315d Analysis of Local and Global Structure during Densification of Non-Spherical Particulate Materials

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While the structure of random sphere packings has been widely studied, the behavior of non-spherical particles is not well understood. In this work, we present research on short cylindrical particles as a prototype system for studying a number of important phenomena. In particular, while the packing density of compact cylinders is similar to the value for spheres, other factors differ significantly: the range of attainable densities is broader, orientational effects and anisotropy become increasingly important, and positional and orientational ordering can occur over quite large characteristic lengths.

The first part of the work involves computer simulations of periodic packings of compact cylinders. These simulations show that the theoretical packing limit for equilateral cylinders is 65% (solid volume fraction), which is close to the limit for spheres. As the cylinders become elongated, there is a slight maximum in packing density. This behavior is similar to what has been observed for sphereocylinders and ellipsoids, but much less pronounced. The reason for the more subtle effect is that cylinders retain orientational freedom even in the compact limit (i.e., length/diameter equals unity).

In the second part of the work, we present x-ray microtomography data of equilateral cylinders at different packing densities. A novel approach is used in which the image data are reconstructed to obtain position and orientation on a discrete, cylinder-by-cylinder basis. This development is significant because it allows an in-depth analysis of ordering and anisotropy in experimental systems. The results also display a number of complex and important phenomena that occur in real systems but which are not captured in computer simulations. Analyses of the real materials include the following: 1) the radial distribution function (and how it evolves with density); 2) changes in quantitative measures of local orientational ordering, and 3) density limits associated with the onset of ordering. It was determined that subtle ordering occurs in the bulk region, with much more pronounced ordering and anisotropy effects in the near-wall region.