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ESC Annual Report 2009

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Introduction

In modeling highly filled polymer composites, the goal is to treat the behavior of the composite on many different length scales ranging from molecular to macroscopic in a unified manner. The disparity of length, energy, and time scales involved precludes a direct numerical approach to this problem, especially in the dynamic response regime. The Probabilistic Crack Occurrence (PCO) model is a statistical technique which is designed to connect the polymer network scale modeling of EPnet with the 2Scale FEM modeling technique performed at significantly larger size scales. In the 2Scale FEM simulations, only the larger HMX inclusions are explicitly modeled, while the smaller inclusions are treated as dirty binder. The goal is to open cracks in the dirty binder at appropriate strain levels. The PCO model is used to generate a spatially-dependent failure strain criterion for the 2Scale FEM simulation. The strain level at which cracks open must be determined outside of the FEM modeling since continuum models are unable to provide predictions of cracking behavior. In addition to the nonuniform failure strain criterion, the 2Scale FEM modeling effort also requires an initial state of a highly filled random packing of HMX crystals, something which is not straightforward to prepare. Dense random packings of particles with complex shapes are needed as input for both the 2Scale FEM initial state and the PCO modeling effort.

Modeling Description

Probabilistic Crack Occurrence

The PCO model is based on a material containing inclusions of two widely differing sizes. The small inclusions are assumed to be part of a background matrix, which is normally represented as a homogeneous substance by a standard FEM mesh. PCO is designed to reintroduce inhomogeneity in the background matrix in a controlled, statistical manner by providing a space-dependent criterion for the strain at which a crack should be opened in the FEM matrix based on the small scale properties of the material. PCO employs a statistical technique known as the weakest link approach. The most likely locations for cracks to form will depend on the details of the random arrangement of large inclusions in a physically meaningful way. Use of the PCO model requires both a knowledge of the locations of explicitly represented grains in the matrix as well as the statistical distribution of spacings between the small grains which are not explicitly represented in the FEM technique. Information from the PCO model is combined with failure strain information obtained at the polymer-scale level through EPnet modeling.

Assume that exactly two sizes of randomly placed inclusions are present in the material, one of which is significantly larger than the other. For any given large inclusion I_1 , identify the closest large inclusion I_2 along the direction perpendicular to the applied strain. The distance between these two inclusions is L . The probability that a crack will

initiate somewhere in the region between I_1 and I_2 can be determined by a statistical technique known as the weakest link approach. Treat the length L as composed of n elements of length l_0 , such that $L=nl_0$.

Assume that failure on the small scale (within the dirty binder) occurs when the matrix connecting two small inclusions i_1 and i_2 breaks apart. The weakest link picture suggests that the failure will occur for smaller strain as the distance l between the small inclusions (in the direction parallel to the applied tension) increases. Thus, we need to identify the largest length $l_{\max}$ occurring in a region of length L .

Writing the probability distribution function (p.d.f.) of l as $f(l)$, the p.d.f. of $l_{\max}$ is given by

$$g_n(l) = n f(l) (F(l))^{n-1}$$

where the cumulative distribution function

$$F(l) = \int_{-\infty}^l f(l) dl.$$

The form of $f(l)$, the probability that two small inclusions will be spaced a distance l apart, can be derived analytically or numerically from the radial distribution function $G(r)$, which could be measured in experiment. In practice we obtain this distribution from simulations of small scale packings. The results of the PCO analysis are placed on the FEM mesh using one of two programs developed for this purpose: PCOMesh or PCOPolyMesh.

As an example of the type of distribution obtained by the PCO analysis, consider a Poissonian distribution of lengths l :

$$f(l) = \frac{e^{-l/a_0}}{a_0}$$

where a_0 is the characteristic length scale of the distribution. Then,

$$g_n(l) = \frac{n e^{-l/a_0}}{a_0} (1 - e^{-l/a_0})^{n-1}$$

Identify the most likely value of $l_{\max}$ from g_n , obtained by setting $\frac{dg_n(l)}{dl} = 0$. Skipping the details, the result factorizes to

$$0 = \frac{n}{a_0^2} e^{-l/a_0} (1 - e^{-l/a_0})^{n-2} (n e^{-l/a_0} - 1)$$

The physical solution is given by

$$l_{\max} = a_0 \ln n.$$

The solution has the expected property that $l_{\max}$ increases with n ; thus, as L increases, the matrix between the two large inclusions becomes weaker.

DiskPack

The Diskpack program is based on an advanced Brownian dynamics simulation technique, and uses a series of simulated annealing procedures to construct dense random packings of disks which have the desired spatial filling fraction and which are drawn

from the appropriate disk size distribution.

We simulate a two-dimensional multidisperse system of N disks of size $L \times L$ with boundary conditions that are either periodic in x and y (for PCO input; see Fig. 1) or bounded by hard walls on all sides (for FEM input). The particles are modeled as repulsively harmonically interacting disks of radii R_i with a size ratio determined by an input file; we use the size distribution given in the Skidmore data set (Fig. 2). We artificially inflate the size of all disks slightly such that the inflated disks should be at least as far apart as the minimum size required for the FEM mesh. The disk packing is obtained by placing the disks in non-overlapping locations and then shrinking all disks, adding a few additional disks, and reexpanding all disks while thermally agitating the disks. This process is repeated until the desired density of uninflated disks is obtained. After the disk configuration is generated, it is inspected to ensure that the spacing between adjacent disks does not fall below the size required by the FEM meshing process. Disks that are too close are reduced slightly in size. The constraint introduced by the minimum spacing between disks generally reduces the density of very dense packings and effectively places a limitation on the densest packing that can be generated from a given particle size distribution.

PolyPack

The DiskPack program has now been extended into PolyPack, which transforms the dense random disk packing into a dense random polygon packing with the same area size distribution. This is achieved in several steps (see Fig. 3). First, the disk packing is tessellated using the Voronoi construction in order to form polygons. Each polygon is then rescaled in size to have the same area as the original disk at that location. The polygons are rotated through randomly chosen angles in order to prevent the appearance of parallel polygon sides throughout the packing – parallel sides introduce an undesirable artifact. Through simple trial I found that an angular rotation range of 5 to 10% produces packings that have a strong visual resemblance to micrographs of the actual material (see Fig. 4). The final, and most complex, step is the removal of polygon collisions introduced by the rotation process.

Results & Discussion

During FY09, the Diskpack program was used to generate a series of packings at 77% filling in a 1500 x 1500 micron sample for use as RVEs in the FEM modeling effort. The size distribution of the disks was taken from the available Skidmore data set, the best available representation of the true size distribution in the actual material. As FEM work proceeded, a further series of disk packings at 65% and in a considerably smaller sample size of 500 x 500 microns were generated. A strong limitation on the packing density was the requirement by the FEM mesh that a particular minimum spacing between disks be maintained (this spacing was iterated in a series of packings provided for FEM); the Diskpack program was able to meet this minimum spacing requirement but was limited in the density of packings that could be generated as a result. One of the 65% disk pack meshes was filled with failure strain criteria values from the PCOMesh program using the output of the PCO model developed previously.

Due to concern about changes in strain state that might be introduced by using disk shaped inclusions instead of the more realistic polygonal shaped HMX inclusions, an investment was made in developing the Polypack program. This program transforms the disk packings generated by Diskpack into dense random packings of polygons. Polygon sides shorter than a cutoff length are removed in order to avoid the generation of very small FEM mesh elements; this procedure was found to be necessary after testing of the polygon packings with the FEM meshing process. The resulting polygon packing is then provided in appropriate format to the FEM modeling effort. Both disk and polygon packings were compared directly (Fig. 5); in each case, the original size distribution was well preserved (Fig. 6).

A series of polygon packings of different densities and sample sizes were generated for FEM input, including a very large 3 mm x 3 mm packing (Fig. 7). The large packing was used as a source for multiple RVEs by cutting windows of a smaller size from the packing. This made it possible to test RVE size effects using only a single packing instead of generating a series of packings. The PCOMesh program, originally written for disk packings, was extended to PCOPolyMesh. This program determines failure strains from the PCO modeling based on the distance between a binder mesh element and the two closest polygon sides. An example of the filling of the FEM mesh with failure strains taken from the PCO model is shown in Fig. 8.

Some runs performed this FY included the introduction of a weakened interface region around each explicit grain in the FEM modeling. This successfully reduced the failure strain of the entire sample; however, care should be taken in following such an approach. Due to the highly filled nature of the sample, virtually the entire sample consists of interface; most of this interface is not explicitly represented in the FEM model because it falls within the dirty binder. The goal of the PCO modeling approach is to capture the effect of the weakened interface in a statistical way without directly employing large scale interface weakening.

Note that by replacing the disks in the packing with polygons, a significantly lower failure strain was obtained without needing to place weakened interfaces into the sample. Thus, geometric strain focusing is probably more of an issue in this respect than the lack of explicit weak interfaces.

Conclusions

The PCO program suite and DiskPack initialization routines have been expanded to polygon packings (PolyPack) and iterated with the 2Scale FEM modeling effort during the past year in order to coordinate the input and output requirements and formats. The polygon shapes of the grains give significantly better agreement with experimental data sets than the disk shaped inclusions, which do not focus strain to the same extent. A series of 2Scale FEM meshes, generated using both Diskpack and PolyPack input, were filled with strain criteria based on PCO and EPnet scale modeling input, and strained to failure in FEM modeling (Fig. 9).

Figure 1: Example DiskPack calculation of dirty binder material for input to the PCO analysis. The size distribution of the spacing between grains $f(l)$ is obtained from packings such as this one and used in the extreme value calculation.

Figure 2: Portion of the Skidmore data giving the distribution of grain sizes in PBX 9501. This portion of the distribution is used in the explicit portion of the FEM analysis.

Figure 3: Illustration of PolyPack procedure. Upper left: Voronoi tessellation of a DiskPack packing produced at a specified density. Lower left: The Voronoi polygons are all rescaled so that they are equal in area to the disks originally present in the packing. Upper right: The polygons are each rotated through a random angle chosen within a 10 degree range in order to eliminate parallel sides from the packing. Lower right: Collisions between polygons introduced by the rotation process are resolved and the final polygons are adjusted in order to maintain a minimum spacing between polygons as required for the FEM meshing process.

Figure 4: PBX 9501 micrograph from Cary Skidmore; the sample was pressed to density 1.835 g/cc.

Figure 5: Left: Diskpack-generated packing of a 500 x 100 micron area at approximately 50% filling with particles of diameter 40 to 250 microns drawn from the particle size distribution. Right: Same packing after processing by Polypack program to give a random polygon packing with the same particle size distribution. These two packings were generated to test the effect of inclusion shape on sample response.

Figure 6: Comparison of the original Skidmore size distribution with the final size distribution of polygons in a PolyPack packing. Agreement is generally very good; the excess small polygons are a result of the minimum spacing requirement which caused some polygons to shrink below their original sizes.

Figure 7: 3mm x 3mm PolyPack packing at 71% filling. This packing was used as a template for cutting out smaller RVE elements for FEM analysis.

Figure 8: Failure strain from PCO analysis placed on FEM mesh for a polygon packing at 71% filling.

PBX9501 93% HMX, [0.65 HMX + 0.35DB(0.8HMX+0.2B,l=1.2)]
DNS+FAILURE USING PCO (DAVE+CYNTHIA)

Figure 9: EPIC results of failure in a 500 x 500 micron 65% disk packing sample populated with failure strain criteria taken from the PCO model.