Particle modeling of random crack patterns in epoxy plates

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Abstract

This paper employs particle modeling for simulation of dynamic fragmentation in (elastic–brittle) epoxy plates (8.25 cm × 33.02 cm), containing non-uniformly distributed circular holes [Al-Ostaz A, Jasiuk I. Crack initiation and propagation in materials with randomly distributed holes, Eng Fract Mech 1997;58:395–420]. Since the experiments on nominally identical specimens resulted in a range of different crack patterns, the model focuses on matching the most dominant experimentally observed cracks. Indeed, this is achieved with lattices having several different mesh resolutions. Next, by introducing very weak, microscale perturbations in the material properties, it is found that the stiffness has a stronger effect on the deviation from the dominant crack pattern than does the tensile strength.

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1. Motivation

This paper has been motivated by a challenge to develop a model of experimentally observed dynamic fragmentations of elastic–brittle plates perforated with holes [1]. The typical experiment involved a number of nominally identical plates (8.25 cm × 33.02 cm), each of a uniform thickness 0.38 cm, and made of epoxy (PSM-5), Fig. 1. Each plate had the same non-periodic, non-uniform distribution of 31 randomly distributed circular holes of the same size. The locations of holes’ centers were generated according to a Poisson point field with exclusion (so as to prevent hole overlaps) by a random number generator, so that, strictly speaking, this was one specific (apparently deterministic, i.e. non-random) realization of a random system. The holes were 1/4 in. in diameter.

Each plate was subjected to a uniaxial tensile loading in the y-direction at a constant displacement rate of 2.0 mm/min (~0.03 cm/s) initially, and then decreased to 0.1 mm/min (~0.0017 cm/s) in order to capture more details of the fracture process. Clearly, it was a quasi-static loading, while the fragmentation was a dynamic fracture event, occurring very suddenly at a load level somewhat variable from one specimen to another.

Fig. 2 is the photograph of final crack patterns in two such epoxy plates, while Fig. 3 is the sketch of final crack paths superposed from seven specimens. The main observation is that no two plates displayed the same crack pattern! In fact, the variability of those patterns was considerable, although a dominant region could roughly be identified where the majority of crack paths would occur.

The basic question that arose was this: “Why did the cracks follow so many different paths?” The authors of the said study concluded that this non-uniqueness of the crack patterns in the perforated specimens was due to minute material and geometric imperfections that influence “which crack path will actually take place in a particular specimen that is nominally (on the macroscopic scale) the same as the rest of the specimens” [1].

The ensemble of seven plates is, in effect, a random system, where the (most likely) very small – and very hard to detect – microscale material randomness has a significant effect on the macroscale response. One might argue here that there are many paths cutting the specimen in the direction normal to the principal loading direction, which only differ by small differences in their energies of fracture. Thus, many paths are almost equally likely to happen. On that basis, one can then set up a model in the vein of maximum entropy formalism [2]. The limitation of such a model is that it is much more suited

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Fig. 1. Dimensions of the epoxy sheet were 3.25 in. × 13 in. × 0.125 in., where the middle square shows the area of placement of Poisson points.

to dealing with quasi-static rather than dynamic fracture, while the problem at hand was a dynamic one.

The dynamic character of fracture in these experiments, combined with the presence of multiple incipient spots, was also the challenge in several computational mechanics models reported in [1] employing commercial finite element programs, as well as in an independent study using a meshless element program [3]. Upon trying various failure criteria [4], various numerical methods (e.g. spring networks [5]), and even being forced to initialize the cracking process by a subjective choice in the meshless model [3], the modelers (including the first co-author of this paper) have run into uncertainty as to which modeling aspect is more critical, and whether there is a way to clarify it.

The present study was motivated by this outstanding challenge, and offered a way to test a recently developed particle model (PM) [6,7], which is an improvement upon the earlier models [8,9]. Unfortunately, the term PM is confusing because it appears synonymous with meshless methods [12].

The PM is fully dynamic with particles (or “quasi-particles”) placed at the nodes of a periodic (equilateral triangular) lattice. Any potential can be specified for particle–particle interactions, and, in the case of lattice spacing decreasing to a few Angstroms, we recover a molecular dynamics (MD)
model at zero kelvins with, say, a Lennard-Jones potential. We developed this method to the stage of real applications in that we formulated four conditions to determine the continuum-level Young’s modulus and tensile strength, while maintaining the conservation of mass and energy of the particle system and satisfying the laws of interaction between all the particles in the PM model for a given MD model [6]. More specifically, the PM was developed to simulate comminution processes of minerals on centimeter-to-meter scales, with a goal of predicting the dynamic crushing/break-up of rocks and liberation from the matrix of, say, gold particles.

Clearly, the preparation of mineral specimens – involving measurement of highly heterogeneous and multiphase microstructures – for a direct comparison with the model prediction is very hard. Thus, we can apply the model to the well described plate with 31 holes and follow this strategy:

(i) decrease the lattice spacing until we attain mesh-independent crack patterns;
(ii) find out whether the lattice of (i) will also result in the most dominant crack pattern of Fig. 3;
(iii) assuming the answer to (ii) is positive, introduce weak perturbations in the material properties – either stiffness or strength – to determine which one of these has a stronger effect on the deviation away from the dominant crack pattern, i.e. on the scatter in Fig. 3.

2. Model formulation

The elastic–brittle character of the epoxy plates can be seen from Fig. 6. It shows experimentally obtained stress–strain curves of the seven epoxy specimens. Following Al-Ostaz and Jasiuk [1], the average Young modulus of the epoxy is adopted as $E \approx 3.26$ GPa, while the Poisson ratio is 0.38. Now, to resolve the $8.25 \times 8.25$ cm domain – which is the central portion with 31 holes in Fig. 1 – our model employs a planar equilateral triangular lattice with central force interactions. This implies an effective Poisson’s ratio $\nu = 1/3$ in the 2-D (plane stress) elasticity interpretation. A different Poisson ratio could be modeled by introducing angular bonds, or three-point potentials of Kirkwood or Keating type [10], but we choose not to do this in the present study.

From Ashby and Jones [11] we find the epoxy’s tensile strength $\sigma_{TS} = 62.86$ MPa, and mass density $\rho \approx 1.1$ g/cm$^3$. The latter quantity is used to assign the mass to each quasi-particle in accordance with the hexagonal-shaped area that it occupies. Using $\sigma_{TS}$, from Hooke’s law, we determine the failure strain $\varepsilon_{max}$

$$\frac{r_{max} - r_0}{r_0} = \varepsilon_{max} = \frac{\sigma_{TS}}{E}$$  

and the displacement threshold for fracture to occur, $r_{max}$. We find $r_{max} = 0.019r_0$, with $r_0$ being the equilibrium spacing between contiguous particles.

The elastic–brittle law of particle–particle interactions is written as

$$F = \begin{cases} \frac{-2S_0(r - r_0)}{0.0} & \text{for } |r - r_0| \leq \varepsilon_{max} \cdot r_0 \\ 0 & \text{otherwise} \end{cases}$$

with $F$ being the interaction force and $r$ the distance between two particles and the stiffness $S_0 = E r_0^2/2$. Fig. 4 displays the interaction force and potential energy curves at $r_0 = 0.02$ cm.

To assess the mesh dependence, we generate four different mesh resolutions specified by lattice (inter-particle) spacings $r_0 = 0.1, 0.05, 0.02$ and 0.01 cm, see Fig. 5. Obviously, the main obstacle to increasing the mesh resolution is the rise in computing time. For instance, to reach the point in time $T = 5.0 \times 10^{-2}$ s on the SGI Altix 350, it takes $\sim 50$ CPU hours for a lattice with $r_0 = 0.02$ cm, whereas a lattice at $r_0 = 0.01$ cm requires $\sim 150$ CPU hours.

We use the leapfrog time-differencing, equivalent to the Verlet algorithm in physics terminology, to compute the lattice dynamics. Unless we work with a coarse mesh at $r_0 = 0.2$ cm, we cannot apply the very slow loading rate of $\sim 0.0017$ cm/s
used in the experiments. This is so because a low velocity at the boundary translates to very small time increments, and this leads to excessive truncation and round-off errors in the leapfrog scheme. Thus, we work with velocities between 2.5 cm/s and 40.0 cm/s, which still qualify as quasi-static loading processes. Also to speed up the computations, we simply work with the middle section of Fig. 1.

3. Simulations

3.1. Homogeneous material

With reference to Fig. 5(a)–(d), in the table below we give the total numbers of particles and the corresponding time increments at increasing mesh resolutions; all cases are based on a domain 8.25 cm × 12.3 cm. We also provide Fig. 7 to give a better idea of the lattice spacing \( r_0 \) relative to the hole size.

<table>
<thead>
<tr>
<th>Mesh resolution, ( r_0 ) (cm)</th>
<th>Total number of particles</th>
<th>Time increment, ( \Delta t ) (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>11,797</td>
<td>( 3.093 \times 10^{-7} )</td>
</tr>
<tr>
<td>0.05</td>
<td>47,452</td>
<td>( 1.564 \times 10^{-7} )</td>
</tr>
<tr>
<td>0.02</td>
<td>293,287</td>
<td>( 6.301 \times 10^{-8} )</td>
</tr>
<tr>
<td>0.01</td>
<td>1,174,456</td>
<td>( 3.158 \times 10^{-8} )</td>
</tr>
</tbody>
</table>

It is seen that, if the mesh resolution (lattice spacing) improves by a factor of 2, then the total number of particles increases by a factor of \( \sim 2^2 \); this relationship is \( \sim 2^3 \) in 3-D. Correspondingly, the computing increment time increases by a factor of \( \sim 2^2 \) in the 2-D or 3-D case.

A kinematic boundary condition is used at the top and the bottom edges:

\[
\partial B_u : U(t)_{\text{top}} = U(t)_{\text{bottom}} = 0.0, \quad V(t)_{\text{top}} = -V(t)_{\text{bottom}} = V_{\text{def}}
\]
where $U$ and $V$ are the velocity vectors associated with the coordinate directions, $V_{\text{def}}$ stands for the tensile rate on the $Y$-axis.

A zero-traction condition is applied at the side edges:

$$\partial B_t : T_x(t) = T_y(t) = 0.0,$$

where $T_x$ and $T_y$ are the force vectors associated with the coordinate directions.

Fig. 8(a)–(d) show final crack patterns for four different mesh resolutions: $r_0 = 0.1, 0.05, 0.02, 0.01$ cm. We note that the principal crack going across the plate is almost identical in all four cases, and it always falls into the dominant “region 2” of Fig. 3. At two lattice spacings in (b) and (d) we also get extra branches somewhat below that crack. In effect, we have mesh independence of the particle modeling for the generation of crack patterns.

We also investigate the effects of different loading rates on the principal crack patterns, in Fig. 9, with the mesh resolution of $r_0 = 0.02$ cm, and $V_{\text{def}} = 2.5, 10.0, 20.0, 40.0$ cm/s. Clearly, the change in loading rate only has a minor effect on the dominant crack pattern.

3.2. Randomly inhomogeneous material

At this point we choose the lattice with $r_0 = 0.02$ cm to study the effects of microscale inhomogeneities of the
epoxy material on crack patterns. Certainly, the lattice with $r_0 = 0.01 \text{ cm}$ would be even more desirable to work with, but too expensive, recall the Table of Section 3.1. In particular, we now want to study the effect of weak perturbations in two material properties – either stiffness or tensile strength – and determine which one may have a stronger effect on the crack patterns.

The spatial material randomness is introduced according to the simplest model of stochastic solid mechanics: a low noise-to-signal field of independent, identically distributed random variables. Thus, for the modulus $E$ at any lattice bond $i$ we have

$$ E_i = E(1 + r_i) $$

(5)

where $r_i \in [-0.5 \times 10^{-4}, 0.5 \times 10^{-4}]$ or $r_i \in [-0.5 \times 10^{-8}, 0.5 \times 10^{-8}]$ is a uniform random variable, and $E$ is the mean value of Young’s modulus. A completely analogous model is used for the tensile strength $\sigma_{TS}$ at any lattice bond $i$

$$ \sigma_{TS_i} = \sigma_{TS}(1 + r_i) $$

(6)

where $\sigma_{TS}$ is the mean tensile strength.

A local sample of the randomized properties is shown in Fig. 10. The different colors and sizes of particles in the figure signify the positive versus negative sign and the value of the perturbation.

Fig. 11(a), (b) show crack patterns with the perturbation in Young’s modulus $r_i \in [-0.5 \times 10^{-4}, 0.5 \times 10^{-4}]$ and $r_i \in [-0.5 \times 10^{-8}, 0.5 \times 10^{-8}]$, respectively. Fig. 12(a), (b) show crack patterns for analogous perturbations in the tensile strength. Comparing these cracks with those in the homogeneous plate of Fig. 8(c), we observe:

1. Perturbation in the Young modulus has a stronger effect than that in the tensile strength, both perturbations being of
(a) $V_{\text{def}} = 2.5 \text{ cm/s}, T = 7.0 \times 10^{-3} \text{ s}$. (b) $V_{\text{def}} = 10.0 \text{ cm/s}, T = 4.0 \times 10^{-3} \text{ s}$. (c) $V_{\text{def}} = 20.0 \text{ cm/s}, T = 2.0 \times 10^{-3} \text{ s}$. (d) $V_{\text{def}} = 40.0 \text{ cm/s}, T = 1.1 \times 10^{-3} \text{ s}$. Note: (a) is the same as Fig. 8(c).

Fig. 9. Final crack patterns for four loading rates at lattice spacing $r_0 = 0.02 \text{ cm}$ and domain size $8.25 \times 12.3 \text{ cm}$ at respective loading rates and final times to fracture: (a) $V_{\text{def}} = 2.5 \text{ cm/s}, T = 7.0 \times 10^{-3} \text{ s}$, (b) $V_{\text{def}} = 10.0 \text{ cm/s}, T = 4.0 \times 10^{-3} \text{ s}$, (c) $V_{\text{def}} = 20.0 \text{ cm/s}, T = 2.0 \times 10^{-3} \text{ s}$ and (d) $V_{\text{def}} = 40.0 \text{ cm/s}, T = 1.1 \times 10^{-3} \text{ s}$. Note: (a) is the same as Fig. 8(c).

(2) With the decrease of perturbation range down to $[-0.5 \times 10^{-8}, 0.5 \times 10^{-8}]$, the effect of perturbation, either in the Young modulus or in the tensile strength, vanishes, and the crack patterns resemble those of the homogeneous case.

These conclusions were supported by several other cases in the parameter space.

4. Conclusions

In this paper we apply particle modeling to simulate the experimentally observed fracture response of nominally identical elastic–brittle epoxy plates, perforated with randomly distributed holes, subjected to uniaxial tension [1]. The authors of [1] found a definite non-repeatability of the crack patterns in nominally identical specimens, and attributed it to microscale material inhomogeneities in the epoxy material, and/or variabilities such as imperfect fixed-grip conditions or unevenly machined surfaces of holes. When the system was
Fig. 11. Final crack patterns for perturbation in Young’s modulus of (a) $[-0.5 \times 10^{-4}, 0.5 \times 10^{-4}]$ and (b) $[-0.5 \times 10^{-8}, 0.5 \times 10^{-8}]$ at time to fracture $T = 7.0 \times 10^{-3}$ s. Compare with Fig. 7(c).

Fig. 12. Final crack patterns for perturbation in tensile strength of (a) $[-0.5 \times 10^{-4}, 0.5 \times 10^{-4}]$ and (b) $[-0.5 \times 10^{-8}, 0.5 \times 10^{-8}]$ at time to fracture $T = 7.0 \times 10^{-3}$ s. Compare with Fig. 7(c).

studied by finite element or element free methods, a very high sensitivity to meshing or assumed failure criteria was noted.

Our particle modeling approach has been adapted to this problem according to the strategy outlined at the end of Section 1. In the following, we examine each step of that strategy.

(i) Four lattices, at spacings from $r_0 = 0.1$ cm through $r_0 = 0.01$ cm, result in practically mesh-independent crack patterns.

(ii) All four lattices resulted in the most dominant crack pattern seen in the experiments, and in two cases with some extra crack branches present.

(iii) For the sake of economy in simulations we adopted the lattice with $r_0 = 0.02$ cm when studying the effect of weak perturbations in two material properties: either stiffness or strength. We found that the first one of these has a stronger effect on the deviation from the dominant crack pattern, i.e. on the scatter in Fig. 3.

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