diverse contexts for many centuries. The optimal packing of identical objects has been often invoked to understand the nature of low-temperature phases of matter. In celebrated work, Kepler conjectured that the densest packing of spheres is realized by stacking variants of the face-centered-cubic lattice and has a packing fraction of \(\pi/(3\sqrt{2}) = 0.7405\). Much more recently, an unusually high-density packing of \(\approx 0.770732\) was achieved for congruent ellipsoids. Such studies are relevant for understanding the packing of glasses, the storage and jamming of granular materials, and the assembly of viral capsid structures. Here, we carry out analytical studies of the stacking of close-packed planar layers of systems made up of truncated cones possessing uniaxial symmetry. We present examples of high-density packing whose order is characterized by a broken symmetry arising from the shape of the constituent objects. We find a biaxial arrangement of solid cones with a packing fraction of \(\pi/4\).

For truncated cones, there are two distinct regimes, characterized by different packing arrangements, depending on the ratio \(c\) of the base radii of the truncated cones with a transition at \(c^* = \sqrt{2} - 1\).

## Results and Discussion

### Cone Packing

There are three natural close-packed geometries (Fig. 1) of a pair of cones. The space-filling arrangements of the cones shown in Fig. 1 \(d\) and \(e\) are effectively two-dimensional with biaxial order arising from the breaking of the uniaxial symmetry of the cone to achieve close packing.\(^{10}\) A collection of bicones (Fig. 1 \(d\) and \(e\)) or hourglasses (Fig. 1\(d\)) can also exhibit biaxial order. There are other high-density arrangements of cones obtained by first assembling them into basic units and densely packing these units. Fig. 1 \(f\) and \(g\) depicts a helical assembly. Fig. 2 shows a stack of planes with cones arranged as in Fig. 1\(d\).

We will assume that the cones have flat bases with the opening angle \(\alpha\) at their apex and the slant height \(L\). In micelles (20), the solvent induces a tip-to-tip attraction between the cones. Here, we consider the role of base-to-base stacking in facilitating planar packing. The cone volume is given by \(V_{cone} = \pi L^3 \sin(\alpha)\sin(\alpha/2)/6\). For the stack of planes shown in Fig. 2, the volume of a elementary cell is equal to

\[
V_{cell}^{pl} = h d s = \frac{2}{3} L^3 \sin(\alpha) \sin\left(\frac{\alpha}{2}\right),
\]

where \(h, d,\) and \(s\) are the dimensions of the cell as described in Fig. 2. Thus, the packing fraction of the cones in this case is equal to

\[
F = \frac{V_{cone}}{V_{cell}^{pl}} = \frac{\pi}{4},
\]

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2\(^{10}\)The arrangement of discrete cylinders stacked in an Abrikosov lattice is not isotropic in the plane perpendicular to the cylinder axis—rather, it is invariant under discrete rotations (by integer multiples of \(\pi/3\)) with three equivalent directions. We will, anyhow, denote as uniaxial arrangements possessing at least two equivalent directions within the plane perpendicular to the symmetry axis. Biaxial order is one in which a privileged direction exists in that plane so that the only residual symmetry is the invariance under rotations by \(\pi/5\). This broken symmetry arises from the shape of the constituent objects, even though they are uniaxial.

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which is independent of $\alpha$.

Interestingly, there is an infinite degeneracy in the close-packing arrangements of cones stacked in planar layers as in Fig. 2b, due to the possibility of choosing between positive and negative shifts each time a new layer is added to the stack. This is reminiscent of the two-fold stacking choice made at each hexagonal layer in the random hexagonal close packed structure of spheres leading to the stacking variants of the face-centered-cubic lattice that share Kepler’s optimal packing fraction (0.7405) (5). Remarkably, the packing fraction of identical cones, $F \approx 0.78539$, is higher than the latter, in accord with the suggestion that spheres cannot be packed as efficiently as other convex objects (19). The packing fraction of cones is also higher than the maximum packing fraction recently found for dense crystal packing of ellipsoids (0.770752) (11).

It is interesting to compare the packing fraction of this biaxial arrangement with the common assemblies of amphiphile nanoparticles (20): the spherical micelles in a face-centered-cubic lattice arrangement and the hexagonal arrangement of cylindrical micelles. Note that a definitive proof of the most tightly packed arrangement is highly nontrivial. For the simpler case of the packing of spheres, Kepler’s conjecture was finally proved only within the last decade (7). For a spherical micelle, as shown by Tsonchev et al. (20), the number of cones in each sphere is given by $N_s = \lfloor \frac{2\pi}{\sqrt{3}} \rfloor$, where $\lfloor x \rfloor$ denotes the integer part of $x$ and $\gamma = \arccos(\cos(\alpha)/(2 \cos^2(\alpha/2)))$ for small enough $\alpha$ such that the cones (or cone bases) form a hexagonal arrangement in the sphere surface. This assumption is certainly valid when $\alpha \leq \pi/3$ ($N_s = 11$ for $\alpha = \pi/3$), $N_s = 3$ for $\alpha \to 2\pi/3$ from below and equal to 2 for $\alpha$ larger than $2\pi/3$. The packing fraction of spheres in a face-centered-cubic lattice arrangement is $\pi/(3\sqrt{2})$ (5). One therefore finds that the packing fraction of cones in spherical micelles is given by

$$F_{\text{sph}} = \frac{\pi}{24\sqrt{2}} \sin(\alpha) \sin\left(\frac{\alpha}{2}\right) N_s.$$  [3]

For a cylindrical micelle, the number of cones in an elementary cell, defined as a cylinder section of thickness $L \sin(\alpha/2)\sqrt{3}$ (20), is $N_c = [2\pi/\alpha]$, and the volume of such an elementary cell is $V_{\text{cell}} = \pi L^2 \sin(\alpha/2)\sqrt{3}$. The packing fraction of cylinders in a hexagonal arrangement is $\pi/(2\sqrt{3})$. Thus, a hexagonal arrangement of cylindrical micelles formed by flat-based cones yields a packing fraction of

$$F_{\text{cyl}} = \frac{\pi}{36} \sin(\alpha) \left[\frac{2\pi}{\alpha}\right].$$  [4]

Fig. 3 shows that the biaxial arrangements lead to a denser packing than both the hexagonal arrangement of cylindrical micelles (20) and the spherical micelle (20) in a face-centered-cubic lattice arrangement. Note that the use of cones with curved bases improves the packing fraction of both cylindrical and spherical micelles (20).

**Truncated Cone Packing.** We turn now to the more general case of the packing of truncated cones (conical frustum) shown in Fig. 4, which provides a natural bridge between a cylinder ($a = b$) and a cone ($b = 0$).

Following our previous analysis, we arrange the objects in a close-packed planar layer, as in Fig. 5, and then stack consecutive layers on top of each other. A reference frame is attached to each

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**Fig. 1.** Arrangements of solid cones. (a–c) Three close-packed configurations of two identical cones. (a) The cones form a bicone. (b) The cones point in opposite directions. (c) The cones axes are not parallel. (d and e) Two close-packed configurations of many identical cones. Note that both arrangements are necessarily planar to achieve close packing. (f and g) Two views of a close-packed helix, a common motif in biomolecular structure. (h) A linear chain made of four identical bicones. Configurations d, f, and g are viable close-packed arrangements for a chain molecule.
layer, as in Fig. 5, so that the shift between consecutive layers is characterized by \((\Delta x, \Delta y, \Delta z)\), the relative displacement of the two origins. We do not consider rotations (about the \(z\) axis) because they generally lead to a worse packing. Our goal then is to accomplish close packing by minimizing \(\Delta z\) through the appropriate selection of \(\Delta x\) and \(\Delta y\). It is crucial to consider the circles cut out by intersecting the plane \(y = 0\) with successive cone layers in the stacking (see Fig. 6). The condition of mutual tangency of three such circles determines the minimum distance between successive layers [see supporting information (SI) Text for details].

In general, one finds two different degenerate (i.e., yielding the same minimum \(\Delta z\)) solutions: one for \(r < R\) and the other for \(r > R\). They can be thought of as being related by a mirror symmetry \(x \rightarrow -x; y \rightarrow -y\) applied to the second layer while keeping the first layer fixed (see SI Text for details). Note that this choice among two possibilities exists each time a new layer is added to the stack, yielding an infinite degeneracy in the close-packing arrangements of cones stacked in planar layers. Upon choosing symmetrically staggered layers, the centers of the circles cut out in the \(y = 0\) plane form a regular planar lattice. The symmetry displayed in the latter (and in the corresponding triangular tiling of the plane \(y = 0\) obtained by joining the circle centers) is related to the uniaxiality/biaxiality of the corresponding packing arrangement.

Remarkably, the optimal stacking and the related symmetries depend on the value of the ratio \(c = b/a\) with a transition point at \(c^* = \sqrt{2} - 1\) separating two distinct classes of behavior (see Methods for a detailed discussion of symmetries and packing fraction equations in the different regimes). The special case of a cylinder, \(c = 1\), is characterized by the hexagonal Abrikosov lattice, yields a tiling of equilateral triangles. In the cylinder-like regime, \(1 > c > c^*\), isosceles triangles form a rhombic lattice (see Fig. 7), whereas in the cone-like regime, \(0 \leq c < c^*\), right-angled triangles result in a rectangular lattice (see Fig. 8). At the transition point between the two regimes, \(c = c^*\), right-angled isosceles triangles result in a square lattice (see Fig. 9). Cylinders (\(c = 1\)) and truncated cones at the transition point (\(c = c^*\)) are special cases where uniaxiality is maintained since different directions are equivalent in the plane orthogonal to their axes. In all other cases (\(1 > c > c^*\) and \(0 \leq c < c^*\)), no such symmetry is present, implying biaxial order.

Fig. 10 shows a plot of the packing fraction \(f(c)\) as a function of the base radii ratio \(c = b/a\) from Eqs. 5 and 6. The transition at \(c = c^*\) between the cone-like and the cylinder-like regimes is
clearly visible. Most notably, the packing fraction does not increase monotonically with $c$ in either regime so that both the transition point ($c = c^\ast$) and the cone point ($c = 0$) are local maxima for the packing fraction.

**Conclusions**

Truncated cones are inherently uniaxial objects. Since they smoothly interpolate between cylinders and cones, we were able to assess the relevance of shape in dictating the nature of the packing. The rigorous determination of the optimal packing is a formidable problem, and the well packed arrangements we have found can at best be thought of as conjectures of the best optimal packing. The packings we have investigated are all based on the simplifying hypothesis that the optimal solutions are formed from the assembly (stacking) of close-packed planar layers. Within this assumption, we have shown that the optimal packing of uniaxial truncated cones is characterized by broken symmetry and is in general biaxial with the exception of the (degenerate) cylindrical case and of a special value of the “aspect ratio” $c^\ast = \sqrt{3}/3$. We have shown that the tiling of the truncated cone cross-section in the plane orthogonal to their axes is a useful way to understand the nature of the order, allowing one to distinguish between two different regimes, $c > c^\ast$ and $c < c^\ast$. At the transition point separating the two regimes, truncated cones with $c^\ast = \sqrt{3}/3 - 1$ have interesting symmetry properties. The packing fraction that is achieved by truncated cones is remarkably high.

We conclude with a speculation pertaining to the building blocks of protein native state structures—uniaxial helices and
AEG triangles are "full." The triangle AEF (red line, cone-like regime) and Trovato  

\[ V_{\text{cell}} = h \Delta z (a + b) \]  

isosceles, since two of the circles have the same radius \( r = a \) or \( r = b \). Note that, for these solutions, the only effective mirror  

\[ F = \frac{\pi}{6} \, \frac{1 + c + 1/c}{\sqrt{1 + 2/c}}. \]  

For the limiting case of a cylinder \( (a = b) \), we correctly obtain  

\[ \frac{\pi}{(2\sqrt{3})} = 0.9069 \ldots \]  

and the triangle defined above becomes equilateral. The restoration of uniaxiality in this limit is underscored by the invariance of the resulting triangular tiling of the \((x, z)\) plane, under rotation by an integer multiple of \( \pm 60^\circ \).  

The breaking of the uniaxial symmetry occurs as soon as \( b \) is strictly smaller than \( a \) and it is accompanied by (i) all of the triangles becoming isosceles and (ii) only half of them being
associated with the mutual tangency condition (see Fig. 7), yielding the two-fold degeneracy discussed above. Note that, upon moving along the $y$ axis, the circles formed in the $(x, z)$ plane change their radii.

**Cone-like regime:** $c < c^*$. The packing fraction is

$$F = \frac{\pi (3 + c)(1 + c + 1/c)}{6 (1 + c)(1 + 2/c)} \quad [6]$$

Note that, for these solutions, the only effective mirror symmetry is $y \rightarrow -y$, because $\Delta x = a + b$ or $\Delta x = 0$ (see Figs. 8 and 11).

In the limiting case of a regular cone ($b = 0$), we correctly obtain $F = \pi/4 = 0.7854 \ldots$.

The triangles defined above are always right-angled but never isosceles. The triangular tiling of the $(x, z)$ plane thus results in a rectangular tiling. Again, only half of the triangles are associated with the mutual tangency condition (see Fig. 8) and uniaxial symmetry is broken (i.e., no rotation symmetry is present in the plane).

**Transition point:** $c = c^*$.

The special value $c = c^*$ [i.e., $b = (\sqrt{2} - 1)a$] separates the two above regimes. At $c = c^*$, the packing fraction is

$$F = \frac{\pi}{6} (3 - \sqrt{2}) = 0.8303 \ldots \quad [7]$$

The triangles defined above are isosceles right-angled, and the degeneracy disappears. Indeed, the two degenerate solutions merge one into the other, and one obtains a square tiling in the $(x, z)$ plane (see Fig. 9). Uniaxiality is restored in this special case because the square tiling is invariant under rotation by an integer multiple of $90^\circ$. The triangles are no longer isosceles, and the square tiling becomes rectangular for any $c < c^*$ (see Fig. 8), whereas the triangles are no longer right-angled for any $c > c^*$ (see Fig. 7).

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