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Mapping Particle Size Distributions into Predictions of Properties for Powder Metal Compacts

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Abstract

Discrete element analysis is used to map various log-normal particle size distributions into measures of the in-sphere pore size distribution. Combinations evaluated range from monosized spheres to include bimodal mixtures and various log-normal distributions. The latter proves most useful in providing a mapping of one distribution into the other (knowing the particle size distribution we want to predict the pore size distribution). Such metrics show predictions where the presence of large pores is anticipated that need to be avoided to ensure high sintered properties.

Keywords: discrete element analysis, particle packing, pore size distribution, mechanical properties, computer model

1. Introduction

Random and ordered packing are two very different structures. A random packing is constructed by a sequence of events that are not correlated with one another - by definition the assembly process involves random events. This results in a structure without long-range repetition. Generally, random structures have a lower packing density than attainable with ordered structures. For a one-dimensional packing the concept is often related to parking automobiles along a curb, where an unmarked curb can have a wide variation in coverage. An ordered structure occurs when objects are placed systematically into periodic positions. In three dimensions this is how the bricks in a wall or atoms in a crystal structure are placed in precise repetitive patterns. In a two-dimensional packing, this corresponds to how tiles are placed to cover a floor or wall. In a one-dimensional packing it is simply the analog to a pearl necklace, where each pearl is abutted against the next.

Formally, an ordered packing is recognized by the fact that each object is located by a simple mathematical translation of steps from every other particle. Some examples are shown in Figure 2.1 to illustrate the cases involving linear translations. Besides linear displacements, structures can be created by rotational translations as well as via mirror images.

Although many particle packing problems are considered in three dimensions, there are many reasons to consider other levels of packing. Indeed, problems with dimensions greater than three have been treated in pure mathematics and have proven useful in designing systems for digital communications. At the other extreme are the one- and two-dimensional packings treated here prior to three-dimensional packings. The one-dimensional parking problem is a useful means to understand general concepts in packing. Likewise, another useful conceptualization is the necklace problem, since bead placement on the string determines the coverage. Random placement of beads leads to an imperfect necklace.

In a one-dimensional packing, each segment is defined in size by its end points, or length. The segment packing problem is fairly easy to solve for the ordered structure, where the maximum attainable coverage is 100%. Perfect segment alignment gives end-to-end alignment. Even if the segments differ in length, it is still possible to generate 100% coverage. However, with a random placement of the segments, the coverage is less than complete. The most common problem is for monosized segments where each segment is the same length.

The one-dimensional packing is determined by two points along the line, the distance between the two points being equal to the size of the segment, effectively the diameter of the 0-sphere. An ordered packing of segments can attain a fractional density ρ of 1.00; this corresponds to total coverage of the line. Alternatively, a random packing of monosized segments attains a fractional density ρ of approximately 0.75. There are unfilled gaps, too small to fill with another segment, that lower the coverage from that of an ordered packing. The reduction in packing efficiency directly results from the random fill process.

Random packings lack the coverage attained with ordered packings. The maximum attainable packing density to decrease as the dimensionality of the problem increases, being 1.000 for one-dimensional, 0.9069 for two-dimensional, and 0.7405 for three-dimensional packings.

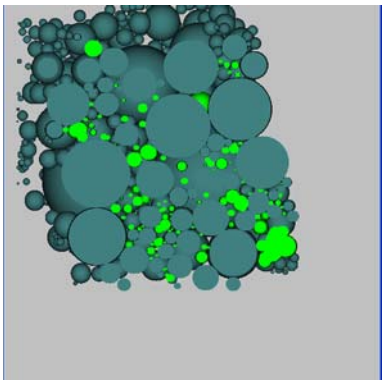
2. Key Findings

Particle size distributions were input into a discrete element particle packing simulation. Many variants were explored in this research:

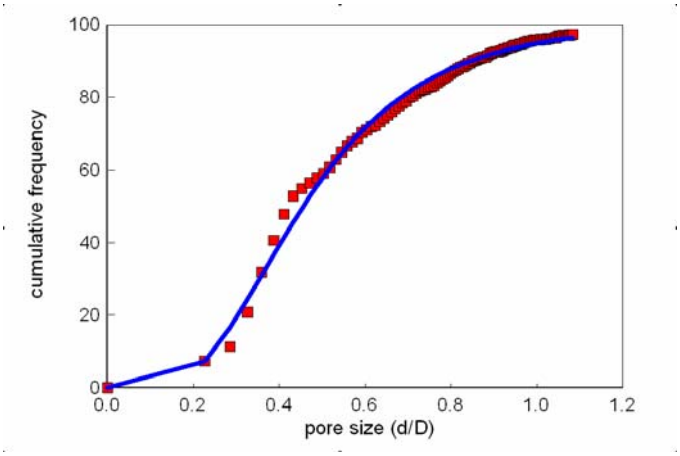
1-dimensional monosized packing of segments
2-dimensional monosized packing of circles
3-dimensional monosized packing of spheres
3-dimensional packing of bimodal spheres
3-dimensional packing of log-normal spheres

Each of the packing structures was first tested for packing density against experimentally and analytical solutions. The findings were consistent with typical expectations; for example monosized spheres packed to a fractional density of 0.58 to 0.64 depending on the container size and shape. Normally the monosize sphere packing is 0.60 for loose random and 0.64 for dense random, large container trials.

Each packing was then analyzed for the in-sphere pore size distribution. The in-sphere represents a fitting of an imaginary sphere into the void space between the particles. Once the void space is filled, the in-sphere size distribution is extracted as a measure of the pore size distribution. Fitting routines are used to measure the pore size distribution and determine the best fitting parameters. An image of the sectioned particles and in-sphere filled pores is given below.



From such a build and fill sequence, it is possible to link and map the input particle size distribution with the resulting pore size distribution. Various log-normal input particle size distributions were used and various degrees of densification via compaction and sintering were applied to the packed particles. From this it was possible to realize a few significant findings. First, large pores form in the packings, often larger than the particle sizes. Second, the pore size distribution tends to be log-normal. Both aspects are evident in the pore size distribution shown below for a monosized sphere loose packing (cumulative fraction versus size d/D where d = pore diameter and D = particle diameter).



In this plot the square symbols are the actual data and the blue line is a log-normal distribution fit to those points. Most significant is to realize the input was a monosized powder which resulted in a broad pore size distribution, with a few pores larger than the particles.

3. Conclusions

As the packing density increases, the median pore size decreases and as the width of the particle size distribution increases the median pore size decreases. However, the spread in the log-normal pore size distribution is invariant with respect to the input particle size. This is a most significant finding. With respect to mechanical properties, the large pores are the major causes of failure. This study shows that for press-sinter processing, the largest gains in properties would come from increasing the density and reducing the median particle size, with a broad dispersion in particle size. Small particles form pore size distributions with the same dispersion, but the overall mean and maximum pore sizes scale with particle size. A high content of small particles induces more sintering that improves properties while helping to remove detrimental large pores. In these systems, lower compaction pressures can be used, since small powders do not deform in compaction, since they rely on a binder for green strength. Compaction then is a shaping step with reduced green density gradients that enable more uniform sintered dimensions. For example, 316L stainless steel pressed and sintered from a 32 μm powder sintered to give 505 MPa tensile ultimate strength, and 65% tensile elongation. The sintered tensile strength from press-sinter 100 μm particles (with large residual pores) is 140 MPa and from injection molded 16 μm particles is 230 MPa. So clearly it is not the press-sinter route that leads to low properties, but the large residual pores.